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TOPICAL REVIEW

Numerical relativity: a review

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Abstract

Computer simulations are enabling researchers to investigate systems which are extremely difficult to handle analytically. In the particular case of general relativity, numerical models have proved extremely valuable for investigations of strong-field scenarios and been crucial in revealing unexpected phenomena. Considerable efforts are being spent to simulate astrophysically relevant simulations, understand different aspects of the theory and even provide insights into the search for a quantum theory of gravity. In this paper I review the present status of the field of numerical relativity, describe the techniques most commonly used and discuss open problems and (some) future prospects.

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1. Introduction

The beginnings of the 20th century witnessed a major revolution in our understanding of gravitation. Einstein's theory radically changed the way we conceive gravity and its effects. Unravelling the messages that his theory contains requires the ability to solve a coupled nonlinear system of ten partial differential equations. These are 'special' equations as they govern the very structure of the spacetime itself (as opposed to other theories where the fields evolve 'on top' of an unchanging spacetime).

For about six decades, only in special situations were researchers able to obtain solutions to these equations. These assumed the existence of symmetries and/or concentrated on asymptotic regimes that allowed considerable simplifications of the equations reducing them to a manageable (and solvable) system. Although certainly considerable 'new' physics has been learned from Einstein's theory, its full implications remain elusive.

The last decades of the 20th century witnessed another revolution. This one, the 'computer revolution', was spurred by the computational capabilities that powerful computers provided researchers. This new tool allows the study of systems which would otherwise be impossible (or extremely involved) analytically. Simulations not only are letting researchers tackle difficult

problems but also allow for a nice visualization of the outcome. These simulations serve as theoretical laboratories for general relativity (GR), where, the past impossibility of constructing a gravitational laboratory prevented data-driven research from aiding in our explorations of the theory. We have already witnessed some of the benefits that these 'numerical laboratories' can provide, for instance, they have demonstrated the existence of critical behaviour in general relativity and naked singularities in gravitational collapse; the possible appearance of toroidal event horizons; indicated generic properties of singularities in cosmological contexts; provided more accurate understanding of rapidly rotating neutron stars and shed light into the structure of singularities.

The continuous improvements in computer power coupled with the gained (and being gained) experience in simulating Einstein's equations signal that, after almost a century, we are on the path to unveiling what these equations have so far kept hidden.

Computer simulations are and will increasingly be of crucial importance in letting us study strongly gravitating systems such as those containing massive stars and/or black holes; spacetimes on the verge of black hole formation; investigation of cosmological scenarios, studies of structures of singularities and even for investigations of different aspects of possible quantum theories of gravity.

Clearly, understanding these issues is very important academically since it will definitively advance our scientific knowledge. Additionally, a thorough understanding of some of these systems is also relevant from a 'more practical' point of view. Technology is also setting us at the verge of being capable, for the first time, to directly test general relativity in the strong-field limit and use it to obtain a new window with which to scrutinize our universe. The beginnings of the 21st century will witness the operation of several highly sensitive gravitational wave Earth- (and probably space-) based detectors [1–5]. These detectors will allow researchers to study signals produced from strong-field systems and therefore will provide a chance to test a theory which has so far proven very successful in weak-regime scenarios. These signals carry specific signatures of the system that produced them and therefore their detection and analysis will represent a new form of astronomy, 'gravitational wave astronomy' [6, 7]. This astronomy will require accurate models of the sources and the waveforms they produce to decode the information carried by gravitational waves. These models will be provided by numerical relativity.

The importance of numerical models of relativistic systems cannot be overestimated. This has been reflected in the growing interest in numerical relativity since its first tentative steps in the late 1960s. Perhaps this growth is better described by noting that a review on the status of numerical relativity 30 years ago would have been dedicated to describing what the pioneers of this field, Hahn and Lindquist [8]; Smarr [9] and Eppley [10] studying black hole spacetimes and Wilson [11] investigating neutron stars were doing back then. These pioneers foresaw the importance of computers in modelling otherwise intractable problems. These first ventures spurred throughout the years a large number of projects in many different directions. Consequently, a comprehensive review would demand a complete edition of *Classical and Quantum Gravity* to justly describe most efforts and directions being studied at present. This, naturally, speaks well for the status of the field, signalling how much momentum has gathered in the past few decades and how an increasingly important role is being played by present-day gravitational research. Unfortunately, lack of space will not allow for a fair addressing of all 'flavours' of numerical relativity research. The vast number of areas renders covering all of them impossible; as much as I tried to present a comprehensive overview, some topics or a more detailed presentation of others are not included and I apologize in advance for this. In particular, I very much regret not being able to extensively cover areas such as relativistic hydrodynamics, critical phenomena and computational cosmology in this paper. Fortunately,

excellent recent reviews are available on these subjects (and I will refer the reader to them as I briefly go through the subjects). This review should be considered complementary to these. I will put more emphasis on areas which I consider basic to understanding the present status of the field (and that are common to all areas of numerical relativity) and to serve as guidance to researchers and students willing to immerse themselves in this wonderful (and relatively) new discipline in GR.

The *main goal of numerical relativity* is to provide a description of spacetime by solving Einstein's equations numerically. This numerical implementation provides the metric g_{ab} on, at least, some region of the manifold $\mathcal{M}$ ($\mathcal{M}$ being an orientable, n-dimensional manifold of all physical events and g_{ab} a Lorentzian metric tensor). This manifold is assumed to be simply connected and globally hyperbolic, therefore, given appropriate data on an initial hypersurface, its future development can be obtained by means of solving Einstein's equations [12]. (Although analytical extensions of non-globally hyperbolic formulations can be obtained, the numerical treatment of such situations is much more complex and has so far not been considered).

Perhaps an obvious point sometimes overlooked when thinking of numerical models to solve a given problem is that *computers are not magic!* Although our computational resources give us a powerful tool with which to attempt solving a problem, it certainly does not provide a magical solution. One must worry about the 'standard points' proper of the traditional 'pencil and paper method' but also keep in mind that a numerical simulation will be employed, which adds a new dimension to the specification of the problem. Hence, before attempting any computation one must carefully:

- choose an appropriate form of equations and set of variables that govern the system;
- adopt a suitable reference frame with respect to which to describe the system;
- define initial and/or boundary conditions.

In a numerical approach, the aforementioned points should be chosen in a way that will possibly aid, or at least not harm, the numerical implementation. This introduces a new set of choices:

- discretization strategy;
- specific algorithms.

I will organize the presentation following this rather natural path. I review in section 2 the basic arena, giving an introductory description concerning the issues involved in obtaining the system of equations, choice of coordinates and initial and boundary conditions. Then, in section 3, a more detailed presentation of the three main avenues towards implementing Einstein's equations presently employed is presented. In each case, a particular representative system is discussed as an example, how coordinate systems can be chosen and the initial and boundary values specification are addressed. (Here for the sake of clarity I will concentrate on the vacuum case.) Section 4 is devoted to some generic aspects related to numerical techniques, while section 5 is devoted to particular issues related to the numerical implementations (separately addressing particulars of the three avenues presented in section 3). In section 6, I discuss the main aspects and techniques related to non-vacuum problems. Then, in section 7 a (partial) list of the main past accomplishments of the field are presented, while section 8 comments on the major current problems and results. Towards the end, in section 9, I describe a few efforts towards employing numerical simulations as a complementary technique to fully describe binary systems from their very early stages to the final merged object. Finally, in section 10, I briefly comment on the main problems for the future and conclude in section 11.

Note that when writing this paper I had three audiences in mind. Researchers outside the field who just want to get a current glimpse on the main issues and approaches of the field

to whom I would recommend sections 1 through 3, 7, 8, 10 and 11. Another group is those interested in getting involved in numerical relativity, who additionally might find sections 4 and 6 useful in 'breaking the ice'. And finally practitioners of the field who I hope will benefit from a comprehensive literature survey throughout the paper, specific discussions in sections 5 and 9 and the 'broad picture' of future possible directions presented in section 10.

Throughout this paper I adopt geometric units where $G = c = 1$. Additionally, lowercase Latin letters in the first half of the alphabet range from 1 to 4 and those from i on range from 1 to 3, unless otherwise indicated.

2. The arena

System of equations

The theory of general relativity clearly stands out from all others by the fact that the spacetime, defined as the pair $(\mathcal{M}, g_{ab})$ is 'obtained' from Einstein's equations all at once. What one solves for is the geometry, not for a particular metric tensor (since two tensors differing by a diffeomorphism describe exactly the same geometry). The 'unknown variables' do not 'live' on top of the spacetime, but rather they are precisely the spacetime. Hence, right from the start, the problem of even posing the equations is not a straightforward one. Einstein's equations, $G_{ab} = 8\pi T_{ab}$, (with G_{ab} the Einstein tensor and T_{ab} the stress–energy tensor) are completely independent of any coordinate system. The lack of a preferred frame of reference, which is a natural manifestation of the equivalence principle, is at the very core of the theory. The complete freedom in the choice of frame is in practice exploited to express the equations in a more convenient way which has led to several formulations of general relativity. Roughly speaking, a notion of time is introduced and the level surfaces defined by this time can be spacelike (giving rise to a *'3 + 1' or Cauchy approach to GR*), null (defining a *characteristic approach*), or of more generic type (which yield the approaches such as the *conformal Einstein equations*; *Cauchy-characteristic matching*, etc).

Once the system of equations is chosen, as is the case with any simulation, care must be taken with adopting (I) a preferred set of suitable coordinates (so that from the equivalence class of metric tensors defining the same geometry a single one is obtained) and (II) appropriate initial and boundary data for the problem under consideration.

Suitable coordinates

When Einstein's equations are recast in a way amenable to a dynamical description, one coordinate, say x^0, is chosen to play the role of 'time' with respect to which the dynamical evolution will be referred to. Then, $n - 1$ additional coordinates, x^i $(i = 1, \ldots, n - 1)$, are introduced at the level surfaces (Σ_t) of the time parameter. These coordinates could be standard ones such as Cartesian, spherical, cylindrical, etc or others better suited for specific problems. Note that one still has quite some freedom left, namely the rate of change of the time coordinate need not be uniform as a function of x^i. Additionally, the x^i at different values of the time coordinates might not be constant along the direction normal Σ_t, i.e. it might be 'shifted'. Exploiting this freedom has proven useful in numerous analytical studies (e.g. the use of harmonic coordinates renders Einstein's equations into an explicitly hyperbolic form which is convenient to analyse properties of the expected solution). In numerical implementations this freedom can prove crucial and the adoption of convenient coordinates is a very delicate (and important) problem which has no 'clear cut' solution. These 'ideal' coordinates satisfy the following properties.

- *Singularity avoidance properties (A) or amenability for singularity excision (B).* Spacetimes containing singularities can be approached by either 'slowing down' the rate of change of time in a region near the singularity so that the evolution is 'frozen', thus avoiding the evaluation at singular regions (A) or excising the singularities from the computational domain, thus getting rid of the problematic region; this can safely be done assuming the singularities are not 'naked' due to the event horizon hiding the excision process (B).
- *Simplification of variables.* Properly chosen coordinates might simplify the metric tensor. For instance, in the presence of a symmetry, by choosing a coordinate adapted to the congruence defined by such a symmetry the metric tensor does not depend explicitly on such a coordinate.
- *Degrees of freedom.* Adopting coordinates that manifest the true degrees of freedom might help in obtaining accurate physical predictions.
- *Radiation propagation.* When gravitational waves are sought for, coordinates adapted to a natural radiation gauge can considerably simplify the numerical treatment [9, 13, 14].

With prior knowledge of the dynamics of the system it is certainly easy to come up with coordinate prescriptions satisfying these properties. However, we need numerical simulations to obtain this knowledge! A great deal of effort has been put into obtaining reasonable recipes to choose coordinates appropriately and I will outline several proposals in this direction. However, our present knowledge on this subject is still rather limited; the field would certainly benefit from further research in this direction.

Initial conditions

Specifying of the initial and boundary data determines the physical situation under study. In general relativity, a theory with only two degrees of freedom 'hidden' in the six components of g_{ab} (assuming four are fixed by coordinate conditions), it is not expected that all can be specified freely at the initial time; rather, there must be constraints limiting the possible choices. Consequently, before starting the evolution problem, one must take care of the initial-value specification which requires careful examination of the constraint problem. Additionally, even when the equations defining consistent initial data can be readily solved (in terms of some freely chosen functions), these must be chosen so that they represent the targeted physical system.

Boundary conditions

As important as the initial-value specification is that of the treatment of the possible boundaries. These boundaries can be at the 'outer edge' of the computational domain (referred to as *outer boundaries*) or inside the computational domain (referred to as *inner boundaries*). Not only must the prescription of boundary data correspond to the physical situation in mind, but also its implementation must not give rise to spurious reflections which could contaminate the described physics or, even worse, render the simulation unstable. Properly addressing the boundary implementation is a highly non-trivial problem even in simple systems. For instance, when modelling the simple wave equation in dimensions higher than one, correct boundary value specification requires a non-local procedure which represents a significant computational overhead [15]. In nonlinear systems, where backscattering is expected, this problem becomes very difficult and a general solution is not known even at the analytical level. Clearly, the numerical treatment of the boundary value problem is a delicate issue, and I will review the present way of handling it in the next sections.

In the following section I will comment on how the above-mentioned problems are addressed in the different formulations that have made their way into numerical relativity[1].

3. Formalisms: initial/boundary data and coordinate conditions

3.1. Cauchy approach to GR

3.1.1. Formalism. In the three-dimensional (3D) Cauchy (or '3 + 1') formulation of Einstein's equations, one foliates $\mathcal{M}$ with a parametrized (with parameter t) set of spacelike, three-dimensional hypersurfaces Σ_t and chooses coordinates x^i ($i = 1, \ldots, 3$) to label points on each one. Thus, the spacetime points have coordinates $x^a = (t, x^i)$. The standard 3 + 1 decomposition presented in [16–18], chooses n^μ as the future-pointing timelike unit normal to the slice, with

$$n^\mu \equiv -\alpha \nabla^\mu t, \tag{1}$$

where α is the *lapse function* defining the proper interval measured by observers travelling normal to the hypersurface. Since coordinates need not be chosen to remain constant along the normal direction (as they can be freely specified at each Σ_t), they are related by a *shift vector* defined as

$$\beta^\mu \equiv t^\mu - \alpha n^\mu, \tag{2}$$

where

$$\beta^\mu n_\mu \equiv 0; \tag{3}$$

so, in this frame, $\beta^a = (0, \beta^i)$. If the (Euclidean) metric of each Σ_t is given by γ_{ij} (defined as the pull-back of g_{ab} onto Σ_t) the spacetime metric results in

$$\mathrm{d}s^2 = -\alpha^2 \,\mathrm{d}t^2 + \gamma_{ij}(\mathrm{d}x^i + \beta^i \,\mathrm{d}t)(\mathrm{d}x^j + \beta^j \,\mathrm{d}t), \tag{4}$$

where γ_{ij} is regarded as a fundamental variable, while α and β^i are mere manifestations of the coordinate freedom proper of general relativity. When writing down Einstein's equations in this approach, a second-order partial differential equation (PDE) system results where, in particular, six equations contain second time derivatives of γ_{ij} (obtained from $G_{ij} = 8\pi T_{ij}$). In order to properly specify the initial-value problem, the first time derivative of γ_{ij} must also be specified at an initial hypersurface. Instead of this, one usually provides K_{ij} defined by

$$K_{ij} \equiv -\tfrac{1}{2}\mathcal{L}_n \gamma_{ij}, \tag{5}$$

where $\mathcal{L}_n$ denotes the Lie derivative along the n^μ direction. From K_{ij} the first time derivative of γ_{ij} is readily obtained but K_{ij} is preferred (as it has a natural geometrical interpretation, being the second fundamental form or extrinsic curvature of Σ_t embedded in the four-dimensional spacetime). With these definitions, Einstein's equations are expressed (with the aid of the Gauss–Codazzi–Ricci conditions) as

$$d_t \gamma_{ij} = -2\alpha K_{ij}; \tag{6}$$

$$d_t K_{ij} = \alpha \left[R_{ij} - 2K_{i\ell}K^\ell_j + K K_{ij} \right] - D_i D_j \alpha; \tag{7}$$

where $d_t \equiv \partial_t - \mathcal{L}_\beta$; D_i and R_{ij} are the covariant derivative and Ricci tensor compatible with γ_{ij} and $K \equiv K^i_i$.

[1] For the sake of keeping the presentation short, I will restrict to the vacuum case until section 6. However, most of what I describe here applies to the non-vacuum case, the additional problem is the accurate treatment of the equations governing the matter variables.

Hence, γ_{ij} and K_{ij} are the set of initial data that must be specified for a Cauchy evolution of Einstein's equations. Equations (6) and (7) constitute the evolution equations which are used to obtain the spacetime to the future of the initial hypersurface. There still remain four extra equations which we have so far not been considered (from $G_{0i} = 8\pi T_{0i}$, which do not contain second time derivatives of γ_{ij}). These equations are

$$R + K^2 - K_{ij}K^{ij} = 0, \tag{8}$$

and

$$D_j \left(K^{ij} - \gamma^{ij}K\right) = 0. \tag{9}$$

Equation (8) is referred to as the *Hamiltonian* or *scalar constraint*, while (9) are referred to as the *momentum* or *vector constraints*. These equations impose conditions that γ_{ij} and K_{ij} must satisfy and therefore restrict their possible values. Fortunately, only at the initial hypersurface must one worry about satisfying the constraint equations as the Bianchi identities guarantee that they will be preserved on future slices of the evolution. Providing data satisfying the constraint equations is not a trivial task, we will return to this issue in section 3.1.3.

This Cauchy or '3 + 1' formulation is customarily called ADM in numerical relativity jargon[2] and has until recently been the system that has received the most attention in numerical relativity. However, this system is by no means the only '3 + 1' approach. Many related formulations can be readily obtained from the ADM. For instance, one can choose (i) to use a different combination of variables; (ii) the constraints can be freely added to the equations (pre-multiplied by arbitrary functions) and (iii) extra variables can be introduced to eliminate second-order spatial derivatives (with the consequent enlargement of the system of equations). (Note that these in turn can be expressed in terms of tensor, frame or tetrad components).

Several of these options have been exploited to come up with new, and of course, physically equivalent re-formulations which explicitly display some desirable properties. Among those, a number of symmetric hyperbolic formulations[3] have been presented (using (i)–(iii)) and are starting to make their way into numerical relativity (see, for instance, [20–24]). These formulations are written in first-order form and the standard mathematical machinery for PDEs can be used to determine the well posedness of the problem under study; whether the characteristic speeds of the system are physical (lie inside the null cones) and furthermore, determine which combination of variables are ingoing and outgoing with respect to a given boundary. This plays an important role when imposing boundary conditions (see the next section). Additionally, other, 'less ambitious' systems (obtained using (i) and (ii)) aimed towards isolating the physical modes of the solution have recently become quite popular in numerical relativity. This approach known as BSSN is displaying in a number of cases better behaved evolutions than those obtained with the ADM formulations [25–27][4].

3.1.2. Coordinate conditions. In this approach, adopting coordinates conditions means providing a prescription for α and β^i (the lapse and shift vector). One would like this prescription to be ideally suited for the simulation; however, as mentioned previously, this is not generally possible without prior knowledge of the expected dynamics. To achieve this, one can somehow 'tie' the coordinate conditions to the dynamics of the fields so as to obtain some 'feedback' on how these coordinates should be chosen. In practice, either 'evolution' equations

[2] For the formulation introduced by Arnowitz, Deser and Misner [16]; although it is related to it by using K_{ij}, instead of the ADM conjugate momentum π_{ij}.

[3] For a recent review of hyperbolic systems in general relativity see [19].

[4] Systems of this type have also been introduced which can be rendered symmetrically hyperbolic by appropriately adding the constraints [28].

or equations at a given surface (elliptic) are employed for this purpose. The former approach, although sound in principle, should be treated with special care, as some choices might lead to coordinate pathologies [29–31]. The latter option involves solving elliptic equations which are computationally expensive, but nevertheless have proven quite useful. In the following we will present some of the options being pursued.

These can be grouped into three different strategies: 'geometrical', 'simplifying' and 'cost-reducing' conditions. The division between the first two is clear in methodology but not necessarily in the final results since, as we will see next, some conditions are obtained with either strategy. In the third group, I gather computationally less expensive conditions defined (I) to retain some of the properties of those in the first two groups, while at the same time simplifying their numerical implementations or (II) derived from known solutions.

