# Snowmass2021 Cosmic Frontier White Paper: Numerical relativity for next-generation gravitational-wave probes of fundamental physics

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#### Abstract

The next generation of gravitational-wave detectors, conceived to begin operations in the 2030s, will probe fundamental physics with exquisite sensitivity. These observations will measure the equation of state of dense nuclear matter in the most extreme environments in the universe, reveal with exquisite fidelity the nonlinear dynamics of warped spacetime, put general relativity to the strictest test, and perhaps use black holes as cosmic particle detectors. Achieving each of these goals will require a new generation of numerical relativity simulations that will run at scale on the supercomputers of the 2030s to achieve the necessary accuracy, which far exceeds the capabilities of numerical relativity and high-performance computing infrastructures available today.

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#### 8 List of Endorsers

# **1** Motivation

Gravitational waves are ripples of warped spacetime that travel at the speed of light. In 2015, a century after Einstein predicted their existence, the Laser Interferometer Gravitational-Wave Observatory (Advanced LIGO) discovered gravitational waves from a merging binary black hole as the waves passed through Earth [1]. Two years later, LIGO and Virgo observed gravitational waves from merging neutron stars [2], a collision also observed by telescopes spanning the electromagnetic spectrum [3]. These events, together with the dozens of gravitational waves that LIGO and Virgo have observed, have inaugurated the era of gravitational-wave astronomy [4–6].

The next generation of gravitational-wave detectors will use gravitational waves from sources throughout the cosmos to probe fundamental physics with unprecedented sensitivity, as discussed in a separate Snowmass White Paper [7]. Proposed detectors on Earth include LIGO Voyager [8], Cosmic Explorer [9], Einstein Telescope [10], and NEMO [11]; future ground-based gravitational-wave facilities are described in a separate Snowmass [12]. In space, the Laser Interferometer Space Antenna (LISA) [13], the DECi-hertz Interferometer Gravitational-wave Observatory (DE-CIGO) [14], and TianQin [15] will observe gravitational waves at frequencies too low to ever detect on Earth because they would be obscured by seismic noise.

Next-generation gravitational-wave detectors are anticipated to begin observations in the 2030s. Their observations of coalescing binary neutron stars and black-hole/neutron-star binaries will measure the equation of state of dense nuclear matter in the most extreme environments in the universe, and their observations of gravitational waves from merging black holes—which contain the strongest spacetime curvature in the universe—will put general relativity to the strictest tests. These future gravitational-wave detectors might also enable observations that use black holes as cosmic particle detectors, potentially giving new, complementary insight into the nature of dark