'Geometrical' prescriptions

Lapse condition: maximal slicings. The first of these prescriptions was suggested by Lichnerowicz [32] and later extended by York [17], and is known as the family of 'maximal slicings'. These slices maximize the 3-volume of the slices, hence the name. This condition translates into slices that effectively deform so that $K \equiv \gamma^{ij} K_{ij} \equiv F(t)$ which in turn implies a non-uniform α. A straightforward evaluation of the trace of equation (7) (and using the Hamiltonian constraint to re-express the Ricci tensor in terms of K_{ij}), provides the elliptic equation for α,

$$\Delta\alpha = \alpha K_{ij} K^{ij} - K_{,t}. \tag{10}$$

Although it is not clear that a solution to the above equation will always exist, in present and past applications (in the particular case of $K = 0$) it has proven quite useful. Not only does it provide a usable definition for the lapse, but the resulting slicing tends to 'avoid the singularities' [17]. Note that from equation (6) one straightforwardly obtains the equation $\partial_t(\log\sqrt{\gamma}) = -\alpha K + D_i\beta^i$, which describes the evolution of the determinant of γ_{ij}. In the case where $\beta^i = 0 = K$ the singularity avoidance property of this slicing is clear as the variation of the local volume remains fixed. This effectively slows down the evolution in regions of strong curvature, while the simulation proceeds in the further regions. Unfortunately, this feature comes at a price. The same property that makes it enticing carries the crux when attempting long simulations of singularity-containing spacetimes. As the evolution proceeds, the slices 'pile-up' in regions of high curvature, while not in weaker curvature regions. The sequence of slices that result are considerably 'bent' and large numerical gradients are induced (this problem is usually referred to as 'grid stretching'; however, the grid clearly does not stretch, rather the proper distance between grid points become large). As the evolution proceeds these gradients become larger and ultimately the evolution crashes. In almost all implementations employing maximal slicings, the choice of $K = 0$ has been adopted. Recently, the properties of slices with non-vanishing K have been analysed in one dimension (1D) illustrating the potential advantages of such a choice [33].

Shift conditions: minimal strain and minimal distortion. A shift condition known as 'minimal strain' was introduced by Smarr and York [34] through a set of elliptic equations obtained via a minimization of the hypersurface strain. Minimizing an action defined with g_{ij} and $\mathcal{L}_n g_{ij}$ with respect to β^i yields the (elliptic) set of equations,

$$D_i D^i \beta^j + D_i D^j \beta^i - 2D_i(\alpha K^{ij}) = 0. \tag{11}$$

A related condition known as 'minimal distortion' is obtained by considering a different action defined in terms of a 'distortion tensor' $F_{ij} = \gamma^{1/3}\mathcal{L}_n\tilde{\gamma}_{ij}$ (with $\tilde{\gamma}_{ij} = \gamma^{-1/3}\gamma_{ij}$) [34],

$$D^j D_j\beta^i + \tfrac{1}{3}D^i D_j\beta^j + R^i_j\beta^j - 2D_j(\alpha[K^{ij} - \tfrac{1}{3}K]) = 0; \tag{12}$$

(this result can also be obtained by $D_j(\tilde{\gamma}^{ij}_{,t}) = 0$).

Recently, Brady *et al* [35] extended the minimal strain prescription by minimizing the action with respect to both α and β^i obtaining (11) and the lapse condition

$$K^{ij}\left(-2\alpha K_{ij} + 2D_i\beta_j\right) = 0. \tag{13}$$

The coupled system (11), (13), is referred to as 'generalized Smarr–York conditions'. Recently, Garfinkle *et al* have studied the question of existence and uniqueness of this system [36]. The authors conclude that although there is a potential case for non-uniqueness, this problem can be avoided by an appropriate choice of slice and boundary conditions.

These conditions have the desirable property of reducing the possible distortion in the spatial coordinates due to the 'evolution' of the spatial slices [17]. Additionally, they minimize the rate of change along $(\partial_t)^a$ which is indeed appealing as the metric variables should vary slowly in the resulting coordinates.

'Simplifying' prescriptions

Coordinate conditions: 'symmetry-seeking coordinates'. Recently [35, 37], prescriptions have been obtained by demanding the existence of some 'approximate' symmetries. In [37] the authors approached the problem by demanding the coordinates be chosen such that, if the spacetime has an approximate timelike Killing vector, they adapt to the (approximate) symmetry. This (pseudo-)symmetry was expressed in terms of a homotetic Killing vector X^a, satisfying

$$\mathcal{L}_X g_{ab} = 2\sigma g_{ab} \tag{14}$$

(with $\sigma = 0$ if X^a is a Killing vector). The homotetic condition gives rise to evolution equations for g_{ab} which, in turn, imply equations for (γ_{ij}, K_{ij}); namely

$$\mathcal{L}_X\gamma_{ij} = 2\sigma\gamma_{ij}, \tag{15}$$

$$\mathcal{L}_X K_{ij} = \sigma K_{ij}. \tag{16}$$

For the coordinate conditions to follow closely the evolutions of the metric variables, equations (15) and (16) are combined with the evolution equations (6) and (7) to obtain a constrained system (since 12 equations are obtained but only four variables are to be fixed). There is clearly a vast range of possibilities; some of the proposed options for the lapse are:

- contraction of (15) with K_{ij}, giving rise to $\alpha = (K^{ij}D_i\beta_j - \sigma K)/(K^{ij}K_{ij})$ (which will not be useful if $K^{ij}K_{ij} = 0$);
- contraction of (16) with γ_{ij} which results in $[-D_iD^j\alpha + (R + K^2)\alpha + \beta^i D_i K + \sigma K] = 0$;

and for choosing the shift:

- divergence of (15), resulting in $D^i\mathcal{L}_X\gamma_{ij} = 0$, which is precisely the 'minimal strain shift' condition;
- divergence of (16), which yields $D^i(\mathcal{L}_X K_{ij} - \sigma K_{ij}) = 0$.

These are elliptic equations and therefore must be supplemented by boundary conditions. Reasonable conditions for an asymptotically flat spacetime are $\alpha \to 1$, $\beta^i \to 0$. Additionally, inner boundary conditions might be required (for instance, in the case of singularity excision). These might be specified by Newman or Robin boundary conditions to enforce a $1/r$ behaviour [17]. However, further studies in this direction are needed since, other options might be better suited to 'follow' changes in the dynamics. For instance, in the case of an orbiting system, co-rotating coordinates should simplify the simulation, and β^i at the boundary must be chosen to reflect this fact. (see for instance [35]).

Most of the coordinate conditions presented above involve elliptic equations which might be computationally quite demanding in 3D. In practice, either approximations to these elliptic equations are used or they are promoted to parabolic equations which are added to the set of evolution equations under study.

Coordinate conditions: 'cost-reduced conditions'

Several prescriptions exist that attempt to keep the main properties of the aforementioned prescriptions, while at the same time reducing the computational cost of their implementations. Among them, are the following.

LAPSE

- Geodesic slices: defined by the simple option $\alpha = 1$, $\beta^i = 0$ (also known as Gaussian normal coordinates). Although this choice considerably simplifies the equations, the resulting coordinates tend to converge producing coordinate singularities.
- Harmonic slices: these are defined by $\nabla^a \nabla_a x^b = 0$. This option enlarges the evolution system with four extra equations and it might lead to coordinate pathologies [30, 31]. However, it has proved quite useful as they help simplify the evolution equations and have been valuable in analytical investigations of the system [17]. An extension of these conditions, referred to as 'generalized harmonic slicing' is defined by $\nabla^a \nabla_a x^b = F^b$. With F^b a source function chosen to provide more flexibility and possibly avoid problems encountered with $F^b = 0$.
- *'log' slices*: this family of slices is introduced by $d_t \alpha = -f(\alpha)\alpha^2 K$ with f an arbitrary function [21]. In particular, for $f = 0, 1$ one recovers the geodesical and harmonic slicing conditions, respectively. For the case $f = n/\alpha$ (with $n \in N$), the resulting slicing 'mimics' the maximal one close to large curvature regions (in the sense that the lapse collapses to zero), but in this case through an evolution equation.
- *'Evolving' the elliptic conditions:* in [38] it is proposed to promote the elliptic conditions to evolution equations. This idea is basically the way elliptic equations are solved through an associated parabolic equation. For instance, $L(u) = 0$ is solved by considering instead $\partial_\lambda u = \epsilon L(u)$, with λ a relaxation parameter and ϵ an arbitrary parameter. λ is chosen to be the time parameter and the equation for the slice is treated as another evolution equation. The main disadvantage is that for a stable discretization of the parabolic equation a very small time step might be required (to satisfy the CFL condition [39]) and hence render the implementation too costly. However, one might choose to relax this equation until some not too severe threshold is satisfied; the associated cost might be acceptable compared with that for the elliptic equations as illustrated in [38].
- *Approximate maximal slicings:* the maximal slicing equation (10) for the case $K = 0$ is modified to approximately satisfy this condition, giving rise to a parabolic equation [40].

- *Slices induced by analytical solutions:* when the system under study is 'close' to an analytically known solution, lapse conditions induced from this solution provide an inexpensive prescription which can prove useful [41].

SHIFT

- *Pseudo-minimal distortion:* a condition simpler than the minimal distortion is obtained by replacing the covariant derivative D_i by ∂_i. For cases where the spatial variation of the metric is 'small', this condition yields a workable approximation to the minimal distortion shift [42]. A similar condition is obtained in [40], slightly simplified by considering a modification of the action defined in [17].
- *Shift conditions induced by analytical solutions:* same as the slicing condition induced from analytical solutions.
- *Shift conditions tailored for dynamical variable control:* these are conditions derived by demanding the shift vector be such that some of the dynamical variables are kept constant in time or driven to a specific value. Having control on the behaviour of particular variables through the evolution can be extremely important. For instance, by demanding that the time derivative of a particular combination of connection coefficients be 'driven' to zero a hyperbolic condition is obtained and the overall evolution is notably improved [43].

These coordinate conditions are generic in the sense that they can be applied in any dimension. For spacetimes with exact symmetries (such as spherical symmetry and axisymmetry) further conditions exist which exploit this property. Particular examples obtained when spherical coordinates are used are: polar slices (obtained by enforcing $K = K^r_r$, yielding a parabolic equation for α [44]); radial or 'areal' gauge (so that the area of surfaces at $r =$ constant is exactly $4\pi r^2$), providing parabolic equations for β^i [44].

3.1.3. Initial and boundary data

Initial data

The theory of setting initial data was laid out by Lichnerowicz [32] and further refined and expanded by York [45]. (For a recent comprehensive review of the initial data problem and its numerical implementation refer to [46]). Here I will just mention the main aspects of this problem. The Cauchy initial-value problem requires prescribing γ_{ij} and K_{ij} on an initial hypersurface. However, not all these variables are independent. Namely, we know there are *four* constraints to be satisfied and so, only *eight* out of the 12 in the $\{\gamma, K\}$ pair need be specified. Care must be taken to 'single out' four 'preferred' variables since under a coordinate transformation the components will mix. This problem is addressed by the Lichnerowicz–York approach which extracts one quantity out of γ_{ij} (by expressing $\gamma_{ij} = \phi^4\hat{\gamma}_{ij}$ in terms of a freely specifiable $\hat{\gamma}_{ij}$) and three out of K_{ij} (by expressing the trace-free part of K_{ij} in terms of a transverse-traceless tensor plus a 'longitudinal part' which is in turn expressed in terms of a vector W^i, which becomes the unknown). An elliptic system of equations for the variables $\{\phi, W^i\}$ is obtained that, assuming proper boundary conditions and the freely specifiable data are prescribed, can be solved to yield consistent initial data to start the evolutionary problem. Of course, the 'free data' must be given in such a way as to conform to the physical system under study. Spurious radiation on the initial surface should be minimized and boundary conditions to enforce appropriate asymptotic fall-off rates be defined [45].

Additionally, when dealing with spacetimes containing singularities, special care must be exercised to handle the singularities. In practice, either the solution is renormalized, effectively

factoring out the divergent part [47], or a region containing the singularity is excised which requires introducing an inner boundary where data must be provided as well [17, 48, 49].

Inner boundary conditions

A particularly delicate issue when dealing with black hole spacetimes is the presence of singularities. Clearly, a simulation will not be able to handle the infinities associated with them. In practice, one could use a slicing that effectively freezes the evolution near the singularities (such as the maximal slicing condition), but as discussed earlier, the simulation will not proceed for long. Cosmological censorship [16] implies that singularities must be hidden inside the event horizons. Moreover, the event horizon hides anything inside it; so, in principle, an inner boundary could be chosen to lie inside the event horizon surrounding the singularity. The presence of the inner boundary, would prevent the simulations becoming 'too close' to the singularity and the simulation should perform well. This idea, originally suggested by Unruh [50] known as *singularity excision* is at present the most promising strategy to deal with the singularities that might be present in the simulation. There are two basic issues in implementing this idea. First, since the concept of an event horizon is a global one, it can only be found *after* the evolution has been carried over. In order to obtain a 'local' notion (i.e. on each hypersurface), in practice one looks for trapped surfaces; in particular the outermost one which is referred to as *apparent horizon*. Under certain reasonable conditions, one can prove that indeed the apparent horizon, if it exists[5], will always lie inside the event horizon [12]. Thus, the apparent horizon location is used as a 'marker' and the region inside it is excised from the computational domain, defining an *inner boundary* which is either spacelike or null. The second issue, which is a delicate one, has to do with the fact that somehow values at this boundary must be prescribed. The basic strategy for this is quite simple; since the past domain of dependence at this boundary is 'tilted' off this boundary (reflecting the causal structure of the spacetime interior to the event horizon), one could provide these values using the evolution equations. The numerical implementation of this strategy, on the other hand, is quite difficult as it must be capable of dealing with moving boundaries (resulting from singularities moving through the grid); merging of initially disconnected inner boundaries (such as those present in binary black hole spacetimes); 'sudden' appearance of inner boundaries (which would result in collapse situation); etc. The numerical implementation of the singularity excision strategy is a delicate issue and considerable effort is being spent in this direction. We will revisit this issue in our discussion of the particulars of numerical implementations (section 5.1)[6].

Outer boundary conditions

The spacelike slices in '3 + 1' implementations extend to spacelike infinity i^o. Assuming, as it is always the case in numerical relativity, that the spacetime is globally hyperbolic; data

[5] Note, there is no guarantee that there will be an apparent horizon on any hypersurface, for instance even Schwarzschild spacetimes admit a, granted odd looking, hypersurface without an apparent horizon [51]. However, all counter-examples of this type require quite 'perverse' looking slices that one can 'hope' that for reasonable slices one will be found.

[6] Note that the presence of the event horizon *does not* allow one to specify arbitrary conditions and claim they will be hidden by it. In fact, different conditions will represent different field configurations at earlier times, describing for instance gravitational waves. Part of these will 'fall' into the horizon providing the 'desired' values at the inner boundary while others will remain outside. Hence, different inner boundary conditions will provide, in general, field configurations outside the horizon representing different physical scenarios. An alternative way of addressing the assignment of inner boundary values is being developed by Eardley [52, 53]. This approach explicitly uses the equation determining the apparent horizon (which is assumed to define the inner boundary) supplemented with some geometrically motivated conditions to obtain a 2D elliptic set of equations which can be solved to obtain inner boundary values. (Note: since this approach is not yet fully developed it has not been attempted so far; but it certainly has appealing properties and should not be forgotten.)

on a given initial hypersurface completely determines the unique geometry to the future of it. In order to have a simulation be able to handle these 'infinitely large' hypersurfaces, one can in principle, compactify the spacetime to deal with a 'finite domain' and gain access to infinity (where, for instance, the concept of asymptotically flatness can be used to provide boundary data). However, the numerical implementation of this strategy is complicated. Namely, spacetime points are separated by increasingly larger distances (in particular, the boundary point is infinitely far from the nearest inner neighbour!). Consequently, there is a clear loss of resolution which considerably complicates the stability of the scheme. This is a real problem as ripples in the metric variables 'pile-up' and there cannot be enough points to accurately resolve them. High-frequency modes ('noise') is generated which usually drives the simulation unstable[7]. An approach which has not yet been pursued, is to consider more generic slices, which asymptotically become null, that end at future null infinity. In this case, assuming coordinates have been chosen adapted to the propagation of radiation, the ripples should appear fairly constant, and the loss of resolution should not be a problem (therefore compactification should be possible). As future null infinity is approached, terms in the equations tending to $0/0$ will arise, which will require special care. Assuming this can be done, it would be interesting to see how a '3 + 1' simulation would proceed when the slices end at $\mathcal{I}^+$.

Because of the potential problems associated with the compactification of spacelike hypersurfaces, the most common approach is to '*cut*' the hypersurfaces and bound them with a timelike boundary Γ. Although this trivially takes care of defining a finite domain for the simulation, it brings about a non-trivial one, i.e. *how to define appropriate boundary conditions*. The problem lies in the fact that appropriate boundary conditions are simply not known! All we know from analytical studies corresponds to *asymptotic fall-off rates* at spacelike or null infinity under certain assumptions on the 'isolated' source [55–58]. In practice several strategies are in use.

Simplistic approach. The simplest approach is to place the boundaries 'as far away as possible' and provide data on Γ by simple-minded prescriptions such as 'freezing' their values, setting them to 'educated' guesses on what they should be, etc. Although this approach provides, at best, approximate values in generic cases, by placing the boundaries far enough from the region one is most interested in, the error introduced should influence late times. Hopefully, by then, the 'interesting' part of the problem has already happened and one need not worry about the boundaries. This approach clearly is 'too dirty' for anyone's taste; yet, when dealing with simulations that are plagued by instabilities the philosophy has been to try to invest time improving the treatment of the '*interior*' before that at the boundary (if, of course the boundaries are not to blame for the instability, which is a *big if*). Additionally, numerical techniques can be used to (try to) minimize the reflections; the most commonly used ones are 'filters' such as the *sponge filter* [59, 60] and the *blending boundary condition* [61], which slightly modify the right-hand side of the equations in a 'thick' region next to the boundary, where the reflections are dumped.

Radiation boundary conditions. A less 'crude' approach is to use the fact that when boundaries are placed in the radiation zone the system must describe (neglecting backscattering) purely outgoing waves. This in turn, can be exploited to prescribe approximate boundary conditions. For instance, imposing Sommerfeld-type (outgoing wave) conditions on

[7] Yet, 'noise' that this loss of resolution creates, could be handled by carefully filtering it out so as to minimize its influence on the rest of the spacetime. This approach has been used in [54], which reported good results for relatively moderate amounts of time.

all variables has been the preferred choice in most numerical applications (e.g. [26,42,62–64]). An interesting option, which has so far not been applied in non-flat spacetimes, is to chose a slicing where the spacelike surfaces asymptotically approach null ones at the outer boundaries. The strategy behind this approach is quite simple, the lapse/shift are chosen in such a way that, asymptotically, both the hypersurface and lines at constant x^i approach null ones [65]. The outer boundary is effectively 'pushed' further away and the loss of resolution is not too severe as outgoing fields vary slowly on 'close to null' trajectories. For massless and massive Klein–Gordon fields propagating on a flat background this approach has been shown to clearly outperform Sommerfeld-type conditions [65]. It would be interesting to investigate this strategy in more generic scenarios; with properly chosen coordinate conditions, this strategy can be really helpful. (Note that providing data on all variables independently is not consistent as will be discussed later in this section.)

Perturbative boundary conditions. Boundary conditions have been derived by matching Einstein's equations to a set of linear equations obtained from linearized perturbations over curved backgrounds [66, 67]. This approach neglects the effects of non-linear terms outside the outer boundary introducing errors which do not decrease with resolution but should become smaller as the outer boundary is moved further out. So far, applications of this technique have been restricted to linear and quasi-linear waves in flat spacetime yielding the expected results [67]. Outgoing waves propagate through the boundaries leaving behind a small reflection which can be further reduced by numerical filtering.

Simplistic approach and hyperbolic formulations. The use of strongly/strictly/symmetric hyperbolic formulations clearly distinguishes the *incoming variables* at a given boundary. Efforts based on these formulations [20] adopt the standard strategy of providing 'simple-minded' or constrained boundary values (see below) but in this case *only* to the *incoming* variables.

Constrained boundaries. There is an important point to be raised here. So far, we have not taken into account that there are only *two* degrees of freedom and imposing boundary conditions to most variables is not, in general, consistent. Although in most cases it is difficult to distinguish these two degrees of freedom, at least we can use the fact that the variables are related by constraints to partially restrict the data to provide. For instance, if Γ is at $x^1 = L$, the constraints would be $G_{a1}|_\Gamma = 0$. Whether these constraints are satisfied at the boundary by the above prescriptions is not clear *a priori*. A few studies have been carried out towards specifying boundary conditions satisfying the constraints.

One of them [68] has presented an approach to incorporate the constraints (induced on a timelike boundary) into a 3D ADM evolution code. This work was specifically tailored for linearized perturbations of flat spacetime and with the shift set to zero; however, this work evolved the system for about 1000 crossing times (as opposed to 100 with Sommerfeld conditions), showing that a more consistent approach to the boundary problem might be quite helpful in a simulation (for a discussion considering a similar approach see [69]). Another [23], employs the Hamiltonian and momentum constraint (i.e. the constraints on the spacelike hypersurfaces) to determine boundary values in a 3D code by implementing a symmetric hyperbolic formulation of Einstein's equations. Preliminary tests indicate better behaved evolutions are obtained. Also, in 1D, constraints have been used to provide boundary values and compare with the simple-minded approach [20]. For the case of a Schwarzschild spacetime, this work illustrates how, in the tested cases, the prescription of 'constrained boundary values'

indeed provides stable implementations, while the simplistic approach to freezing incoming field values at the outer boundary fails.

Additional support for the use of constrained boundaries has been presented in the 1D case. Here a couple of works have chosen boundary conditions defined in a way such that the time derivative of the constraints remain zero (and therefore they are satisfied throughout the evolution), achieving stable evolution of black hole spacetimes perturbed with a minimally coupled scalar field without the need for specially designed gauge conditions [70, 71].

Recently, Stewart presented a systematic study of the well posedness question of the *initial boundary value problem* [72]. This required analysing the properties of the evolution system (in this case the symmetric hyperbolic formulation introduced in [73]) coupled to the boundary value specification. He found that well posedness is obtained if these boundary data are specified so that the constraints are satisfied at the boundary.

A deep insight into the initial boundary value problem both from the mathematical point of view (i.e. well posedness) and its physical interpretation has been presented by the work by Friedrich and Nagy [74]. Through a careful analysis of the properties of the system, taking into account the presence of a timelike boundary, they conclude that, as expected, only *two* variables might be freely specified (related to the two polarizations of the incoming radiation). Although the conclusions obtained in this work should be extendible to all formulations (after all it is a statement about the *physics* of the problem) the extension is far from straightforward when not dealing with symmetric hyperbolic systems. Clearly, a more systematic study of the role played by boundaries in GR and their role in numerical implementations is needed.

Another alternative, is to dispense with the outer boundary completely; two options for achieving this are: Cauchy-characteristic matching [75–79] or the conformal field equations (see section 3.3). While the latter implies using a completely different formalism to study the spacetime (and will be presented in detail in section 3.3), the former supplements the '3 + 1' formulation with a characteristic one (see section 3.2). Basically, in the region exterior to the boundary to future null infinity, one introduces a foliation along outgoing characteristics and Einstein's equations are written adapted to this foliation. Since the phase of the 'ripples in the metric' is nearly constant along these null surfaces, the Penrose compactification technique [80] is used to deal with a finite computational domain. Just as several coordinate patches are required to deal with non-trivial topologies, patching together regions of spacetime treated with different approaches can provide a clean treatment of the problem.

The '3 + 1' approach has been that receiving the most attention in numerical relativity (NR); however, several other alternatives have been implemented successfully in several systems. These alternatives are the characteristic formulation of GR and the conformal Einstein equations.

3.2. Characteristic formulation

3.2.1. Formalism. The characteristic formulation of GR was introduced by Bondi [14] and Sachs [81] in the 1960s. The main strategy of this approach is the use of a foliation by a sequence of (outgoing or incoming) null hypersurfaces which made it an ideal arena to understand the key issues regarding gravitational radiation. There are several 'variants' of this approach yielding slightly different systems of equations; however, they all have in common that only *two first-order* evolution equations and *four* 'hypersurface' equations[8] need be solved (which are essentially ODEs). Here I will present the one first implemented in 3D [82], which adopted the Bondi approach to characteristic GR, but several other efforts have implemented characteristic approaches in 2D [79] or 3D [83].

[8] Equations relating quantities only on a given hypersurface.

In the Bondi approach a coordinate system adapted to the null foliation is chosen in the following way: the outgoing (incoming) lightlike hypersurfaces emanating from a timelike geodesic or worldtube are labelled with a parameter u; each null ray on a specific hypersurface is labelled with x^A ($A = 2, 3$) and r is introduced as a surface area coordinate (i.e. surfaces at $r =$ constant have area $4\pi r^2$). In the resulting $x^a = (u, r, x^A)$ coordinates, the metric takes the Bondi–Sachs form [14, 81]

$$ds^2 = -\left(e^{2\beta}V/r - r^2 h_{AB}U^A U^B\right)du^2 - 2e^{2\beta}\,du\,dr - 2r^2 h_{AB}U^B\,du\,dx^A + r^2 h_{AB}\,dx^A\,dx^B. \tag{17}$$

Six real field variables appear in this form of the metric[9]: V, β, U^A and h_{AB}. They have a straightforward physical interpretation: h_{AB} represents the conformal intrinsic geometry of the surfaces defined by $dr = du = 0$ and contains the two degrees of radiative freedom. The field β represents the *expansion* of the light rays as they propagate radially. V is the analogue of the Newtonian potential, and its asymptotic expansion contains the mass aspect of the system. Note that the coordinate system is tied to null surfaces which can intersect due to caustics or crossovers. In these cases, the coordinate system becomes singular! So, it is clear that this approach cannot be used for arbitrary systems. However, as we will discuss in section 5.2, one has several options to address the caustic/crossover problem in a number of cases, thus extending its range of applicability.

Einstein's equations in the vacuum case, $G_{ab} = 0 = R_{ab}$, decompose into hypersurface equations, evolution equations and conservation laws. Bondi designated as the 'main' Einstein equations [14] those which correspond to the six components of the Ricci tensor, R_{rr}, R_{rA} and R_{AB}.

The hypersurface equations, given by R_{rr}, R_{rA} and $h^{AB}R_{AB}$, can be written as

$$\beta_{,r} = \tfrac{1}{16}r h^{AC}h^{BD}h_{AB,r}h_{CD,r}, \tag{18}$$

$$(r^4 e^{-2\beta}h_{AB}U^B_{,r})_{,r} = 2r^4\left(r^{-2}\beta_{,A}\right)_{,r} - r^2 h^{BC}D_C h_{AB,r}, \tag{19}$$

$$2e^{-2\beta}V_{,r} = \mathcal{R} - 2D^A D_A\beta - 2D^A\beta D_A\beta + r^{-2}e^{-2\beta}D_A(r^4U^A)_{,r} - \tfrac{1}{2}r^4 e^{-4\beta}h_{AB}U^A_{,r}U^B_{,r}; \tag{20}$$

and the evolution equations, given by $R_{AB} - h_{AB}h^{CD}R_{CD}/2$, are expressed as

$$\begin{aligned} r(rh_{AB,u})_{,r} - \tfrac{1}{2}(rVh_{AB,r})_{,r} = {} & \left(2e^{\beta}D_A D_B e^{\beta} - r^2 h_{AC}D_B U^C_{,r} - \tfrac{1}{2}r^2 h_{AB,r}D_C U^C\right. \\ & + \tfrac{1}{2}r^4 e^{-2\beta}h_{AC}h_{BD}U^C_{,r}U^D_{,r} - r^2 U^C D_C h_{AB,r} \\ & \left. - 2rh_{AC}D_B U^C + r^2 h_{AC,r}h_{BE}(D^C U^E - D^E U^C)\right) \\ & - \tfrac{1}{2}h_{AB}\left(r^2 h^{CD}_{,r}\left(h_{CD,u} - \frac{V}{2r}h_{CD,r}\right) + 2e^{\beta}D_C D^C e^{\beta}\right. \\ & \left. - D_C(r^2U^C)_{,r} + \tfrac{1}{2}r^4 e^{-2\beta}h_{CD}U^C_{,r}U^D_{,r}\right); \end{aligned} \tag{21}$$

where D_A is the covariant derivative and $\mathcal{R}$ is the curvature scalar of the 2-metric h_{AB}. There is a natural hierarchy to integrate these equations; namely, assuming h_{AB} and consistent boundary values are known, the integration sequence (18)→(19)→(20), completely determines the metric on a given hypersurface. Lastly, equation (21) is integrated to obtain h_{AB} at the next hypersurface and the process starts again [84].

[9] Note that the areal r coordinate requirement in turn implies that $\det h_{AB}$ be that of the unit sphere metric; thus there are only two independent fields for h_{AB}.

So far, we have accounted for six hypersurface and evolution equations. Together with the equations $R^r_a = 0$, they form a complete set of components of the vacuum Einstein equations. Given that the main equations are satisfied, the Bianchi identities imply they are satisfied on the spacetime provided they hold on a single spherical cross section. By choosing this sphere to be at infinity, Bondi identified these three equations as conservation conditions for energy and angular momentum.

3.2.2. Coordinate conditions. It is also possible to obtain a geometrical insight into the fields by analysing the intrinsic metric of the $r =$ constant surfaces,

$$\gamma_{ij}\,\mathrm{d}x^i\,\mathrm{d}x^j = -\mathrm{e}^{2\beta}\frac{V}{r}\,\mathrm{d}u^2 + r^2 h_{AB}(\mathrm{d}x^A - U^A\,\mathrm{d}u)(\mathrm{d}x^B - U^B\,\mathrm{d}u). \tag{22}$$

In analogy to the 3 + 1 decomposition of the Cauchy formalism [16], a 2 + 1 decomposition of the timelike worldtube geometry leads to the identification of $g_{AB} = r^2 h_{AB}$ as the metric of the 2-surfaces of constant u which foliate the worldtube, $\mathrm{e}^{2\beta}V/r$ as the square of the lapse function and $(-U^A)$ as the shift vector. However, there is a clear difference. Inspection of the system (18)–(20) reveals 'hypersurface equations' for the gauge variables; which result from the fact that the slices are to be null. Consequently, the issue of 'coordinate freedom' in characteristic numerical relativity is not as 'open' as in the Cauchy case, and this freedom is to be fixed at a given timelike or null worldtube.

Little has been explored about this choice, most analytical studies have concentrated on defining the problem at $\mathcal{I}^+$ and integrating the equations radially inwards. Numerical applications do the opposite, i.e. integrate the equation outwards. Additionally, the remarkable robustness displayed by all characteristic implementations (in the vacuum case) to handle superluminal shifts have not prompted the need to introduce shift choices that would simplify the dynamics.

LAPSE. Lapse choices have been induced from analytical solutions [79, 82, 83, 85] or by matching to a Cauchy evolution [79, 82]. Additionally, models describing the geometry of a fissioning white hole have been introduced [86, 87] in which the parametrization of the null generators can be used to induce lapse conditions for a double null evolution [88].

SHIFT. Although vacuum codes routinely handle superluminal shifts without problems, simulations of non-vacuum systems [89] might benefit from a convenient choice. For instance, when modelling a 'star' orbiting around a black hole, a shift can be used so that the angular coordinates rotate around the inner boundary 'following' the orbiting star which, in the resulting coordinates, will remain (approximately) fixed [90].

3.2.3. Initial and boundary data

Initial data

A distinctive feature of the initial data problem in the characteristic formulation is that data on a given initial hypersurface are generally not enough to determine the solution (not even locally). This is due to the fact that the domain of dependence of a single *non-singular* null hypersurface is empty! In order to obtain a well defined problem the null hypersurface must either be completed to a caustic-crossover region or an additional boundary must be introduced (which defines an S^2 cross section at the intersection). In present numerical applications the latter option is pursued where the boundary is either null or timelike. Assuming the constraints

are satisfied in this inner boundary at the S^2 intersection, one can freely chose h_{AB} on a given surface (albeit subject to a regularity conditions at the intersection), integration of the ordinary differential hypersurface equations yields perfectly valid initial data *without* having to solve an elliptic problem. The non-elliptic character of these equations is a consequence of their application on a null surface, rather than a spacelike one. For the case where the boundary is null, the system is well posed [91]; for the timelike case, only existence and uniqueness have been proven [92, 93].

Although there is no difficulty in obtaining 'valid' initial data, the important issue is to have these data be 'physically relevant'. Cauchy formulations can look to post-Newtonian approximations for guidance in the search for physically relevant data, in the characteristic case, an approximation approach based on a family of null cones with the speed of light being a varying parameter [94] has been introduced to make contact with Newtonian theory. This approach guarantees that for weakly radiating systems the obtained waveforms are, to a first-order approximation, given by the quadrupole formula.

Boundary data: inner boundary

In implementations, when the inner boundary is timelike, the data have been defined by either known analytical solutions [85, 95, 96] or through matching to a 3 + 1 evolution being carried out in the interior (we will discuss more on matching in section 5.2) [97, 98]. These options guarantee the extra four equations ($R^r_a = 0$) are satisfied at the boundary. In the case where the inner boundary is null, since whichever data have been given on the initial null hypersurface cannot interact with the boundary, these can be easily specified. In particular, applications, the inner boundary has been chosen to coincide with the past null horizon of a Schwarzschild spacetime [77, 82, 83]; an incoming null surface (outside the event horizon) of a Kerr spacetime [85] or in a double null problem where the inner boundary corresponds to a fissioning white hole (this case will be discussed later in more detail in section 5.2).

Boundary data: outer boundary

Another property that makes this formulation appealing is that the outer boundary is $\mathcal{I}^+$, the hypersurfaces define cuts at $\mathcal{I}^+$ which is a flat $S^2 \times R$ null manifold, defined by the end points of outgoing null curves. No boundary condition is needed as the evolution proceeds along $\mathcal{I}^+$ at this boundary. Since gravitational waves have constant phase on null hypersurfaces the compactified spacetime can be safely implemented numerically without the risk of a loss of resolution affecting the evolutions. Additionally, having access to future null infinity brings about extra benefits, such as the possibility of rigorously obtaining the gravitational radiation, mass and angular momentum [14, 81, 84, 99]; also, when studying asymptotically flat spacetimes, the metric variables have a well known asymptotic dependence which has been exploited to aid the numerical implementations [79, 82, 83].

3.3. Conformal Einstein equations

3.3.1. Formalism. A further approach used in numerical relativity is known as the 'conformal Einstein equations approach' and was introduced by Friedrich in the early 1980s [100]. The main peculiarity of this approach is that instead of solving for the spacetime (M, g_{ab}), it first obtains the description of a larger one $(\tilde{M}, \tilde{g}_{ab})$. As a result, one can foliate the spacetime $\tilde{M}$ with a sequence of spacelike; null or more generic hypersurfaces. Although the latter option has not been pursued to date, the former approach has been adopted in all efforts. Naturally,

this approach is also of Cauchy type but I have chosen to present it separately as it has a few notable differences from those from section 3.1. The larger spacetime is determined by the conformal Einstein equations which can be expressed as

$$\tilde{\nabla}_a \tilde{R}_{bc} - \tilde{\nabla}_b \tilde{R}_{ac} + \tfrac{1}{12}\left((\tilde{\nabla}_a \tilde{R})\,\tilde{g}_{bc} - (\tilde{\nabla}_b \tilde{R})\,\tilde{g}_{ac}\right) + 2\,(\tilde{\nabla}_d \Omega)\,d_{abc}{}^{d} = 0, \tag{23}$$

$$\tilde{\nabla}_d d_{abc}{}^{d} = 0, \tag{24}$$

$$\tilde{\nabla}_a \tilde{\nabla}_b \Omega_a + \tfrac{1}{2}\,\tilde{R}_{ab}\,\Omega - \tfrac{1}{4}\tilde{\nabla}^a \tilde{\nabla}_a \Omega\,\tilde{g}_{ab} = 0, \tag{25}$$

$$\tfrac{1}{4}\tilde{\nabla}_a\left(\tilde{\nabla}^b \tilde{\nabla}_b \Omega\right) + \tfrac{1}{2}\,\tilde{R}_{ab}\,\tilde{\nabla}^b \Omega + \tfrac{1}{24}\,\Omega\,\tilde{\nabla}_a \tilde{R} + \tfrac{1}{12}\,\tilde{\nabla}_a \Omega\,R = 0, \tag{26}$$

$$\Omega d_{abc}{}^{d} + (\tilde{g}_{c[a}\tilde{R}_{b]}{}^{d} - \tilde{g}^{d}{}_{[a}\tilde{R}_{b]c}) + (\tilde{g}_{c[a}\tilde{g}_{b]}{}^{d})\tfrac{1}{6}\tilde{R} - \tilde{R}_{abc}{}^{d} = 0, \tag{27}$$

$$\Omega^2 \tilde{R} + 6\,\Omega\,\tilde{\nabla}^a \tilde{\nabla}_a \Omega - 12\,(\tilde{\nabla}^a \Omega)\,(\tilde{\nabla}_a \Omega) = 0. \tag{28}$$

A solution of this system provides the metric $\tilde{g}_{ab}$ (defining a unique covariant derivative $\tilde{\nabla}_a$), the traceless part of the Ricci tensor $\tilde{R}_{ab}$, the Weyl tensor (of $\tilde{g}_{ab}$) $\Omega d_{abc}{}^{d}$ and $\tilde{R}$ (the Ricci scalar). The physical spacetime M ($\subset \tilde{M}$) is defined by $M := \{p \in \tilde{M} | \Omega > 0\}$ ($\Omega = 0$ represents the boundary of M). The metric $g_{ab} := \Omega^{-2}\tilde{g}_{ab}$ is a solution of Einstein's equations on M. It is worth pointing out that the (degenerate) physical metric at $\Omega = 0$ is also obtained, thus, one straightforwardly gains access to future (or past) null infinity and quantities such as gravitational radiation and tidal forces at infinity are obtained by straightforward algebraic evaluations. Although this system seems more complex, it is also amenable to a sort of 3 + 1 decomposition [101] in much the same vein as that presented in section 3.1. $\tilde{M}$ is sliced with a parametrized (with parameter t) sequence of spacelike hypersurfaces Σ_t. The unit normal to Σ_t given by n^a, allows one to adopt the intrinsic and extrinsic curvatures of Σ_t, denoted by h_{ab} and K_{ab} as the main variables. Additional variables are introduced to re-express the system in first-order form and obtain a symmetric hyperbolic system of equations for the variables (h_{ab}, K_{ab}, γ^a_{bc}, Ω, Ω_0, Ω_a, ω, E_{ab}, B_{ab}, R^*_a, R^*_{ab}). Here γ^a_{bc} is the 3-connection of h_{ab}; E_{ab} and B_{ab} are the electric and magnetic parts of d_{abcd}; $\Omega_o = n^a \tilde{\nabla}_a \Omega$; $\Omega_a = h^b_a \tilde{\nabla}_b \Omega$ and R^*_{ab}, R^*_a are particular projections of $\tilde{R}_{ab}$. Clearly, the system contains many more variables than the traditional ADM approach. However, it is important to point out that: (i) some of the variables are directly related to the gravitational radiation (and there is no extra work to obtain it from the evolved data) and (ii) the system is well posed, and the number of variables is certainly comparable to (most) well posed formulations obtained in the traditional '3 + 1' approach.

Aside from the 'standard gauge freedom' described by the lapse and shift vector, there is a further one in any conformal approach. Note that the conformal and the physical metric are related by a rescaling which is essentially arbitrary, as two solutions ($\tilde{M}$, $\tilde{g}_{ab}$, Ω) and ($\tilde{M}$, $\bar{g}_{ab}$, $\bar{\Omega}$) with ($\bar{g}_{ab}$, $\bar{\Omega}$) = ($\theta^2 \tilde{g}_{ab}$, $\theta\Omega$) and a positive function θ describe the same physical spacetime. Under the rescaling θ, the Ricci scalar R changes. Specifying either Ω or R fixes this freedom.

I have presented the conformal equations in the 3-tensor formalism simply because it is the one that yielded a 3D implementation and its 'closeness' with the '3 + 1' presentation of section 3.1. However, the equations have also been presented in the spinorial [102] or frame formalisms [100, 103].

3.3.2. Coordinate conditions. Choosing gauge conditions for the conformal equations is a similar problem to the '3 + 1' approach. Care in this case must be taken so that the foliation

crosses $\mathcal{I}^+$ and not $\mathcal{I}^-$ as one tries to avoid going through i_o (among other reasons so that boundary conditions on the unphysical spacetime will not propagate into the physical one).

LAPSE. The options for the lapse used so far have been obtained from analytical expressions; derived from harmonic conditions [102] or from the condition $\alpha = e^s\sqrt{\det(h_{ab})}$ (with s real) [104]. At first sight, this last condition appears awkward as it would suggest that evolution is 'accelerated' when $\det(h_{ab})$ becomes large. In simulations of Schwarzschild spacetimes [105], this has not represented major difficulties since the initial slice is chosen to be 'far' from the singularity. Nevertheless, as more generic initial data are considered, the need for alternatives for the lapse would likely be greater.

SHIFT. A particularly interesting choice for the shift, is one which keeps the location of $\mathcal{I}^+$ at a constant grid location [102]. This addresses a common criticism to this formulation where future null infinity can move inwards in the grid and therefore, computational resources are wasted more and more since the unphysical space becomes larger (with respect to the grid). This choice introduced by Frauendiner has been successfully implemented in 2D to study vacuum spacetimes with toroidal null infinities and read-off the gravitational radiation at $\mathcal{I}^+$ [102].

As mentioned previously, numerical implementations have also been presented in the *frame* formalism [100, 103], which can be more 'flexible' with respect to gauge choices.

3.3.3. Initial and boundary data

Initial data

The literature on choosing initial data is not as extensive as in the traditional '3 + 1' approach as the numerical implementation of the conformal approach is considerably 'more recent'. However, the picture does resemble the '3 + 1' approach as constraint equations limit the possible configurations of the initial data (h_{ab}, K_{ab}, γ^a_{bc}, Ω, Ω_0, Ω_a, ω, E_{ab}, B_{ab}, R^*_a, R^*_{ab}). As proven in [106, 107], only a subset of data need be solved, namely by solving an elliptic system for (h_{ab}, K_{ab}, Ω, Ω_0) simple contractions on the remaining constraints yield the complete set of variables. Hence, the initial data problem, at least from the elliptic system to be solved, is by no means more complicated than that in the traditional system. In fact, it would be reasonable to assume that much of the numerical expertise gained in solving the traditional system should be 'transferable' to the conformal approach.

Inner boundary data

Just as in the previous formulations, if the hypersurfaces contain singularities one can use singularity excision techniques to excise the singularities from the computational domain as was done for the 1D scalar field collapse presented in [103]. Another option which, in fact, has been the preferred one in the 3D simulations of Schwarzschild spacetime [108] has been to use slices that do not contain the singularity; namely the foliation was chosen so that the slices cross both $\mathcal{I}^+$s of the Kruskal extension [12] of the Schwarzschild spacetime without 'hitting' the singularities. Clearly, this approach is sound and could also be used in the '3 + 1' approach (assuming variables can be properly renormalized at i^o or $\mathcal{I}^+$, the latter case being more or less straightforward in the conformal approach); however, the simulation is making roughly twice therequired work (there is no need to evolve sector IV in the notation of [12]). Moreover, it is not clear whether a spacetime with two black holes would be amenable to such

a strategy since the gauge conditions will have to be carefully tuned so that the slices avoid both singularities.

Singularity excision would seem to be better adapted to handling more generic situations. Incorporating this technique into the conformal approach should be expedited by the expertise (being) gained in this area in the '3 + 1' approach.

Outer boundary data

The spacetime under study in this case is larger than the physical spacetime. Consequently, the outer boundary lies beyond future null infinity. At first sight it would appear awkward to set up conditions at this boundary since it is not known what boundary conditions are to be specified there. However, this need not be a problem, since $\mathcal{I}^+$ is an incoming null surface and the space beyond $\mathcal{I}^+$ is causally disconnected from the physical spacetime. Thus, this formulation manages to get rid of the boundary problem by 'hiding' the boundary from the region of interest. There is a price to pay for this feature, namely that the implementation spends time evolving points that are of no interest and there is therefore extra computational overhead. In principle, this can be minimized by adopting an appropriate shift conditions [102] that keeps the location of $\mathcal{I}^+$ at a constant coordinate value.

4. Some ado about numerics

Now, suppose that one has (i) decided for a given system of equations for a set of variables; (ii) adopted suitable coordinates and/or coordinates conditions and (iii) defined the equations which determine the initial and boundary data and feels 'ready' to implement (i)–(iii) numerically. The question to ask is: *how does one proceed to obtain such an implementation?*

First, a 'finite' representation of the (continuous) $(n-1)$-dimensional hypersurfaces is obtained by defining a (not necessarily uniform) grid or lattice whose vertices can be labelled by a discrete set of points $(x^1_{i_1}, \ldots, x^{n-1}_{i_{n-1}})$ (with $i_j = 1, \ldots, N_j$). Then, a finite representation for the field variables is obtained by either (I) representing the variable by its value at points in the grid $\Psi^n_{i_1 \ldots i_{n-1}} \equiv \Psi(t^n, x^1_{i_1}, \ldots, x^{n-1}_{i_{n-1}})$ or (II) expanding the variable on a finite set of trial functions; i.e. $\Psi(t^n, x^1, \ldots, x^{n-1}) = \sum_l^N C^n_l \phi_l(x^1, \ldots, x^{n-1})$. The finite representation is then given by values of the variables themselves, $\{\Psi^n_{i_1 \ldots i_{n-1}}\}$ (case I) or the coefficients $\{C^n_l\}$ (case II).

These two different strategies yield, as expected, two very different approaches. *Finite-difference approximations* belong to case (I), while *Finite-difference elements*; *spectral methods*; *multiquadrics*, among others, belong to case (II). Irrespective of the method used, the 'end' result is an algebraic problem, which, in the limit of infinite resolution (i.e. grid points spacing $\to 0$, for case (I) or $N \to \infty$ for case (II)) the algebraic system should reduce to the original PDE system[10].

4.1. FDA: a couple of useful points

Finite-difference approximations (FDA) are widely used in computational physics and are so far the most popular choice in numerical relativity. The details of this technique can be found in most numerical analysis books (for instance, [39, 109, 110]); here I will comment on two important points that are not often discussed.

[10] This is known as a *consistency* requirement; although I would prefer the term *absolute* condition, since otherwise one is not studying the system of interest!

A finite-difference approximation entails replacing all derivatives operators by discretized counterparts. These discrete operators approximate the derivative of functions using the grid values $\{\Psi^n_{i_1\ldots i_{n-1}}\}$ and can be obtained through formal Taylor expansions. There are an infinite number of combinations that *a priori* can be used to approximate the original system. Unfortunately, the majority of these combinations result in unstable implementations. This is often reflected in the high-frequency components of the solution growing without bound. In practice, stable implementations often 'control' this potential problem by dissipating the high-frequency modes. In nonlinear systems, this proves to be very important since, even when the initial data do not contain high-frequency modes, these will likely be generated by the low-frequency ones.

Extensive analysis of dissipative schemes to obtain stable discretization of wave equations was performed by Kreiss and Oliger [111]. They showed how the addition of dissipation could become crucial when treating nonlinear systems. The value of such techniques have been validated over the past 50 years since they were first proposed by Von Neuman and Richtmeyer [112] to solve the classical Euler equations. In numerical relativity their use can be traced back to Wilson's implementation of the relativistic hydrodynamic equations [113]. In more recent times, dissipation techniques have been shown to be of great help in achieving stable discretizations in computational relativity, for instance in [62, 114, 115].

Additionally, the use of dissipation can play a crucial role in achieving stable discretizations for initial boundary value problems. This is highlighted in the work by Oliger [116] who considers the equation

$$F_{,t} = aF_{,x} + b(x,t) \tag{29}$$

in the domain $[L_1, \infty)$ where inner boundary conditions at L_1 are expressed as

$$F^{n+1}_{ib} = \Sigma^m_{k=0} A_k F^n_{ib+k} + g^n_k; \tag{30}$$

with m indicating the number of points to the right of $x_{ib} = L_1$ involved in the scheme. For instance, a particular case of equation (30) would be

$$F^{n+1}_{ib} = F^n_{ib} + \frac{\Delta t}{\Delta x}(F^n_{ib+1} - F^n_{ib}). \tag{31}$$

Oliger proved the following theorem [116]. *If the approximations for the initial-value problem and for the approximation at the boundary (30) are* stable *and, further, (30) is* dissipative *then, the implementation of the initial boundary value problem is stable.*

This result shows the following: (I) stability of the initial boundary value problem can be assessed by providing boundary conditions written in PDE-like form. (II) The stability and dissipative properties of this equation can be readily obtained which coupled to the stability of the initial-value problem provide a stable implementation.

Naturally, it would be desirable to have similar results tailored to the more complicated systems considered in numerical relativity. I doubt that this will be achieved since the nonlinearities and coupling of Einstein's equations make a similar analysis quite difficult. Nevertheless, as we will see later in section 5.1, the equations are customarily recast in a form somewhat closely related to equation (29) and it is important to keep this theorem in mind. The use of dissipative inner boundary conditions has not yet been generally pursued; however, I am aware of a few systematic efforts in this direction reporting considerable improvements [117–119]. The advantages gained from the use of dissipation both in the absence and presence of boundaries indicates that implementations can benefit considerably from its use.

As mentioned, FDA have been the preferred choice in numerical relativity, their ease of use; transparent interpretation of its strategy and power certainly make them very attractive.

This is illustrated by their use in all areas of numerical relativity; i.e. initial data problem, evolution and 'physics' extraction. There are a few criticisms which have led people to other choices.

- Appropriateness of its use on arbitrary variables: basically, when using Taylor expansions up to order n, one *exactly* accommodates for polynomials up to the nth order. However, this might not be the ideal 'basis' to express certain functions at particular places. For instance $1/x$ near $x = 0$ is not conveniently represented by polynomials (of positive integer). A solution to this problem is to re-express variables so that they are better represented by polynomials; thus if a given function F is expected to behave like $1/x$, re-expressing the equations in terms of a variable $\tilde{F} = xF$ improves the obtained results. This technique has been used in a limited number of cases [47,54,83,96] yielding excellent results. However, this approach requires some 'prior' knowledge of the field dependence.
- Awkward use at non-regular boundaries: as discussed, the variables are represented by their values at grid points; when dealing with irregular boundaries where values and derivatives might be required, an often complicated set of interpolations must be carried out. This introduces high-frequency modes which bring about all sort of nightmares. Dissipation of these modes could take care of this problem but requires carefully designed algorithms. As the grid is refined, this problem might become less severe. Refining a grid (i.e. adding more points to it) increases the computational cost considerably; however, the use of *adaptive mesh refinement* can help to alleviate this problem by refining the grid locally only where needed (for more on this technique see section 4.3).

Certainly, these criticisms can be addressed but, undeniably, some situations might be better handled by other methods. For instance, expansion in terms of spherical harmonics of a regular enough variable, say the electromagnetic potential of the localized distribution of charges, might yield an accurate and inexpensive representation nicely adapted to a particular problem. In cases like this, the use of appropriately chosen basis functions is of great help. There are several approaches based on this idea being used in numerical relativity [120] and next I briefly review some of them.

4.2. Beyond FDA

4.2.1. Finite elements. The use of finite elements (FE) in numerical relativity has so far been restricted to the solution of the initial-value problem of the '3 + 1'. Here, the flexibility of this approximation to conform to non-regular boundaries is a valuable asset. Namely, the 'discretized' version of the hypersurface constitutes a 'mesh' of, usually, triangles which are not required to be regular. Consequently, hypersurfaces with 'holes' are conveniently covered (which is often more difficult with FDA). Additionally, if steep gradients are expected, smaller sized triangles can be used to accurately represent them. These particularly nice features come at a price, as the solution is obtained through a global minimization of the 'residual'. Roughly, the solution S of the equation $L(S) = 0$ is approximated by

$$\hat{S}(\vec{x}) = \sum_{l}^{N} a_i \phi_s(\vec{x}); \tag{32}$$

where a_i are unknown coefficients and $\phi_i(\vec{x})$ are known basis functions (which are continuously differentiable and integrable functions). The numerical implementation will not, in general, exactly satisfy the original equation but $\hat{L}(\hat{S}) = \hat{R}$ (with $\hat{L}$ the discretized version of L and $\hat{R}$ the residual). By minimizing $\hat{R}$ over the *whole* computational domain an algebraic system for $\{a_i\}$ is obtained. This method has a 'global' flavour nicely suited to the treatment of elliptic

equations. Its flexibility to treat irregular boundaries has been implemented to solve the initial-value problem of Einstein's equations in [121] where multigrid techniques have been used to diminish in part the high computational cost.

4.2.2. Spectral methods. Other interesting options are the spectral and pseudo-spectral methods [122, 123]. Not only have they been used for the initial data problem [124–128], but they are also being employed for the actual evolution part [24, 83, 129]. These methods have the capability of addressing non-trivial boundaries without the overhead required for a minimization procedure (although the goal is to minimize the residual error, as in finite-element methods, this is done only at particular *collocation* points conveniently distributed over the computational domain). In this method, the solution is expanded in terms of a set of basis functions (usually trigonometric functions or Chebyshev polynomials). In spectral methods, the PDE system is Fourier transformed to obtain a simpler one in the frequency space whose solution is then transformed back to produce that of the original system. Depending on the type of PDE under study, this transformation might not yield a simpler system in the frequency space. For these cases, pseudo-spectral methods were introduced. Loosely speaking, in these methods only part of the system is treated in the frequency space, while the other part is solved in the coordinate domain (for instance time derivatives are done in the regular space while spatial ones are considered in the frequency space). The Fourier transformation is in practice carried out in an efficient way through the use of fast Fourier transformations. For problems *with smooth solutions* these methods converge *exponentially* as the number of basis functions is increased. This improved convergence rate comes at a higher computational cost, which is nevertheless justified. Two problems are often cited as the main ones. First, in evolutionary problems, the CFL condition [130] (which requires the numerical domain of dependence to contain the analytical one) scales as N^{-2} (while in general FDA scales as N^{-1}) which can render the application too costly (note, however, that for smooth functions small values of N are usually enough). The second problem relates to the way the collocation points are chosen which requires the computational domain be sufficiently simple. This is a problem when dealing with a spacetime containing irregular boundaries such as those containing more than one black hole. It has been suggested that the use of several overlapping regions (known as domain decomposition) can overcome this problem [125, 129]; and the solutions on each patch would serve as boundary conditions for the other patches. The scheme would involve an iterative procedure which would, hopefully, converge. This suggestion is justified by the fact that this strategy indeed works for the Laplace equation [127, 131]. Considerable progress has been obtained with Einstein's equations and the results obtained are so far very good [24, 128].

4.2.3. Regge calculus. In the 1960s Regge introduced a way of approaching general relativity which by its discrete nature appeared tailored for numerical relativity. Rooted in the ADM formalism, it replaces the dynamical field variables by finite distances by using the following approach. A lattice is introduced and the main variables correspond to the length of (short) geodesic segments defining the legs of the lattice. To date its application has been rather limited; I am aware of its applications to model the Kasner T^3 cosmology and Schwarzschild spacetime [132, 133]. A project to investigate this approach in more general scenarios is underway [134]. Initial data corresponding to gravitational waves on Minkowski and Schwarzschild backgrounds and head-on binary black holes (Misner data) have been obtained tailored for a code implementing Regge calculus. We should soon hear reports on the feasibility of this approach to study generic settings.

4.3. Simulation costs and how to improve the picture: AMR, multigrid, parallelism

Let us estimate the computational cost CC to carry out a 3D simulation, say for instance we want to model a black hole system. To fix our ideas let us assume we will employ FDA and the ADM formulation on a uniform grid with N_p grid points in each direction. The number of operations needed to 'advance' a single time step will be given by $N_p^3 \times$ number of floating point operations per point (CC_1). A back of the envelope estimate for the operations is: number of variables $\times$ number of operations per variable $\times$ number of 'updates' per time step (e.g. if we are using predictor–corrector-type algorithms, this last item would at least be 2–3).

NU $\equiv$ number of 'updates': 3.

NO $\equiv$ number of operations: the Ricci tensor appears on the right-hand side of the equation and its evaluation requires ≈ 2000 floating point operations.

NV $\equiv$ number of variables: 12 (from $\{g, K\}$) + 4 (lapse and shift) + 1 (marking variable to keep track of where the holes are at each step)) (these have to be multiplied by 2 to keep the 'old' and 'new' values). Hence we have of the order of ≈ 30 variables. Thus

$$CC_1 \approx 2 \times 10^5 \frac{NO}{2000} \frac{NV}{30} \frac{NU}{3}. \tag{33}$$

Now, suppose the typical size of the source we wish to include in our simulation is M. We must be capable of placing the outer boundary in the wave zone, which would require our computational domain be at least $[-20M, 20M]$. The resolution to (barely) resolve the system will be $\Delta x = M/4$. Hence $N_p \approx 160$. In order to resolve the first quasinormal modes of the produced radiation, we would like the total simulation length be $\geqslant 100M$. Since, stability requirements would imply (assuming a fully explicit FDA approximation) $\Delta t \approx \Delta x/4$ the total number of time steps required is at least $N_T = 10N_p$. Therefore, the total computational cost would be $CC = 10CC_1N_p^4$.

$$CC \approx 2 \times 10^{14} \frac{NO}{2000} \frac{NV}{30} \frac{NU}{3} \left(\frac{N_p}{160}\right)^4. \tag{34}$$

The most powerful publicly available chips nowadays have peak performance of 10^9 floating point operations per second (1 Gflop/s). Therefore, our full 3D simulation would take 10^5 s $\approx$ 30 h. Memorywise, every real number is at least represented by $R_p = 8$ bytes. Since one usually introduces temporary variables to aid in the calculation, in practice, the total number of variables from the previous estimate at least doubles, so, the memory requirements (MR) would be

$$MR \approx 2 \times 10^9 \left(\frac{N_p}{160}\right)^4 \frac{NV}{30} \frac{R_p}{8}. \tag{35}$$

These numbers are not too bad, but are to be considered as an 'idealized lower bound' since we have considered the minimal required configuration in the vacuum case (for spacetimes containing fluids, Δx is usually required to be much smaller or the dynamics of the fluid will not be represented accurately). Additionally, many simulations will be needed for a reliable configuration space survey and the total computational time invested will increase considerably. Moreover, if we wanted to perform the same simulations with a better resolution, things rapidly increase. For instance, improving our resolution by a factor of 2 would increase the CC by a factor of 16 and MR by 8 (i.e. now we would have to wait 20 days for the results and need eight times more memory). The computational cost of symmetric hyperbolic formulations would be of about the same order (more expensive though), but that for the characteristic simulation would be much less (in this case, arrays need only 2D storage and the right-hand side require about ≈ 200 evaluations).

As we have seen, the computational cost to go beyond the 'bare necessities' of a simulation in 3D rapidly increases. However, there are computational techniques that allow finer resolved simulations be achieved without paying such a high price. Next I will mention a few of these.

Adaptive mesh refinement

When modelling systems, such as gravitational collapse, black hole/neutron star spacetimes, singularity structure, etc, the strength and variability of the field variables are expected to be significant only in a 'small' region. Achieving an accurate model capable of capturing the essential features of the dynamics might require keeping the local truncation error below some threshold. In practical terms, this often requires much more information from the variables in these 'small' regions. Clearly, one can adjust the overall resolution by satisfying the strongest requirement and therefore enough information will be available for all regions. This straightforward approach is evidently sound; however, it might entail wasting computational resources in regions where not much is 'going on'. A more desirable strategy would be to choose a non-uniform grid or definition of collocation points adapted to those regions that need to be resolved better. Here we again face the problem that in general we might not know this *a priori*! One could, in principle, proceed with a coarse grid first, and from the obtained solution deduce properties that a subsequent finer one should have. This strategy has the weakness that the 'coarse' solution might be too crude to produce a good enough solution from which to infer how to proceed. If this is indeed the case, one could discard the 'coarse' simulation and start all over with a finer one.

A more direct approach, and one that in principle should work directly (i.e. without trial and error) is to 'adaptively' increase or decrease the information needed locally by monitoring the solution 'on the fly'. In computational relativity, this approach has so far only been used in simulations using FDA and is known as *adaptive mesh refinement*. This method adds more points to the grid according to some user-defined threshold on the local truncation error. The use of adaptive mesh refinement in 3D numerical relativity is making its first steps [135–138], but its benefits have been dramatically confirmed by the investigations of Choptuik in 1D [62]. Choptuik employed a technique introduced by Berger and Oliger [139] to write a fully adaptive code to solve the Einstein–Klein–Gordon system in spherical symmetry. This allowed him to achieve very high accuracy with relatively low computational cost, and more importantly, to discover critical phenomena in GR. Today, computational speed and memory resources are readily available for very fine 1D simulations without the use of AMR. However, in 3D where one barely has enough resources to achieve crude simulations, the use of AMR would open the door to better resolved simulations, and perhaps, many of the nightmares faced by numerical relativity in 3D would disappear (or be negligible for the desired simulation length). Efforts to implement AMR are today, and will be for several years to come, central.

Multigrid techniques

When solving elliptic problems through standard relaxation schemes, it is often the case that the low-frequency modes of the solution (picturing the solution in Fourier modes) are accurately obtained with relatively little computational effort while the higher modes require substantially much more and are responsible for most of the computational cost. To alleviate this problem, multigrid techniques [140] are introduced. The basic idea of a multigrid is to eliminate the high-frequency components of the error quickly on a fine grid. These modes can be easily isolated by transferring to a coarser grid and comparing the solutions. This strategy is carried out through successive coarsening of grids and the results are transferred back to the fine grid. The use of multigrid techniques has in the past been restricted to the initial-value problem [48,49,121,141]

and to solve the maximal slicing condition in unconstrained implementations [135]; but are now also being employed on partially constrained evolutions in an axisymmetric code [118].

Parallelism

Einstein's equations are ideal candidates for constructing parallel implementations which take advantage of supercomputers. The hyperbolic character of the equations translate into the fact that to update the value of a field at a given point, only a small amount of information from the previous slice is needed. Hence, the computational domain can be subdivided into smaller ones. Different processors/machines solve the equations in these smaller cells and the solution is obtained at a later time after properly communicating data among cells. This strategy would imply that the elapsed time of a simulation T on a single processor could in principle be shortened to T/n (if n is the total number of processors used and neglecting the overhead from the communications). In practice this is not exactly the case but instead $T/(\alpha n)$ (with $\alpha < 1$). Typical implementations give $\alpha \in [0.7, 1)$, which, although not 'perfect' still implies that the more processors used, the sooner the results will be obtained. Equally important is that the total memory available is now $M_T = nM_1$. Hence not only can we obtain our solution sooner but we have much more memory at our disposal to treat larger/more refined problems.

As a last point, I would like to mention that until the very recent past, only very expensive supercomputers provided researchers with enough computational power to achieve large simulations. Unfortunately, these supercomputers were not available to all researchers. Their high cost and laws prohibiting the importation of such machines to many countries prevented many from having access to powerful enough computers. Fortunately, the picture is changing by the possibility of clustering many relatively low-cost machines (such as PCs) in what has been called 'Beowulf supercomputers'. These machines will enable numerical relativists around the world to carry out their research more effectively which will certainly have a positive impact on the field.

4.3.1. Expediting the computational science aspect. A particular aspect when exploiting the available computational power is the design of efficient codes. Writing codes is very time consuming. The resulting product should not only minimize the amount of computation and memory employed but also pay close attention to the way memory is being used (efficient memory usage can speed up the performance considerably); input and output is performed and the way data is to be stored. Taking care of these issues often exceeds the capability or the available time of numerical relativists who need to spend time concentrating on getting the physics correctly. It would be ideal if computer scientists could take care of the code efficiency. Of course, having direct computer science assistance is unlikely to be the case; but fortunately, something is indeed being done in this direction. There exists software designed to expedite writing efficient codes. Namely, these software are capable of managing the memory usage, input/output, parallelization issues, data storage and helping in the implementation of AMR. Among these (freely available) software products are RNPL [142, 143]; PARAMESH [144]; PETSc [145]; KELP [146] and the CACTUS Toolkit [147].

RNPL lets the user simply specify the equations to be solved and how boundary conditions are to be treated and the compiler produces the code. Remarkably, with little effort from the user, a code can be obtained.

PARAMESH is a package of Fortran 90 subroutines designed to provide a relatively easy route to extend an existing serial code (which uses a logically Cartesian structured mesh) into a parallel code with adaptive mesh refinement (AMR).

PETSc provides a suite of data structures and routines to write a parallel implementation of a system governed by partial differential equations.

KELP is a framework to implement parallel applications providing run time support for blocked data decompositions. These block need not be uniform in size and AMR can be easily achieved by appropriately chosen block sizes.

The *CACTUS computational toolkit* was designed as a collaborative tool where users can adopt modules written by others for specific purposes. In its bare bones, the users can choose to have the software handle the parallelization, memory management and input/output and just concentrate on the physics *per se*.

As opposed to RNPL, all other mentioned packages will not write the code but provide an infrastructure which expedites the parallelization of the code, incorporation of AMR and appropriate I/O and memory management.

Although these tools are not ideally suited for all problems; they can certainly help researchers concentrate on the physical implementation without the need to spending too much time on the computer science aspects in a considerable number of situations.

4.4. Analytical properties and numerical implications

The rich theory of PDEs [148, 149] tells us a great deal about generic properties of the expected solution. The distinction of hyperbolic, elliptic and parabolic teach us how the system governs the way signals 'propagate'; which data are needed to obtain a solution, whether this solution exists and is unique, etc. Here I will comment on two particularly interesting issues regarding the interface between PDE theory and numerical implementations.

4.4.1. Well posedness. Of particular importance is the concept of well posedness [150]. A well posed system is such that the solution S (at time t) corresponding to the initial data u (at time $t = 0$) can be bound by

$$\|S\| \leqslant K \mathrm{e}^{at} \|u\|, \tag{36}$$

with $\{a, K\}$ constants independent of the initial data. (Note that this does not rule exponentially growing solutions.) Two points can be cited as the main conclusions to be drawn from this property.

- The growth of the solution is bounded. Although exponentially growing solutions are admitted, there is an 'upper' limit to their growth rate.
- The solution depends continuously on the initial data.

In numerical implementations, clearly, the specified initial data in general will only be an approximation to the desired initial data (since at best it can only be defined up to round-off errors); well posedness guarantees (at the analytical level) that the obtained solution will nevertheless be in the neighbourhood of the solution we seek. Most systems being used in 3D numerical relativity are not known to be well posed (the exceptions being [20, 22, 23] in the 3 + 1 approach, the conformal Einstein equations approach [102, 108] and the double null approach [82, 83]). The 'danger' with systems that are not well posed is that a in equation (36) might depend on the initial data and therefore, the solution might have varying exponential growth rates. In particular, it is often the case that if the initial data are 'pictured' in terms of Fourier modes, different frequencies ω have different values of a and furthermore

$$\lim_{\omega \to \infty} a \to \infty. \tag{37}$$

Note that an unstable numerical implementation exhibits this behaviour even if the system is well posed. Of course, in practice ω does not attain infinity but, as the grid is refined, larger frequencies are allowed and the solution *grows with the number of time steps*! A behaviour of this sort has been investigated in the ADM system [151, 152] for particular gauge choices. The growth of a with respect to ω is not a 'violent' one and, in principle could be controlled with the introduction of dissipation which would keep the high frequencies in check. Further investigations will show if this is indeed the case. I would expect that the discretization of a well posed system *should* simplify the attainment of a stable numerical implementation, even though to date it has not yet clearly shown its advantages in this sense. As we learn more on how to exploit this feature, its role in the simulations will become increasingly useful.

A particular example from which conjectures can be drawn is the wave equation written in well posed form and not. Consider the following two systems obtained from $F_{,tt} = F_{,xx}$.
System (A)

$$F_{,t} = \Phi, \tag{38}$$

$$\Phi_{,t} = G_{,r}, \tag{39}$$

$$G_{,t} = \Phi_{,r}, \tag{40}$$

(where the intermediate variables $\Phi = F_{,t}, G = F_{,r}$ have been introduced to reduce the original system to first order).
System (B)

$$F_{,t} = \Phi, \tag{41}$$

$$\Phi_{,t} = F_{,rr}. \tag{42}$$

System (A) can be easily shown to be well posed while system (B) is not well posed in the usual sense. *Can we at least say something about the expected behaviour of the solutions of system (B), $S(B)$, given that we know how system (A) behaves?* Note that well posedness of (A) means that its solution $S(A)$

$$\|S(A)\| = \|F(t)\| + \|G(t)\| + \|\Phi(t)\| \leqslant \alpha e^{Kt}\big(\|F(0)\| + \|G(0)\| + \|\Phi(0)\|\big); \tag{43}$$

since (at the analytical level) $\|F(t)\| + \|\Phi(t)\| \leqslant \|F(t)\| + \|G(t)\| + \|\Phi(t)\|$ we can infer

$$\|S(B)\| = \|F(t)\| + \|\Phi(t)\| \leqslant \alpha e^{Kt}\big(\|F(0)\| + \|G(0)\| + \|\Phi(0)\|\big). \tag{44}$$

Although these results do not imply well posedness (as the solution of system (B) is not bounded by its initial data), it at least tell us that there is indeed an upper bound for the growth of the solutions. This property could in principle address one of the criticisms of symmetric hyperbolic formulations of Einstein's equations—the large number of variables involved. One could start by considering one of these hyperbolic formulations and then, replace the variables introduced to reduce the system to first order by the original higher-order derivatives. (Note that this 'backtracking' can only be done if constraints were not added to the 'evolution' equations of the intermediate variables to achieve well posedness.) The obtained system would have considerably fewer variables and its solutions should still be bounded. This approach has only recently received attention and it does appear to provide better behaved evolutions [119, 153]. These preliminary investigations have been restricted to 1D, and further studies must be carried out before firmer conclusions can be drawn. At present, a clear advantage exploited from hyperbolic systems is the distinction of incoming variables at a boundary (which are the only ones one is allowed to specify).

4.4.2. Well posedness... is not enough! As mentioned previously, the difficulties observed in the numerical implementations of the ADM equations lead to the formulation of a number of symmetric hyperbolic systems. However, implementations of these systems did not show a significant improvement in the obtained simulations. This is certainly not a surprise as well posedness *does not* rule out the presence of exponentially growing modes. Moreover, in analysing whether a system is symmetric/strongly hyperbolic one concentrates only on the principal part. However, the non-principal part of the system can play a crucial role in the stability of a numerical scheme. As an illustration, consider the following equation:

$$f_{,t} = f_{,r} + f^2, \tag{45}$$

which is strictly hyperbolic and its principal part is just the 1D wave equation. There exists an extensive set of algorithms capable of accurately treating the wave equation, however, the addition of the f^2 term makes implementing equation (45) delicate. In particular, suppose one were to provide as initial data $f(t = 0, r) = r^{-1}$ and the boundary condition $f(t, r = R) = R^{-1}$. The unique solution of such a problem is $f(t, r) = r^{-1}$. Let us consider the linear perturbation of (45) in the neighbourhood of this static solution.

$$\delta f_{,t} = \delta f_{,r} + (2/r)\,\delta f. \tag{46}$$

What kind of solutions are allowed for such an equation? Introducing the Fourier modes $\delta f = \mathrm{e}^{su+\mathrm{i}kr}$, and replacing in (46) to solve for s, one obtains,

$$s = \mathrm{i}k + (2/r). \tag{47}$$

Thus, although the wave equation admits only purely imaginary values of $s = \mathrm{i}k$, our toy model, whose principal part is the wave equation does admit exponential modes. (Note that if we had obtained a negative sign in front of $(2/r)$, we would have exponentially decaying modes and, at least at the linearized level, the system would naturally drive towards the static solution.) In the numerical realm, one can readily see via the usual Von Neuman analysis [130] that a straightforward extension of stable schemes for the wave equation, leads to unstable implementations of equation (45).

The reader at this point might wonder why such a particular example was chosen; after all, one could always perversely modify an equation to display an exponential behaviour. However, it turns out that this simple example has a strong relationship with Einstein's equations expressed in the 3 + 1 approach. Recall equation (7) for the evolution of the extrinsic curvature,

$$d_t K_{ij} = \alpha \left[R_{ij} - 2K_{i\ell}K^{\ell}_{j} + K K_{ij} \right] - D_i D_j \alpha. \tag{48}$$

It precisely has the form

$$\partial_t K_{ij} = \beta^l \partial_l K_{ij} + f_1 (K_{ij})^2 + \text{extra terms}, \tag{49}$$

where i, j are fixed and f_1 is a function of the variables *not including* K_{ij}. If $f_1 > 0$ then an analogous local mode analysis indicates the presence of exponentially growing modes. *Is there anything one can do in this situation to 'change the sign' of* f_1*?* Note that we have at hand the constraints which can be arbitrarily added to the equations. In particular, the Hamiltonian constraint has combinations of undifferentiated extrinsic curvature components and, in principle, by adding it with appropriate factors one can 'effectively' achieve the desired sign change or, the magnitude of f_1 be made much smaller. An illustration of such a procedure has been studied in the 1D case for the simulation of Schwarzschild spacetime [119, 154]. A remarkable improvement is obtained; without the addition of the Hamiltonian constraint to the evolution of the extrinsic curvature, simulations past $500M$ could not be achieved for

all possible evolutions. With the modification of the equations, stable configurations were obtained for all configurations. Note that although the example presented here applies to the ADM formulation; all other 3 + 1 formulations have (at least some) equations containing wave operators in the principal part and nonlinear terms in the non-principal part where a similar structure can be identified.

A related work has been presented in the 3D case with an implementation of a hyperbolic system obtained by modifying the Einstein–Christoffel system [155] by adding the constraints with free parameters [24]. By simply varying the value of these parameters full 3D evolutions of single non-spinning black holes are achieved with evolution times ranging from a few M to $1200M$. These results highlight the need for a deeper understanding on the influence of the non-principal part of the system. Clearly, numerical implementations can benefit considerably from adding the constraints in an appropriate way. Perhaps the simplest and quite general way of choosing 'ideal parameters' would be to do so by monitoring the evolution of the variables in a similar way as artificial viscosity is often added in the numerical treatment of the hydrodynamic equations (see section 6.2.1).

4.4.3. Elliptic equations and black holes. A recurring issue in numerical relativity is the role that constraints play in the evolution of the equations. Analytically, they should be propagated by the evolution equations [45, 156]; numerically, as shown by Choptuik [157] if the equations have been consistently implemented, the constraints should be satisfied to the level of the implementation. These results justify the construction of *free evolution* codes (i.e. not dynamically enforcing the constraints as part of the evolution) and, in practice, the constraints are monitored to show the quality of the obtained solution. The use of free evolutions in black hole spacetimes (where singularity excision is to be used) has also been preferred as it is not clear which boundary conditions are to be specified at the inner boundaries (i.e. those surrounding the excised singularities). Since the constraints are elliptic, the theory of PDE tells us that the choice of boundary condition determines the solution globally (i.e. there is an 'infinite propagation speed of signals'). This being the case the worry is that unless the correct data are known at the inner boundary spurious solutions will result from a *constrained evolution*. In fully or partially constrained systems [60, 158], inner boundary conditions are obtained by employing the evolution equations to define values at the inner points for all variables.

5. Particulars of numerical implementations of Einstein's equations

In this section, I will very briefly review some aspects of the numerical implementation of the formalisms described above.

5.1. 3 + 1 approach

Evolution equations

The evolution equations are implemented through, basically, the following structure:

$$(\partial_t - \mathcal{L}_\beta)F = \mathrm{Rhs}(F), \tag{50}$$

where F denotes the evolution variables and $\mathrm{Rhs}(F)$ collects all extra terms. In order to treat this equation, the terms provided by the Lie derivatives that include derivatives of β are customarily moved to the right-hand side:

$$(\partial_t - \beta^i \partial_i)F = \mathrm{Rhs}(F). \tag{51}$$

This splitting is carried out so that 'standard' techniques developed for the *advection* equation can be used to discretize this equation. The approaches most commonly used can be divided into roughly two main groups: (i) *operator splitting* and (ii) *straight discretization of the right-hand side*. In the operator splitting strategy, the integration is divided into steps involving parts of the original equation. One step integrates the homogeneous equation $(\partial_t - \beta^i \partial_i) F = 0$ while the other the 'source' part $\partial_t F = \text{Rhs}$. Both steps can be intercalated, in different ways to produce an approximation for F to a desired order. For instance,

$$F^* = F^n + \mathrm{d}t\ \beta^i \partial_i F, \tag{52}$$

$$F^{n+1} = F^* + \mathrm{d}t\ \text{Rhs}(F^*). \tag{53}$$

This choice is by no means absolute, other options involve: integrating the source equation first and then the homogeneous one and even proceeding in half steps [159]; treating the transport part via interpolations at the nth or $(n+1)$th level (examples of the algorithms used are the cubic-interpolated pseudoparticle [42], causal-differencing [160–162]; causal-reconnection [163], etc).

The second group involves a straightforward discretization of the right-hand side. The most promising approaches within FDA though, do make a difference in the way the $\beta^i \partial_i F$ term is treated (see, for example, [108, 117, 158, 164]). These terms are discretized using 'up/down wind'-type schemes where the sign of β^i determines whether points to the right or left of that under consideration are used. When using pseudo-spectral methods, the right-hand sides are evaluated straightforwardly and the method of lines is used to advance the solution to the next step [20].

At present '3 + 1' unconstrained simulations are mainly based on a handful of formulations: the ADM [16]; the BSSN (or 'conformal ADM') [25,165], the 'extended Einstein–Christoffel' formulation [24] and the Bona–Masso formulation [21][11]. The last two are symmetric hyperbolic systems while the first two are not. The BSSN system is obtained from the ADM with the addition of extra variables such as the determinant of γ_{ij}; the trace of K_{ij} and Γ^k_{ij}, coupled with a conformal decomposition of the metric and extrinsic curvature and the use of the momentum constraint to replace some terms in the resulting equations. The obtained system resembles the ADM one, but manages to (approximately) separate gauge-dependent variables. When studying linearizations over flat space, the system does indeed show appealing properties [27, 152, 166]. Recently, several works have shown that the BSSN system provides longer evolutions than the ADM one. A peculiarity of the results displayed by simulations obtained with this system is that the errors in the constraints are larger than those obtained with the ADM one; nevertheless, as the evolutions proceed the ADM evolutions crashed earlier than those with the BSSN system [27,152,165]. The fact that the errors are larger could be explained by further discretization errors introduced in the BSSN because of the extra variables evolved. These comparative studies evolved both formulations with the *same* algorithms; however, there is no reason for the same 'numerical recipe' to be a good choice for both. Application of singularity excision in the BSSN system has started recently, in 1D [167] it has shown similar results to those obtained with the ADM one (for a specific way of handling the excision); recent 3D implementations show encouraging results [43].

The Einstein–Christoffel system implementation is presently being pursued using pseudo-spectral methods. Its hyperbolic character has been exploited to simplify the treatment of both the inner and outer boundaries. Kidder *et al* [20] report successful simulations of a single black hole in 1D (which is also 'perturbed' via a Klein–Gordon field). The extension to 3D has been carried over with a related system (the extended Einstein–Christoffel

[11] Preliminary implementations of the Ashtekar formulation [22] have also been presented.

system) achieving evolutions of $1200M$ [24] when constraint-violating instabilities render the simulations inaccurate.

Inner boundary

As mentioned, when singularity excision techniques are used, an inner boundary appears in the computational domain. This boundary is usually defined by finding the apparent horizon [168]. In practice, to allow for displacements of the singularity a 'buffer zone' is employed; i.e. if the apparent horizon is located at $R = R(x^i)$, the inner boundary is placed at $R - \delta$ (with $\delta = n\Delta x, n \in [2, 6]$). This buffer zone also allows the simulation to proceed without needing to 'locate' the apparent horizon at every time step. Finding apparent horizons is an 'expensive' computational task. It involves solving an elliptic equation in 3D which defines a surface whose outgoing null normals neither diverge nor converge (i.e. it is marginally trapped [168]). As usual with elliptic equations, if a 'good guess' is known, the task of solving it might not be so severe. When a single apparent horizon is expected, a rough estimate of the mass of the hole coupled with some notion of where the centre of the horizon might be is exploited to yield fast apparent horizon finders [64, 169–171]. In the generic case, finding the apparent horizon can be a considerably expensive task, not only must the finder be capable of starting with an arbitrary surface (usually chosen close to the boundaries of the computational domain) and flow towards the location of the horizon, but also be capable of handling several distinct apparent horizons. I am aware of only two of such finders [172, 173] which are based in the *flow method approach* outlined in [174]. To reiterate, although finding apparent horizons on a given surface is an expensive computational task, it need not be found at every single time step.

What is done at the inner boundary points? As mentioned, the strategy is to use the evolution equations to update these points. Both strategies employed at the 'bulk' (which we mentioned in the previous point) are suited to implementing this idea. An important requirement is that the shift is conveniently chosen in the neighbourhood of the excised region. Namely, β^i has such that $(\partial_t - \beta^i \partial_i) F = 0$ describes signals propagating *towards* the excision boundary and not *from* it. If this were not the case, then, it will be difficult to prevent signals propagating from regions inside the event horizon to the outside. Although these methods appear to work reasonably well in lower dimensions, their 3D implementations are not yet robust enough (but considerable progress has been achieved over the past year with single black hole evolutions being carried out for times beyond $500M$ [24, 43]).

The goal pursued by all methods is to have an accurate and stable implementation of the equations at the inner boundary (often called the 'excision boundary'). Note that when using finite-difference techniques the right-hand side of the equations cannot be evaluated in a centred way (as there are 'no points' available at the interior of the excision boundary). In practice, interpolation or extrapolation is used; this process must be handled with care as it not only introduces 'high-frequency' features in the solution but it can also render the evolution unstable [167]. There are a number of methods under use, differing in the way the interpolation is carried out and which of the previously mentioned groups (operator splitting or straightforward discretization of the right-hand side) is adopted. The techniques presently used are: causal-differencing [160–162] and more simple-minded excision techniques with up-/down-wind algorithms [117, 164]. With spectral methods, on the other hand, as one counts with a continuous representation, the evaluation of the desired variable and its derivatives can be made at any point without needing to interpolate. Hence, the right-hand sides of the equations are straightforwardly evaluated and the method of lines is used to advance the solution to the next hypersurface [20, 24]. It is important to point out that handling a moving singularity is a crucial test for a robust treatment of the inner boundary (as points will

'pop out' from the excision region and the evaluation of the equations will shift location at different hypersurfaces). Only causal differencing has been shown to be partially successful in this problem. One might argue that with appropriate coordinate conditions, one can 'fix' the singularity in the grid and therefore need not pass such a test. However, it is difficult to imagine that such coordinate conditions will be available for all problems and even if this is the case, treating a moving singularity will probably encounter the limitations of the implementation.

A possible way to 'aid' the numerical implementation is to 'modify' the equations near the excision region. Since, in principle, nothing can escape from the event horizon, one could use this fact to simplify the implementation of the evolution equations; for instance, consider the following variation of equation (51):

$$\partial_t F - (W\beta^i + (1 - W)V^i)\partial_i F = W\,\mathrm{Rhs}(F); \tag{54}$$

where $W = 1$ outside the apparent horizons and smoothly going to zero at the excision boundary. The vector V^i could be chosen appropriately so that signals propagate normal to the excision boundary, be zero so that the values of the variables are frozen, etc. I am aware of the use of an analogous strategy only in the implementations of the conformal Einstein equations [108], except that in this case it was used to control signals from propagating into the physical spacetime crossing $\mathcal{I}^+$.

Initial data

As mentioned, initial data must satisfy four constraint equations. For spacetimes free of singularities, these initial data together with appropriate outer boundary conditions determine a unique solution [17].

When singularities are present, either inner boundary conditions are prescribed or, if possible, the singular behaviour removed from the field variables. In the past, most efforts towards obtaining valid initial data were carried out under certain assumptions which, although restrictive, considerably simplified the treatment and allowed one to gain valuable experience in treating this problem (see, for instance, [47,48]). For instance, the families of Brill–Lindquist [175] and Misner [176] data provide multi-black hole solutions under the assumptions of conformal flatness and time symmetry. Relaxing the time-symmetric assumption, but still keeping conformal flatness, provides more generic multi-black hole solutions referred to as 'Bowen–York' [177] data and 'puncture' data [47].

These data sets have several drawbacks for astrophysically relevant applications. One is the assumption of conformal flatness, as has recently been shown by Garat and Price [178], there exists no spatial conformally flat slicings for the Kerr spacetime. Therefore, even in a spacetime containing a single spinning black hole, the assumption of conformal flatness introduces unphysical radiation. Further questions on the suitability of the Bowen–York solutions for astrophysically relevant simulations have been raised in [179]. By considering the 'particle limit' of these data sets, the authors find that even in the case of a single non-spinning black hole spurious radiation is present. Additionally, these solutions are all obtained on a maximal slice (in the case $\gamma^{ij}K_{ij} = 0$) which allows for the constraint equations to decouple but considerably restricts the available freedom.

The aforementioned initial data sets have proved quite valuable in investigating different aspects of the theory and numerical implementations of black hole spacetimes. As the focus turns to producing astrophysically useful information, a revision of the initial data specification is required. Recently, a number of proposals have been introduced where conformal flatness has been dropped [49, 180–182]. Here, the Lichnerowicz–York approach is still used, the difference lies in the non-flat 'seed' metric $\hat{\gamma}_{ij}$ provided. As a result, the constraint equations

are coupled and must be solved simultaneously. The approach introduced in [181, 183], has recently been fully implemented in 3D where $\tilde{\gamma}_{ij}$ has been chosen to be the superposition of boosted Kerr black holes [183]. By conveniently 'weighting' this superposition, reasonable inner boundary data around each (excised) singularity can be induced from the analytically known single black hole solution.

5.1.1. Examples of implementations

1D

Spherically symmetric spacetimes still offer a rich arena to study strong gravity effects. Applications in critical phenomena, collapse simulations, singularity structure studies, etc are within reach of reliable simulations. Additionally, 1D simulations are useful first steps to test algorithms for more generic spacetimes.

2D

Simulations assuming axisymmetric spacetimes are being carried out to investigate critical phenomena [54, 158], black hole collapse situations, rapidly rotating neutron stars [184], black hole accretion physics, etc. Here, the problem of the coordinate singularity at the symmetry axis must be addressed. This is done by enforcing regularity conditions at the axis [44] or by 'thickening' the direction along the spacelike Killing vector so that enough points are available to take derivatives as if it were a 3D spacetime (and then interpolate the results back to define their values at the axis) [185]. Preliminary investigations of gravitational wave collapse scenarios [54] display critical behaviour of the solution; these simulations are still rather coarse and more definitive results will be obtained with the use of AMR.

3D

3D simulations are mainly targeting black hole/neutron star systems. Studies of collapse of compact objects or collapse of waves onto black hole are being pursued. Considerable progress has been obtained as the first series of simulations are being reported [41–43, 186–188]. As discussed, 3D numerical relativity is very challenging already from the computational-resources point of view; this has restricted the resolution used in all these works. All of the obtained models have been able to simulate the systems under study for moderate amounts of times, enabling preliminary conclusions to be drawn from them. The focus is now to address the observed stability problems and improve the resolutions. Perhaps many of the stability problems faced so far might disappear, or become negligible for the targeted simulation length, when fine enough resolutions can be achieved.

5.2. Characteristic

Evolution equations

The evolution equations in this formulation are implemented by observing that the left-hand side of the equations correspond, roughly, to wave equations in (u, r) coordinates, i.e.

$$2(rh_{AB})_{,ur} - ((V/r)(rh_{AB})_{,r})_{,r} = \text{RHS}. \tag{55}$$

A crucial ingredient is the way tensor fields (and derivatives) appearing on the right-hand side (of the evolution and hypersurface equations) are handled on the spheres $r =$ constant, $u =$ constant and that a single patch cannot be used to cover these sphere. Efficient implementations

have been obtained with the use of *eth*-operators [189], which have been implemented via second-order FDA [95] or through the use of fast Fourier transformations [83]. Recall that inner boundary conditions are required; once these have been specified, integration of the hypersurface equations is carried out by explicit second-order FDA [79, 96], or by an eighth-order Runge–Kutta integration [83] marching radially outwards. Finally, the evolution equations are integrated explicitly in time and no outer boundary conditions are required as the last point on radial lines lies on an incoming null surface $\mathcal{I}^+$.

Caustics

The common disadvantage of all characteristic codes is the necessity to either deal with caustics or to avoid them. It has been proposed to treat these caustics 'head-on' as part of the dynamical problem [190]. Since only a few structural stable caustics can arise, their geometrical properties are well understood and their behaviour could be treated numerically [191]. To date, this option has not been pursued but its beauty and potential cannot be denied. In the mean time, the formulation can be used in the following.

- Spacetimes where caustics will not render the coordinates singular. For instance, when dealing with compact objects, the lens equation provides a rough estimate of when they can appear [90].
- Spacetime *regions* without caustics. Here, the use of Cauchy-characteristic matching (CcM) [76, 78, 97, 98] exploits the main advantages offered by '3 + 1' and characteristic codes. A '3 + 1' formulation is employed to simulate strong curvature regions in a bounded domain, on the exterior (which is assumed to be free of caustics) of that domain a characteristic formulation is employed. The combination manages to cover the entire spacetime, removing the boundary problem for the '3 + 1' code and, the caustic problem for the characteristic one. Although CcM is not yet satisfactorily working in 3D, its successful applications in simpler cases illustrates its usefulness (see, for instance, [98, 192]).
- A combination of regions patched with different characteristic codes. Characteristic–characteristic matching (c2M) [193], can also be used to avoid caustics while simulating the whole spacetime (although it can be used in a more restrictive set of problems than CcM, its implementation in 3D should be rather straightforward [193]).

Initial data

As discussed, another distinctive feature of a characteristic formulation is that the initial data are constraint-free. Namely, the intrinsic (conformal) metric h_{AB} is freely specifiable on an initial hypersurface $\mathcal{N}_0$ and the integration of the hypersurface equations (which are basically ODEs) provide the complete metric on $\mathcal{N}_0$. This trivializes posing consistent initial data; however, the problem of defining data which conforms to the physical situation in mind still remains. For the vacuum case, a convenient option is to set the Weyl component $\Psi_0 = 0$ (in the language of the NP formalism [194]), this choice minimizes the radiation crossing $\mathcal{N}_0$ when the departure from spherical symmetry is small[12]. For the case of spacetimes with non-trivial matter content, a consistent way of defining the intrinsic metric was introduced by Winicour [94]. Contact with post-Newtonian theory is obtained through a perturbative analysis with a varying speed of light. The obtained prescription is such that the radiation observed at $\mathcal{I}^+$ reduces, to first order, to the familiar quadrupole approximation.

[12] Note that if the initial null hypersurface coincides with $\mathcal{I}^-$ this is precisely the condition of no incoming radiation.

5.2.1. Examples of implementations

1D

There is a considerable wealth of 1D characteristic codes which have been applied to this study: the radiation tail decay of spacetimes containing scalar fields [195]; critical phenomena [196–198]; singularity structure [199–202]; scalar fields as precursors of inflationary cosmology [203]; cosmic strings (represented by massive scalar and vector fields coupled to gravity) [204] and self-similar collapse of spherical matter and charge distributions [205], among others.

2D

A 2D characteristic code for twist-free axisymmetric vacuum spacetimes was developed in [206] and recently been extended to handle matter through the use of high-resolution shock-capturing schemes [207]. This implementation is being applied to study neutron stars in full GR. Another implementation that removes the twist-free requirement has been presented [98,208] and is being employed in a larger Cauchy-characteristic matching code (the Cauchy code used is the axisymmetric ADM code introduced in [209]. A double null code (under the assumption that departures from spherical symmetry are small) has been employed to simulate a region exterior to the event horizon of the Kerr–Newman spacetime. The inner boundary is placed at the incoming null surface defined by $r = 3m$ (with m being the mass of the black hole) [85]. Another recent implementation [210] has been used to study scalar field collapse in spacetimes with a negative cosmological constant. Aside from the study of black hole formation, the interest in anti-de Sitter spacetimes from AdS/CFT proposed duality in string theory makes this an important subject [211]. Although the conjectured duality between AdS spacetimes and physical effects in conformally invariant Yang–Mills theories on its boundary is for five-dimensional spacetimes, the work presented in [210] appears as a natural first step for numerical studies of this duality.

3D

There exist two characteristic codes in 3D. The first one, obtained by second-order accurate FDA has been presented in [82, 96] for the vacuum case was used to simulate black hole spacetimes (for 'unlimited times' $\approx 60\,000M$ with M the mass of the black hole) and study scattering off a Schwarzschild black hole in the highly nonlinear regime (stably simulating power outputs up to 10^{60} W). Notably, the transition from 1D to 3D is considerably simplified by replacing tensors by spin-weighted complex scalar fields and angular derivatives by eth-operators [189] (which are in turn implemented by FDA and interpolations between the two patches used to cover spheres at $r =$ constant [95]). At present this 3D code is being extended in two directions. On the one hand, the equations governing a perfect fluid have been incorporated (in a rather crude way) for a feasibility study of simulations of black hole spacetimes containing a companion star. Encouraging results were obtained in collapse of dust or matter with weak pressure onto a black hole [77]. At present, more realistic matter data are being studied and plans for incorporating high-resolution shock-capturing schemes [89] are underway. On the other hand, a project aimed towards obtaining gravitational radiation of a binary black hole spacetime is also under development [88]. Here, the spacetime is envisioned in a time-reversed point of view. This is motivated by the possibility of posing a double null problem whose inner boundary corresponds to a fissioning white hole [86, 87] (which from a time-reversed point of view corresponds to merging black holes) and the other corresponds to $\mathcal{I}^-$. An inverse scattering process can be formulated to obtain the radiation produced by a binary

black hole collision [212]. Preliminary investigations of this approach have targeted a 'close limit approximation' yielding excellent results [213].

In an independent 3D implementation [83], a characteristic code has been developed not in Bondi–Sachs coordinates but rather using a null-quasispherical gauge [214]. In this gauge, the angular part of the metric is effectively a unit sphere metric (this can always be done as surfaces at $u = \text{constant}, r = \text{constant}$ have S^2 topology). The angular coordinates transformation (which naturally depends on time), encodes the radiation content of the spacetime. The numerical implementation is obtained through: (I) a clever combination of FDA, fast Fourier transforms and spectral decomposition of tensors in terms of spin-weighted spherical harmonics to handle fields on the spheres; (II) an eighth-order Runge–Kutta integrator for the hypersurface equations and (III) the method of lines with a fourth-order Runge–Kutta time stepper. This code has been used to study (linear to mildly nonlinear) scattering off a (mass M) Schwarzschild black hole. The resulting simulations exhibit very high accuracy and evolutions for about $100M$ are reported, the evolution terminates at late times close to the event horizon where the null-quasispherical gauge apparently breaks down.

5.3. Conformal

Evolution equations

The evolution equations formally look very much like those discussed in section 5.1. Codes implementing the conformal evolution equations have been obtained using standard FDA for both the time and spatial derivatives [102] (in 2D) or have employed the method of lines [108] (in 3D), where FDA approximations are used for the spatial derivatives, while the time integration is carried over by a standard fourth-order Runge–Kutta algorithm.

Outer boundary

Specifying boundary values for the evolution part is simplified in this formulation as we do not need to conform to the physical problem in mind. This might appear puzzling at first sight but let us not forget that the outer boundary is causally disconnected from the physical spacetime; hence, in principle one can pose arbitrary conditions as long as this is done in a stable manner. Furthermore, even the equations might be modified in the unphysical region to aid in this task. In [108], the evolution equations are modified (beyond $\mathcal{I}^+$) to mimic advection equations describing signals propagating towards the outer boundary and therefore 'numerical diffusion' which could leak into the physical spacetime is minimized.

Initial data

Initial data are obtained by solving the Yamabe equation (obtained from the Hamiltonian constraint) [215] in such a way that their degeneracy at the boundary is properly addressed. Pseudo-spectral methods are employed which aid in obtaining solutions with the proper regularity conditions [125, 126]. Data corresponding to flat spacetime, vacuum spacetime with toroidal infinities [216] and Schwarzschild spacetime [217], among others, are available.

5.3.1. Examples of implementations

1D

Scalar field collapse situations were studied by Huebner in [218], reproducing the scaling law behaviour obtained by Choptuik [62], but in this case, being able to simulate the full spacetime.

2D

Frauendiener [102] implemented a 2D code to study A3-like spacetimes [216]. These provide the first examples of vacuum spacetimes with gravitational radiation. Although the toroidal topology of future null infinity imply that they cannot be used as models of isolated systems, they provided a rich arena to investigate the system and calibrate the implementation in higher dimensions.

3D

Quite recently, a 3D implementation was used to simulate the Schwarzschild spacetime [105]. In particular, the full Kruskal diagram was targeted and encouraging results were obtained as a significant portion was accurately simulated. Additionally, the code has been used to study initial data sets departing slightly from flat spacetime [104]. The simulation is able to reproduce the rigorous analytical results from Friedrich [219] (and related to those of Christodoulou and Klainerman [220]) that these initial data should evolve in such a way that a regular i^+ should exist. The entire future of the initial hypersurface is accurately obtained and the radiation at $\mathcal{I}^+$ is extracted; to date this is the most complete simulation of this kind of system.

6. Beyond the vacuum case

6.1. Scalar field models

Although scalar fields have not been observed in nature so far, their study has been carried out since the 1960s [221, 222]. The original motivation was to consider the existence of bosonic counterparts of observed fermionic objects (such as neutron stars). These objects can provide useful physical insights on a variety of fronts since they are sources of scalar gravitational radiation and can collapse to form black holes. More recently, these objects have been suggested as candidates for dark matter [223]; thus being 'promoted' from purely theoretical toy models to perhaps real physical objects. An important feature of the scalar field models under study is that they do not develop shocks or discontinuities (if these were not already present in the initial data) which simplifies their numerical simulation. Not only have scalar field models been useful to investigate: 'stability' of Minkowski spacetime; critical phenomena; singularity structure; cosmological models; alternative theories of GR; etc, but they have also served well to test codes for their use in relativistic hydrodynamics.

A large number of scalar field models exist, these have been introduced considering both real and complex fields which can be massive and/or charged. For simplicity, next I will consider a simple case, that of the massive Einstein–Klein–Gordon field [12] to illustrate their use. The real scalar field Φ, satisfies the equation

$$\nabla^a \nabla_a \Phi = m^2 \Phi \tag{56}$$

which is derived by minimizing the action

$$S = \int \left[R - \left(\tfrac{1}{2} \nabla_a \Phi \nabla^a \Phi + m^2 \Phi^2 \right) \right] \mathrm{d}V \tag{57}$$

with R the Ricci scalar and m the mass of the field. The stress–energy tensor T_{ab} is given by

$$T_{ab} = \nabla_a \Phi \nabla_b \Phi - \tfrac{1}{2} g_{ab} (\nabla_c \Phi \nabla^c \Phi + m^2 \Phi^2). \tag{58}$$

The dynamics of the scalar field is governed basically by a wave equation in a curved spacetime (56). Particularly interesting is the possibility of stable (or long-lived) compact configurations of complex massive scalar fields known as *boson stars*. These are local equilibrium solutions

of the system in which the spacetime is static (although the real and imaginary components of the field oscillate). These 'stars' are 'similar' to neutron stars in the sense of having a maximum mass marking a transition from stable to unstable states. Additionally, there exists a family of solutions known as *multi-scalar stars* which are quasiperiodic compact solutions to the Einstein–Klein–Gordon systems. This class of solutions contains boson stars and *oscillating soliton stars* (periodic solutions of systems with a single real scalar field). The study of boson stars in fully general relativistic scenarios was started by Seidel and Suen [224, 225] to investigate their role as a possible source of dark matter. Since then, numerical simulations have been directed towards analysing the stability of boson stars and critical phenomena [226, 227]; to investigate possible 'boson halos' around galaxies and their influence on them [228]; and to simulate the collision of 'boson stars' [229].

6.2. Relativistic hydrodynamics

In the non-vacuum case a fluid is characterized by its velocity u^a, pressure p, enthalpy ϵ and rest mass density ρ defined in a locally inertial reference frame. The general relativistic hydrodynamic equations consist of the local conservation of T_{ab} (a direct consequence of the Bianchi identities) and of the current density $J^a = \rho u^a$ (the continuity equation),

$$\nabla_a T^{ab} = 0, \tag{59}$$

$$\nabla_a J^a = 0. \tag{60}$$

These equations determine the dynamics of the fluid, while Einstein's equations (appropriately modified to include the corresponding components of T_{ab} on the right-hand sides) determines the geometry. When neglecting non-adiabatic effects (such as viscosity or heat transfer) the stress–energy tensor for a perfect fluid is

$$T_{ab} = \rho h u_a u_b + p g_{ab} \tag{61}$$

with h the relativistic specific enthalpy given by $h = 1 + \epsilon + p/\rho$. In order for the system be solvable, the five equations (59), (60) must be supplemented with *two* extra conditions. One of these is $u^a u_a = -1$ and the other is an equation of state $p = p(\rho, \epsilon)$.

An accurate simulation of this system is a challenging task even in Newtonian gravity. The difficulty lies in the fact that the system develop shocks, rarefraction waves and contact discontinuities which are difficult to handle (which, because of the nonlinear character of the equations governing the fluid, can develop even though they were not present in the initial data). To simplify the treatment of the system, equations (59) and (60) are rewritten in explicit conservation form. This requires introducing intermediate variables which are integrated over time, and the primitive variables are recovered at each step by an, often expensive, inversion method. Flux-conservative systems are formally simpler to handle and simplify implementations where variable grid spacing is employed.

Most ways of expressing the equations were obtained for the 3 + 1 approach (namely the ADM one). Recently, interest in covariant expressions which could be applied in different approaches resulted in a number of reformulations [89, 230].

In [89], the spatial components of the 4-velocity u^i together with ρ and ϵ are taken as primitive variables. The intermediate variables are $V^A = (\rho u^0, \rho h u^0 u^i + p g^{0i}, \rho u^0 u^0 + p g^{00})$, $(A = 0, i, 4)$. In terms of V^A, the equations take the form

$$\partial_o(\sqrt{-g} V^A) + \partial_j(\sqrt{-g} F^j) = S, \tag{62}$$

with

$$F^j = (J^j, T^{ji}, T^{j0}) = (\rho u^j, \rho h u^i u^j + p g^{ij}, \rho h u^0 u^j + p g^{0j}), \tag{63}$$

$$S^A = (0, -\sqrt{-g}\Gamma^i_{ab} T^{ab}, \sqrt{-g}\Gamma^0_{ab} T^{ab}). \tag{64}$$

After integrating these equations, the value of the primitive variables are recovered typically by a root-finding algorithm such as the Newton–Rapson one [109]. This feature is computationally expensive and might even lead to a loss of accuracy. However, in the case where a characteristic formulation is employed, $g^{00} = 0$ which allows for an explicit recovery of the primitive variables [89].

6.2.1. FDA and relativistic hydrodynamics. As mentioned in section 4, FDA algorithms are obtained by formal Taylor expansions, this naturally carries the implicit assumption that the variables are smooth enough for such an expansion to be valid. Clearly, discontinuities do not satisfy this requirement and in practice are 'smoothed-out' via the addition of artificial viscosity terms to the stress–energy tensor in the following way:

$$T_{ab} \rightarrow T_{ab} + Q_1 u_a u_b + Q_2 g_{ab}, \tag{65}$$

with Q_1, Q_2 'viscosity controlling functions' which can be chosen independently. For instance, in the Wilson formulation [11] $Q_1 \equiv 0$, while in that by Norman and Winkler [231] both Qs are allowed to be non-zero. These extra terms are such that, as the grid is refined, they tend to zero (and therefore one does have a consistent approximation to the original system). In order to avoid dissipation in regions where the solution is smooth, Qs are defined to be non-zero only in places where the solution has large gradients.

Clearly, the magnitude of these terms must be carefully chosen so that the necessary amount of dissipation is introduced but, at the same time, excessive smearing of the discontinuities is avoided. Assuming this can be done, artificial viscosity is indeed very appealing as it is straightforward to implement and computationally efficient. For these reasons, this technique has enjoyed an absolute popularity for more than three decades. It has only been until recently that other options, the *high-resolution shock-capturing schemes* [232], have become popular. These methods exploit the hyperbolic character of the equations and explicitly use the characteristic speeds and directions to solve (exactly or approximately) the Riemann problem at every interface of the numerical grid [233]. This property guarantees that physical discontinuities are treated consistently, producing stable and sharp discrete shock profiles while providing good accuracy order. To illustrate the spirit of this technique, let us take the 1D case and define $\Omega = \{(x, t), t \in [t, t + \Delta t], x \in [x_o, x_o + \Delta x]\}$; consider,

$$\partial_o(\sqrt{\gamma} V) + \partial_x(\sqrt{-g} F) = S \tag{66}$$

can be formally integrated as

$$(\bar{U}\,\Delta)|_{t+\Delta t} - (\bar{U}\,\Delta)|_t = -\left(\int_{L_1} (\sqrt{-g}\hat{F})\,\mathrm{d}t - \int_{L_2} (\sqrt{-g}\hat{F})\,\mathrm{d}t\right) + \int S\,\mathrm{d}t\,\mathrm{d}x \tag{67}$$

with $L_1 = (x_o, t)$, $L_2 = (x_o + \Delta x, t)$ $(t \in [t_o, t_o + \Delta t])$

$$\bar{U} = \frac{1}{\Delta V}\int_{\delta V} (\sqrt{\gamma} U)\,\mathrm{d}x, \tag{68}$$

$$\Delta V = \int_{x_o}^{x_o+\Delta x} \sqrt{\gamma}\,\mathrm{d}x, \tag{69}$$

where $\hat{F}$ are the fluxes across the numerical cells which depend on the solution at the interfaces. At them, the flow conditions can be discontinuous and can be obtained, as Godunov suggested [234] by solving a collection of *local* Riemann problems. In practice, the continuous solution is locally averaged over the numerical grid, leading to discontinuities at cell interfaces. Accurate knowledge of the Riemann problem's problem is exploited to obtain the solution at the later time. Dissipation is still added in the process but the information of the local characteristic of the fluid is used to do so in the 'correct' amount.

6.3. Other options

Two approaches have been considered which can be regarded as hybrid combinations of FDA for the geometric variables and a 'particle' approximation for the fluid variables. These approaches are known as: *smooth particle hydrodynamics* and *particle mesh*.

6.3.1. Smooth particle hydrodynamics. In the smooth particle hydrodynamics (SPH) method, the fluid is modelled as a collection of particles which are represented by smoothed values. That is, given a function $f(x^i)$ its mean smoothed value $\langle f(x^i)\rangle$ is obtained from

$$\langle f(x^i)\rangle \equiv \int W(x^i, \hat{x}^i; h) f(\hat{x}^i)\sqrt{\gamma}\, \mathrm{d}^3\hat{x}^i, \tag{70}$$

where $W(x^i, \hat{x}^i; h)$ is the kernel and h is a smoothing length. The kernel satisfies

$$\int W(x^i, \hat{x}^i; h)\sqrt{\gamma}\, \mathrm{d}^3\hat{x}^i = 1; \tag{71}$$

gradients and divergences are also represented by smoothed counterparts; for instance,

$$\langle \nabla f(x^i)\rangle \equiv \int W(x^i, \hat{x}^i; h)\nabla f(\hat{x}^i)\sqrt{\gamma}\, \mathrm{d}^3\hat{x}^i. \tag{72}$$

After introducing the density distribution of particles,

$$\langle n(x^i)\rangle = \Sigma_{a=1}^{N} \frac{\delta(x^i - x_a^i)}{\sqrt{\gamma}} \tag{73}$$

with $\{x_a^i\}_{a=1,\ldots,N}$ (the collection of N particles where the functions are known). These approximations are used to derive a smoothed version of the general relativistic hydrodynamics equations (59) and (60). The explicit formulae are reported in [235]. Again, viscosity terms must be introduced to deal with simulations where shock waves arise [236]. The integration of the hydrodynamic equations via this method reveals only pairwise particle interactions among particles inside the compact support of the kernel. The drawback is the need to search among all N particles those N_h in a given kernel. The use of hierarchical grid methods [237] makes the search an $\mathrm{O}(N \ln N)$ task; once the search is performed, the update takes only $\mathrm{O}(N_h N)$. Studies of tidal disruptions by supermassive black hole spacetimes have been presented in [235, 238] where the background is kept fixed. I am not aware of SPH being used to study a fully relativistic problem as yet.

6.3.2. Particle mesh. In this approach, the fluid is treated as a 'collisionless gas of particles'. The stress–energy tensor is expressed as

$$T^{ab} = \Sigma_A m_A n_A u_A^a u_A^b, \tag{74}$$

where m_A, n_A, u_A^a are the rest mass of the particle, the number density in the comoving frame and the 4-velocity of each particle. Each particle's evolution is determined by the geodesic equation. The integration of the geometric variables using FDA requires an interpolation of the stress–energy tensor onto the grid points. Additionally, the evolution of the particles requires interpolating the metric variables onto the particle's trajectory. This method has been extensively applied by Shapiro and Teukolsky to investigate stellar dynamics [239], collapse of dense star clusters to supermassive black holes [240] and the formation of naked singularities [241].

6.4. Initial-value problem

Most works dealing with non-vacuum spacetimes and targeting astrophysically relevant simulations employ 3 + 1 formulations[13]. Next I will comment on how initial data for these simulations are obtained.

In the non-vacuum case, the Hamiltonian and momentum constraints must be solved, taking into account the corresponding terms of (the now non-vanishing) stress–energy tensor. From the implementation point of view, little changes. Given appropriate definitions for the matter fields (ρ, $p(\rho, \epsilon)$, ϵ, u^a) the same modules used for the vacuum case can be used to obtain the gravitational data. However, one is usually interested in situations where both matter and geometry are in (or close to) equilibrium. That is, the spacetime is assumed to (approximately) have a timelike Killing vector.

6.4.1. Isolated neutron stars. For an isolated star, apart from the timelike Killing vector T^a, a further assumption is the existence of a spatial Killing vector (ϕ^a) corresponding to an azimuthal symmetry. The 4-velocity of the fluid is expressed as

$$u^a = u^t T^a + u^t \Omega \phi^a, \tag{75}$$

with Ω the angular velocity of the matter as measured at infinity. For a perfect fluid, equation (59) can be expressed in differential form as

$$\mathrm{d}p - (\rho + p)(\mathrm{d} \ln u^t - u^t u_\phi \, \mathrm{d}\Omega) = 0, \tag{76}$$

which is referred to as the *relativistic Bernoulli equation*. Two cases are distinguished: *uniform rotation*, $\mathrm{d}\Omega = 0$ where equation (76) can be trivially integrated and *differential rotation*, where the integrability condition $u^t u_\phi = F(\Omega)$ is used to perform the integration. $F(\Omega)$ describes the *rotation law* of the matter [243].

The simplest model for stars was introduced by Oppenheimer and Volkoff [244], corresponding to non-rotating spherically symmetric configurations parametrized by a single variable determining how relativistic the system is. Due to the Birkhoff theorem, the solution outside the star is the Schwarzschild one. This model constitutes a valuable test for general relativistic hydrodynamic implementations and is customarily used for this effect.

In general, isolated neutron stars will be rotating and the hydrostatic equilibrium equations must be solved in conjunction with the constraints (8) and (9). For uniformly rotating stars, the obtained solutions (for a given equation of state) are parametrized by Ω and the value of the central density which serves as an indication of how relativistic the solutions are. For differentially rotating stars, the rotation law must be specified. As mentioned, data must be specified to solve the constraints and different choices have led to a number of approaches. Some examples of them are [245–250]. (For a recent review on the subject see [251].)

6.4.2. Binary neutron stars. Binary systems cannot rigorously be in equilibrium as they emit gravitational radiation. However, when the members of the binary are far apart (beyond the *innermost stable circular orbit*), the gravitational radiation reaction time scale is much longer than the orbital period and a reasonable assumption is to consider that the stars are in a quasi-equilibrium state. This state is reflected in an approximate Killing vector in a frame co-rotating with the binary, i.e., if the binary rotates with angular velocity Ω, this Killing vector is

$$\hat{T}^a = T^a + \Omega \xi^a, \tag{77}$$

[13] The exception being [89, 90, 242] which adopt a characteristic formulation.

where ξ^a is the generator of rotations about the rotation axis and $T^a = (\partial_t)^a$. Numerical implementations of binary systems were initiated by Wilson and Mathews [252] where the fluid variables are not prescribed enforcing hydrostatic equilibrium. Rather, an initial guess for the density profile is specified and the system is evolved until equilibrium is reached. In order to have a clearer physical picture of the initial configuration hydrostatic equilibrium can be enforced at the initial time. Work on obtaining equilibrium configurations has concentrated on two different assumptions leading to considerably different solutions: (I) *co-rotation* where $u^a \propto \hat{T}^a$ and the individual stars in the binary do not rotate with respect to the co-rotating frame defined by $\hat{T}^a$ and (II) *counter-rotation* where the individual stars do not rotate with respect to the rest frame of the binary.

Corrotating binaries

With respect to the co-rotating frame, the stars appear to be in a (extremely slow) head-on trajectory; hydrostatic equilibrium is specified by solving the relativistic Bernoulli equation (under the assumption $\mathrm{d}\Omega = 0$) together with the constraints [253]. The main drawback of this approach has to do with its relevance for astrophysical purposes. The viscosity of the fluid composing the neutron stars is not expected to be large enough for the spin to 'lock' with the orbit (as is the case in the Earth–Moon system) [254, 255]. If the spins of the neutron stars are small, for close binaries, *irrotational* fluid models are expected to provide a more reasonable approximation.

Irrotational binaries

Irrotating (also referred to as counter-rotating) binaries are obtained assuming the matter has irrotational flow [256–258]. This assumption allows one to express the velocity of the fluid in terms of a 'vector potential' Φ,

$$hu_a = \nabla_a \Phi \tag{78}$$

where h is the enthalpy. When expressing u_a in this way the Euler equation (59) is automatically satisfied, leaving only the continuity equation to be solved (60), which can be expressed as a Poisson equation for Φ. The quasistationarity condition is expressed as

$$hu_a \hat{T}^a = \text{constant}, \tag{79}$$

which is readily obtained from the Killing equation [257]. The continuity equation coupled with appropriate boundary conditions at the surface of the stars and the constraints are then solved simultaneously to yield quasi-equilibrium counter-rotating configurations. Numerical implementations have been presented in [256, 259, 260].

6.5. Black hole/neutron star binary

The first (and as far as I know only) data set describing a system containing a non-spinning black hole and a polytrope star (which is taken to approximate the neutron star) has been presented recently by Miller [261]. The method combines the puncture method [47] to specify the black hole with the assumption of corrotation to treat the fluid describing the star [253]. It produces accurate initial data to study the system approximately assuming quasi-equilibrium [261], or as initial data for a complete description of the system through a 3 + 1 code. This is an important first step, and will probably lead to more realistic initial data when the irrotational case is considered.

7. Main accomplishments

Perhaps the most spectacular accomplishment to date is the discovery of critical phenomena in general relativity by Choptuik [62] and analogous behaviour in a wealth of different systems discovered though numerical models [262]. This and several other important achievements illustrate the potential of numerical relativity, to name a few.

- *Bagels might form when black holes collide/form*: in the early 1990s Shapiro and Teukolsky studied a system containing a toroidal distribution of particles [263]. These simulations followed the collapse of these particles and the resulting event horizon was obtained by tracing (past directed) null rays from the end of the simulation [264]. Strikingly, what they found was that early phases of the horizon topology corresponded to a *toroidal horizon*, while at late times, as expected, to a *spherical horizon*. This at first sight was puzzling as this toroidal horizon appeared to leave room for violations of cosmic censorship. Shortly after these results, an analytical model studying the caustic/crossover structure of null surfaces showed that indeed this toroidal topology was the correct picture [265]. Cosmic censorship is not violated as the 'hole of the torus' pinches off faster than the speed of light. Additionally, recent analytical models have shown that a toroidal structure of the early phase of colliding black holes might indeed be the *generic* behaviour [86,87,266]. It will be a 'nice' challenge for numerical simulations to reproduce this expected feature.
- *Head-on collision of black holes*: a two-dimensional code was used to simulate the head-on collision of non-spinning black holes [267, 268]. Not only were these simulations capable of accurately following the evolution past merger for a decent amount of time but also of extracting the gravitational waves, observing the ring-down of the merger hole for several periods and reconstructing the event horizon structure (revealing the expected 'pair of pants' [269]). These simulations were carried out with the use of singularity-avoiding slicings (maximal slices). Additionally, the obtained results were successfully corroborated with those obtained from perturbative studies[14]. A remarkable agreement of results obtained with both approaches was achieved [271]. These results have a twofold message, on the one hand, perturbation analysis (used in a regime where one expects it to be valid) can be used to check a numerical implementation; on the other hand, the numerical implementation might show that the regime of validity of the perturbative approach be larger than first expected. Obtaining 'error bars' for perturbative treatments is an involved process requiring working out the following order in the perturbative expansion [272]. A carefully tested simulation can certainly provide these error bars in a much more direct way and be used to decide whether the, cheaper, perturbative method can be used to describe the system at certain stages.
- *Generic single black hole simulations*: simulating stably a single black hole in 3D for unlimited periods was proven to be possible [273, 274]. Initial data corresponding to single Schwarzschild or Kerr black holes plus some amount of gravitational radiation was accurately simulated for tens of thousands of M (M being the mass of the black hole) without signs of instabilities. This work employed singularity excision, highlighting its usefulness. As a test of causality not being violated, different excision regions were defined by choosing the apparent horizon or different types of surfaces (lying inside the apparent horizon but not coinciding with it), physical 'measurements' were carried out in the exterior and the solutions were checked to agree quite well.

[14] For a review on the subject see [270].

- *Qualitative studies of binary neutron star spacetimes:* an approach that has been exploited to gain insight into the behaviour of binary neutron star systems assumes that the system is in *quasi-equilibrium*. Under this approach, the system is assumed to radiate negligible amounts of energy and the system can be, in some sense, approximated by obtaining equilibrium configurations at different separations [253,256,259,260]. This translates into solely having to solve the initial-value problem (i.e. find data satisfying the constraints). This approach has been used to obtain estimates of the location of the innermost stable circular orbit (ISCO) and the behaviour of the central densities of the stars as they approach each other, even closer than the ISCO. It is unclear to me whether this approach can be pushed *this far*, as at the ISCO neglecting gravitational radiation is not consistent and its accounting by means of the quadrupole approximation might not be accurate enough. The results predicted from this approach will eventually be corroborated or not by fully dynamical evolutions.
- *Singularity studies:* understanding whether singularities are hidden, which types they are, etc has been another goal of numerical investigations and important results have been obtained.
  Singularities in collapse situations: naked singularities in gravitational collapse of a scalar field have been found by Choptuik [62] and many others (see for instance [196, 197]), additionally revealing a self-similar or discrete self-similar behaviour of the solution [262].
  Nature of singularities in charged/rotating black holes: spacetimes containing rotating or charged spacetimes possess a Cauchy horizon (CH) [12]. Studies on the effect of perturbations on this CH were initiated (analytically) by Poisson and Israel to check conjectures that these perturbations would drive the CH into a true singularity [275]. Over the last decade a number of numerical investigations were capable of showing this to indeed be the case [199–202]. Moreover, numerical investigations provided the complete picture [202]; that is, generically the CH becomes a null, weak singularity which is a precursor of a strong spacelike singularity.
  Singularities in cosmological models: in homogeneous cosmologies the generic singularity is approached either by the Kasner solution [276] or by displaying Mixmaster dynamics [277]. Furthermore, it has been conjectured that singularities in generic four-dimensional spacetimes are spacelike and oscillatory (Belinski *et al* [278]), while generic spacetimes with stiff fluids (including massless scalar fields) have singularities which are spacelike and non-oscillatory (as conjectured by Belinski and Khalatnikov [279]). Additionally, according to this picture, spatial points decouple near the singularity and the local behaviour is asymptotically like spatially homogeneous (Bianchi) models. Spacetimes with non-stiff matter appear, close to the singularity, to behave independent of the matter and the evolution is determined by the curvature. On the other hand, for stiff matter, this dominates the evolution and is responsible for the oscillatory behaviour. A valuable insight has been provided by numerical simulations that there exist important situations where classes of spacetimes exhibit non-oscillatory behaviour at the singularity even without the presence of stiff matter. For instance, in the Gowdy class of spacetimes, simulations showed no oscillations [280]; this result was later proven analytically [280,281]. Aside from confirmation or not of these conjectures (often referred to as the BKL conjecture) for specific cases, numerical explorations of cosmological singularities have provided evidence that each of the spatial points does evolve towards the singularity independently [277].
- *Critical phenomena:* ever since the discovery of critical phenomena by Choptuik [62], analogous phenomena have been discovered basically in every possible imaginable (and workable) scenario and well over a hundred papers have been published on this

topic[15]. Critical phenomena has been 'observed in the numerical laboratory' in systems containing massive and massless Klein–Gordon fields, in Yang–Mills theory, in spacetimes with perfect fluids, in gravitational collapse in anti-de Sitter spacetimes, self-gravitating nonlinear sigma models, in 6D (assuming spherical symmetry); in full 2D gravitational collapse, etc. I cannot cover here the rich aspects of this problem and I refer the reader to the latest (and continuously updated) review in [262]. Just to show the tip of the iceberg, here I will mention that the work presented in [62] carefully studied the (spherically symmetric) Einstein–Klein–Gordon system on the verge of black hole formation. Namely, in a collapse situation, there could be *two* final states. Either a black hole forms or the field disperses away. At the boundary between black hole or star formation and dispersion a rich phenomena was discovered, where the mass M of the final collapsed black hole obeys a (by now famous) scaling relation $M = C(p - p_*)^\gamma$, where γ results completely independent of the initial data. Moreover, the solution that gives rise to such a relation, displays a scale-periodic dependence for $p \approx p_*$. The existence of such a phenomena was first discovered numerically and it marked the beginning of a new branch of research in numerical and analytical GR. Most of the simulations displaying critical phenomena have been carried out in 1D situations; I am aware of just two published studies displaying this phenomena in 2D [158, 283]. As a last point, it is worth remarking that these phenomena have been simulated with the three formulations presented in section 3. For examples of critical phenomena studied with the '3 + 1'; characteristic and conformal approaches see [62, 284], [197, 198] and [103].

- *Rapidly rotating neutron stars. Secular instability:* studies of rapidly rotating neutron stars provide valuable information on the equation of state of matter at extremely high densities and an insight into them being sources of detectable gravitational waves. In particular, oscillations can become unstable, producing gravitational waves that could be detectable, carrying information on the equation of state. Uniformly rotating, incompressible stars are secularly unstable to bar mode formation; this instability grows in the presence of some dissipative mechanism such as viscosity or gravitational radiation. The instability appears for critical values of β (= *(rotational kinetic energy)/(gravitational binding energy)*). This value depends on the compaction of the star, the rotation law and the dissipative mechanism. Instabilities driven by gravitational radiation have a critical value of $\beta \leqslant 0.14$ as observed in simulations [285, 286]. Viscosity, on the other hand, drives the critical β to larger values [287, 288]. (For a detailed presentation of the subject see [251].)

8. *Current main focus and results*

Most present efforts are concentrated towards obtaining robust implementations of Einstein's equations in 3D, while at the same time extracting physically relevant information with the current (and constantly revised and improved) codes. There already exist robust 3D implementations in the characteristic formulation, but as mentioned they cannot be applied to generic situations. The main targets within this formulation are BH–NS systems and the post-merger phase of BH–BH systems. 3 + 1 and conformal field equations implementations are not yet robust. Existing codes in these approaches can evolve single black hole systems for at most $1000M$. If richer spacetimes (binary black holes, non-vacuum black hole spacetimes, etc) can be modelled for about the same time, useful physical information can be extracted. Thus the current focus it not only to extend the simulation lengths (by re-examining analytical

[15] For an up to date complete review on the subject refer to [262, 282].

and numerical issues), but also to apply the existing knowledge to investigate physically relevant systems.

Of the systems being considered, some have the additional incentive of being important for gravitational wave detection but certainly all entice us by their potential to shed light on our understanding of general relativity in strong-field scenarios and/or the global structure of spacetimes. Some of the current main projects are as follow.

- *Black hole and or neutron stars simulations*
  Several efforts worldwide are being directed towards modelling systems containing black hole and/or neutron stars. These simulations will play an important role in the detection and analysis of gravitational waves to be measured by LIGO [1], VIRGO [2], GEO600 [3], TAMA [4], etc. Considerable progress has been achieved in both fronts recently as the first simulations of binary black holes [41, 289] and binary neutron star systems [186, 290] are starting to appear. The simulations have been conceived more as a proof of concept than actual models of realistic scenarios. Nevertheless, they are not only useful in understanding the problems being faced by 3D numerical relativity but also are starting to give actual physical information.
  Binary black hole simulations. The first medium-lived simulations of binary black holes were presented in [289, 291]. This simulation used maximal slicing conditions and zero shift. The (spinning) holes had masses m and $M = 1.5m$ (for a total $M_{ADM} = 3.1$), located at $\pm M$ on the y-axis (i.e. fairly close to each other) and their linear momentum was chosen to be perpendicular to the line of separation. The runs proceeded nicely for about $30M_{ADM}$ and the first period of the gravitational waves produced by the system were obtained. The simulations were obtained using the BSSN approach [27, 165] and outgoing boundary conditions were prescribed. However, the initial data used [47] assume conformal flatness which, as mentioned is not well suited to astrophysically relevant cases. Additionally, the use of maximal slicings prevents long-term simulations. Current work is focused on incorporating singularity excision techniques to extend these runs [117].
  The other set of simulations has presented the first binary black hole simulation with the use of singularity excision [41]. Initial data corresponded to a grazing collision of (two spinning or not) equal mass (m) black holes separated by $\approx 10m$ and with impact parameter of m. Outer boundaries where placed at $20m$ from the 'grid' origin and data were specified there by the 'simplistic' approach. Singularities were excised from the computational domain and the simulations run for about $15M_{ADM}$. It was noted, however, that as boundaries were pushed further, longer simulations were obtained (indicating a strong boundary influence). Initial data were *not conformally flat* [181]. Present efforts are focused on removing the instabilities and improving the outer boundary treatment.
  The main messages from these preliminary simulations are: (I) considerable gravitational radiation might be expected from binary black hole simulations $\approx$1–3% (estimates obtained by analysing the area of the apparent horizons [41, 289] and waveform extraction [289]); (II) excision techniques have been shown to be capable of dealing with singularities, starting on a slice with two separated black holes and following it well past the merger [41].
  Binary neutron star simulations. Models of binary neutron stars systems are also starting to produce simulations describing two 'neutron' stars to the point where the stars begin to merge [42, 186, 292]. The stars are represented by polytropes, have equal masses and the codes have been constructed using the '3 + 1' approach presented in [25, 26].
  In [42], 'conformal' slicing and pseudo-minimal distortion are used to prescribe the shift. The stars have mass $M_\odot$, radius $6M_\odot$, are initially separated by $24M_\odot$ and initial data for co-rotating or irrotating stars are simulated. Instabilities, apparently caused by the slicing

condition used, terminate the runs obtained with this code when the stars are about to merge. This simulation was extremely coarse ($\Delta x^i = M_\odot$) and boundaries where placed $95M_\odot$ from the centre of mass. The authors are working on incorporating maximal slicing in their code and will run their new simulations on a more powerful machine. In [186], maximal slicing is used to foliate the spacetime, the modelled stars had mass $1.4M_\odot$, radius $9M_\odot$ and were separated by $35M_\odot$; they employed their code to investigate a conjecture by Shapiro [293] concerning the non-occurrence of prompt collapse of head-on collision of polytropes. The results in [186] display the formation of a black hole in prompt timescales, although further resolved simulations will be required to put the conclusions on firmer grounds. The simulations presented in [292] describe co-rotating equal-mass polytropes in contact and were capable of describing the system for a couple of dynamical timescales.

Black hole–neutron star simulations. An implementation targeting a binary system containing a black hole and a neutron star is being developed with the characteristic formulation (exploiting the robustness displayed in single black hole spacetimes) [90]. Because of the possible formation of caustics the range of parameters (mass/radius of the star and proximity to the black hole) that can be simulated with this approach is restricted. However, there is an interesting 'window' of allowed values which would enable one to study astrophysically relevant systems and provide not only gravitational wave information but also enable a global description of the system, investigate consequences of different equation of state, the influence of orbit precession on the produced gravitational wave, etc.

Accretion of matter by a black hole. Simulating the process of black hole accretion requires incorporating, among other things, the dynamics of the fluid that describes the accreted material and electromagnetic fields. Numerical models are yet to be completed to incorporate these ingredients into a fully GR code. Achieving such a simulation will be expedited by the considerable experience gained through the use of pseudo-Newtonian models where the gravitational effects of the black hole are included by modifying the gravitational potential and adopting suitable boundary conditions [294–296]. First steps towards a fully relativistic simulation of accretion processes are being carried out by Papadopoulos and Font [242]. Their model at present does not incorporate magnetohydrodynamics effects but is already producing predictions which could bear observational importance. Namely, they find that if mass accretion significantly increases the mass of the black hole during the emission of gravitational waves, the expected damped-oscillatory radiative decay [297, 298] is modulated by the mass accretion rate. This effect could be exploited by gravitational wave astronomy to obtain valuable information on our understanding of black hole birth.

Single black hole simulations. Unfortunately, there still does not exist a code in the 3 + 1 formulation capable of dealing with single black hole spacetimes for unlimited times. However, considerable progress has been achieved in simulating such systems in 3D. Recently, a number of efforts have extended the total simulation length to beyond $600M$ [24, 43]. Given that the quasinormal period of gravitational waves is of the order of $20M$, accurate simulations for at least an order of magnitude longer provide quite a decent setting to study a variety of interesting scenarios. In [43], for instance, the study of collapse of gravitational waves onto a black hole is carried out and the produced waveforms obtained. The evolution of the system is obtained from the early dynamical phase to late times where the black hole has clearly settled into a stationary regime.

Rapidly rotating neutron star simulations. Dynamical instability. Studies of the *dynamical* instability to bar-mode formation of rapidly rotating neutron stars in full 3D are underway [184, 292]. As opposed to the secular instability, the dynamical one is independent of

dissipative mechanisms. Preliminary simulations show the onset of instability for $\beta \sim 0.24$; which is slightly smaller than predictions obtained from Newtonian implementations (see, for instance, [299,300]). Estimates of the gravitational wave amplitude and frequency are $h \sim 10^{-22}$ and $\sim$1 kHz, respectively. Although more detailed simulations need to be carried out, these results do show that fully relativistic simulations of these systems are possible and might be valuable for gravitational wave detection.

- *Dynamical GR—quasi-equilibrium NS*
  As mentioned when discussing the quasistationary approximations of binary neutron star systems one shortcoming of this approach is that the dynamics of the spacetime was neglected. A more reliable description of this system (yet still short of the full numerical modelling of neutron stars) has been recently proposed [301] which employs the quasi-equilibrium sequences described earlier to obtain a description of the stress–energy tensor describing the stars and 'feeds it' to a full GR code. This approach, called 'matter without matter' [302] does, *a priori*, a better job of describing the spacetime since gravitational radiation is not neglected (although its back-reaction on the sources is). However, when obtaining the equilibrium sequences a working assumption has been that the 3-metric is conformally flat throughout all of the sequence. In the GR part of the approach (where Einstein's equations are fully evolved) this is only enforced at an initial slice. It is not clear whether this assumption holds during the evolution. Although conformal flatness is not required, when producing the quasi-equilibrium sequence a (by hand) prescription for the metric is assumed. Throughout the evolution, however, the dynamically evolved metric might not satisfy this assumption. This can be easily monitored and as long as the agreement is acceptable this method can be used to obtain a 'cheaper' simulation.
  Clearly, this will not be generically the case; nevertheless, this approach appears as a natural step towards investigating the system in a more complete way than when using quasi-equilibrium sequences and can serve as additional checks for the fully dynamical codes mentioned in the previous item.
- *Critical phenomena in higher dimensions*
  As mentioned, most of the simulations displaying critical phenomena have been carried out in 1D situations. The first simulation displaying this phenomena in 2D was presented by Abrahams and Evans [283] shortly after Choptuik's discovery. However, the resolution achieved was still quite low to allow for a detailed description. Recently, 2D systems have been revisited and preliminary results display this phenomena [158, 283]. However, these simulations are still rather coarse and do not yet have the desired resolution. The use of adaptive mesh refinement proved important in 1D, but certainly its role in higher dimensions will be crucial.
- *Singularity structure*
  General relativity clearly displays its difference with Newtonian theory in regions where the curvature is large. In particular, in regions close to a singularity the theory displays its full glory. What it can tell us about the structure of singularities is certainly an interesting issue. In particular, we have seen that spacetimes on the verge of black hole formation (and therefore the appearance of a singularity) the rich phenomenology of critical phenomena arises. We would also like to understand the structure of singularities away from this limit case. Studying singularities via numerical implementations is particularly difficult; in fact, singularity excision/avoidance techniques are introduced to get rid of them! However, the promise of unravelling what Einstein's equations have to tell us in the very harshest regime is certainly hard to resist. Answering questions about the existence of naked singularities, whether 'hidden' singularities share some properties, what character do they have (timelike, spacelike or null), etc in generic situations is the goal of numerical studies

of spacetime singularities. These numerical simulations must be capable of describing the singularities by the asymptotic approach to them. Describing the efforts to obtain such simulations and what we have learned from them requires a review completely dedicated to it which goes beyond of the scope of this review. For the interested reader I suggest starting with the comprehensive review in [277].

- *Cosmology*
  Even though gravity is the weakest of the four fundamental forces, its long-range character and the impossibility of shielding anything from its effects imply that general relativity plays a fundamental role governing the structure of the universe. Clearly, numerical relativity has a natural place in efforts towards obtaining reliable models that can account for the observable universe. These models must be capable of describing from the strong-field behaviour at the big-bang epoch, include a possible inflation phase, accommodate for the standard model and the complex physics involved at shortly after the big bang and follow the evolution to the late-time phases corresponding to clusters of galaxies formation and large-scale mass fluctuations. Cosmological simulations enjoy the benefit of comparing the obtained predictions with observations, and will certainly play a fundamental role in our understanding of issues such as the existence of the cosmological constant, topology of the universe, initial singularity, gravitational wave interactions, the model of structure formation, etc. For a recent review of computational cosmology and the role of numerical relativity refer to [303].

9. Working together: complement with other approaches

In the description of binary systems, some distinct phases can be recognized. The first one, is an *adiabatic* or *inspiralling phase*, where the members of the binary orbit around each other while the separation between them slowly decreases as energy is carried away by gravitational radiation. This phase can be described by means of post-Newtonian [304, 305] or quasi-equilibrium [253, 256, 259, 260] methods. This phase ends at the innermost stable circular orbit and a second stage, known as, *plunge and merger phase* takes place in which a single merged object forms (a black hole or a neutron star). Here, numerical simulations appear to be the only way to obtain a complete description for generic situations. The final stage is the *ringdown phase* where the final object settles into equilibrium; perturbative methods (around the expected equilibrium scenario) can be used to describe the system.

Note that, since numerical relativity can in principle fully solve Einstein's equations, simulations could be used to model the *complete* problem (i.e. on all three phases). However, this is not feasible as the computational cost of such an enterprise would be tremendous. It is preferable to have the simulations concentrate on the plunge and merger phase and appropriately matching with the other two. Achieving this 'transition' is not a straightforward task; several questions have to be addressed for such a task.

Pre-merger

In the case of an inspiral phase treated with post-Newtonian approximations, the system is described in a 'point-particle' way and the main variables are the positions, velocities and angular momentum of these 'particles'. However, initial data for the second phase is the geometry of an initial slice which requires a proper 'translation'. For the particular case of non-spinning black holes, Alvi has presented [306] such a translation following the method of [307]. The metric presented in [306] is expressed in terms of a single coordinate system valid up to the apparent horizons of the black holes (in the co-rotating gauge suggested in [35]).

Whether this presentation is well suited for a numerical implementation is not known as it has not yet been implemented. Such an implementation will prove very valuable as it will shed light onto how the matching strategy should proceed.

In the case where the first stage is treated with quasi-equilibrium methods, there is no need for such a translation since it directly provides the metric variables. Some of the metric variables are obtained, as discussed, via a solution of the constraints while the others are provided by hand; the main difficulty of this method is to choose these accurately. So far, almost all methods have provided these assuming conformal flatness [253, 256, 259, 260] (the exception being [308], although still restrictions on the metric are imposed). Information obtained from post-Newtonian approximations should be exploited to provide more consistent data.

Post-merger

The interface with the third stage is certainly more direct as in both phases the geometry is evolved. The difficulty lies in recognizing the background spacetime with respect to which the perturbations are defined. For the case of black hole spacetimes, a useful notion is that of an *isolated horizon* [309] which can be used to provide a rigorous and unique way to determine the parameters describing the black hole. Another issue is that of gauge. Namely, the gauge employed during the numerical simulation need not coincide with that for the perturbative approach. In principle, several slices of the numerical simulation can be used to induce data on the initial hypersurface of the perturbative approach. This is not a trivial task, and will have to be analysed on a 'case-by-case' basis, since, although perturbative approaches have been formulated for a few well defined slicing conditions, numerical implementations will use different slices depending on the physical problem under consideration. Still, a number of scenarios will presumably be simulated and the time spent writing this module can certainly be worthwhile. Additionally, there is an extra 'added bonus' in handing the simulation to a perturbative approach (aside from saving computational costs). The total simulation length might be 'extended' since the full numerical implementation might suffer from instabilities generated by boundary conditions, or late-time exponential modes. If already a perturbative approach can be used where the quality of the simulations at intermediate times is reasonable, the simpler perturbative approach might be capable of producing longer total simulations. A recent work by Baker *et al* [310, 311] (the 'Lazarus approach') has actually shown this can be the case. Namely, they have used an ADM full 3D simulation (with maximal slicing) to model a binary black hole system. Initial data are defined with the Misner solution [176] from a fairly close separation. Although the full 3D simulation crashes a relatively short time after the holes have merged, the perturbative approach is able to continue the simulation for essentially unlimited times [311]. At least for this particular case, the combination of numerical relativity with a post-merger perturbative treatment, has simulated a binary black hole plunge all the way to the final equilibrium stage. Work is underway to study astrophysically relevant scenarios, match to codes using black hole excision, accommodate more generic slicing options, etc.

10. The future role of numerical relativity

As the field matures and enough computational resources become available, the role of numerical simulations in understanding the theory will become increasingly more important. It is hard to imagine all branches where it will be employed, but certainly in astrophysical systems, singularities, cosmology, global spacetime analysis and even quantum gravity.

In the particular case of astrophysical systems, it is worth noting that for decades progress towards achieving astrophysically relevant simulations have proceeded on two fronts. One front has concentrated efforts towards accurately evolving the geometric variables (either assuming vacuum spacetimes or treating the matter in an approximate way), with the other pursuing accurate simulations of the fluid variables (at the cost of treating problems where the geometry was considered fixed or where dynamical effects could be taken care of by pseudo-Newtonian approaches). Recently, these fronts have started converging with renewed hopes for complete studies of physical situations [42, 186, 187, 292] which will provide further insight into these systems. Still, present simulations do not incorporate a number of processes such as neutrino transport, magnetohydrodynamics, etc. Inclusion of these ingredients will greatly benefit from present simulations of systems obtained with Newtonian or pseudo-Newtonian models which have advanced the knowledge of how to accommodate for them (see, for instance, [294–296, 312–314]).

Black holes; neutron stars and beyond

Clearly, any system involving black holes or neutron stars can only be accurately studied by taking into account general relativity. In systems involving a single BH or NS with other much gravitationally weaker and smaller objects, the latter can be reasonably well represented by a point particle following a geodesic path on the spacetime defined by the BH or NS, see for instance [315, 316] (where the backreaction of the 'particle' is accounted for by prescriptions like those presented in [317, 318]) A very different treatment is needed if the system contains binaries (BH–BH; BH–NS; NS–NS) or if a single object is surrounded by a massive accretion disc. X-ray observations already predict a significant abundance of NS–NS and massive accretion discs and quite reasonable models predict a considerable number of BH–NS and BH–BH binaries [319, 320]. A complete study of these systems requires full 3D numerical simulations, which will not only provide important insights into their gravitational wave output but also on the equation of state (for the NS case); active galactic nuclei and quasars; formation of black holes; models of gamma-ray bursts (GRBs) and strong-field gravity.

These simulations must incorporate general relativity, neutrino processes, magnetohydrodynamics and nucleosynthesis and will certainly be quite a challenge for many years to come. However, their pay-off will make the effort very much worthwhile; among them are:

- *Gravitational waves:* prediction of the gravitational waves from these systems will enable one to decipher the information encoded in these waves and let us understand the source system. Masses, spins, equation of state, accretion rate, etc can be readily estimated from the detected waveforms (see, for instance, [321–325]).
- *Merger recoil estimation:* in the coalescence of these strong-field binaries a non-zero recoil will result from the linear momentum carried away by gravitational waves. This effect might be particularly relevant in the case of supermassive black holes believed to exist in most galaxies. When two galaxies collide (and present models predict those at $z \geqslant 3$ participated in a series of mergers! [326]); the non-zero recoil velocity could be large enough that the resulting hole will be dislodged from the centre of the merged galaxy. This effect would explain low-z quasars are asymmetrically located in their host galaxies. Even more spectacular, the recoil might be large enough to eject it out of the galaxy! [326]. Only through numerical simulations will this recoil be quantized.
- *Black hole birth description:* gamma-ray bursts are for a very short time the brightest objects in the universe (much more than the rest of the universe combined). This hints at extreme conditions causing them, and understanding these will tell us a great deal

about GR in strong-field cases. One model for GRBs is that they are produced when a massive disc ($0.1M_{\odot}$) is accreted onto a BH [327]. NS and NS–white dwarf binaries can yield precisely these kind of situations (as could BH systems), thus GRBs might also be signalling the birth of a black hole. Numerical simulations of these systems will provide the ultimate corroboration of this model.

- *Energetics of GRBs:* although the afterglow of GRBs is well described by current models [328]; these models overestimate the GRB energy [327]. Understanding this issue through numerical simulations will certainly be quite a challenge, but a computational approach might be the most reliable way to fully resolve it.

Naked singularities

Since the early attempts to produce naked spindle singularities by Shapiro and Teukolsky [241] an unresolved controversy has existed. On the one hand, analytical evidence against the formation of spindle singularities has been presented [329]. Additionally, it has been conjectured [330] that if this type of singularity could exist, it would disappear or become a black hole by the backreaction of the gravitational waves emitted at the formation of the singularity. On the other hand, numerical investigations [241, 331, 332] point towards their existence *assuming* that the failure to locate an apparent horizon is a good indicator. However, even Schwarzschild spacetime admits slicings without apparent horizons [51], Wald [333] suggests that the singularities found in these simulations are not naked and the apparent horizon has not yet appeared in the slicings considered. This tension can be resolved by further numerical studies, under different slicing conditions and by analysing the structure of the event horizons.

Quantum gravity?

Numerical relativity is making its first steps into the realm of string theory. Computational investigations of the AdS/CFT duality are underway which hopefully will contribute to the understanding of the subject [210]. Additionally, simulations about the stability of black strings are also being considered. As first noted by Gregory and Laflamme a notable difference of gravity in higher dimensions is that black holes are not stable [334]. By perturbative calculations, these authors showed that a 'black string' (the higher-dimensional analogue of a black hole) is not stable under perturbations. Due to their analysis being restricted to linearized perturbations, it was not clear what the 'final' fate of these perturbed black strings was. Recently, in the case where certain assumptions are satisfied, it has been shown that the horizon does not pinch off but rather it apparently settles into some new static black string solution [337]. On a separate treatment (one which does not require the assumptions in [337] to be satisfied but uses a Newtonian approach), it has been argued through a linear perturbation analysis and a Newtonian analysis that the final fate corresponds to a collapse of the spacetime in the string direction [338]. A full numerical solution could certainly shed light on this problem. Preliminary studies of this problem, under the assumption of spherical symmetry, are being carried out with a 2 + 1 code (i.e. radius and 'string' coordinate + time) and hopefully will report interesting results in the near future.

'Conjecture-testing'

Physical intuition has given rise to a number of conjectures, among them: cosmological censorship [168]; the 'Hoop' conjecture [335]; the Belinski–Khalatnikov–Lifschitz conjecture [278, 279]; the 'Shapiro conjecture' [336], etc which have proven very difficult to prove (or disprove). Numerical simulations can shed light on their validity; in particular, they have

already shown the possible existence of naked singularities [62] and Cauchy horizons being driven to true singularities [202].

Global spacetime structure

Numerical relativity can play an important role in global properties of spacetimes with isolated sources. Penrose's realization of asymptotically simple (AS) spacetimes, shows the relationship between Einstein's equations, geometric asymptotics, conformal geometry and the notion of isolated system [80]. In particular, the concept of asymptotically simplicity implies that the Weyl tensor displays a '*peeling behaviour*' of the Weyl curvature and since its introduction a recurrent issue in general relativity has been how general it is. A well known system displaying a peeling behaviour weaker than that implied by an AS spacetime is the 'perturbed' Minkowski spacetime studied by Christodoulou and Klainerman [220] (perhaps a restriction on the initial data considered in [220] might yield an AS spacetime). Numerical investigations might provide valuable indications on spacetime properties on the large scale; a rigorous analysis would demand being able to simulate the whole spacetime; at present, it appears that the conformal field (section 3.3) and Cauchy-characteristic matching approaches are best suited for such a task. Less ambitious estimates, but probably useful ones, can still be made with implementations in the 3 + 1 formulations by studying the fields in the far zone.

11. Conclusions

In the present review lack of space has prevented me from addressing every subject in detail; thus, I have intended this work to be an up-to-date 'tour' through the many aspects present in today's numerical relativity research. In some cases, I have chosen to briefly describe the goal and main aspects of: relativistic hydrodynamics [233]; computational cosmology [303]; singularity studies [277] and critical phenomena [282] and refer the reader to recent reviews on these subjects.

I have discussed the several 'flavours' presently found in numerical relativity. Both from their approach towards Einstein's equations and their numerical strategies to implement them. I have tried to emphasize the ideas, techniques and main problems together with the main accomplishments and outstanding problems which will keep everyone quite busy in the coming years. Yet, this list is by no means exhaustive, we still do not know what treasures have been kept hidden in the theory waiting for us to discover. Certainly, the road in front of us is not an easy one, but is likely to be one with exciting discoveries. As the (translated) words of Antonio Machado tell us: 'Traveller there are no paths, paths are made by walking'.

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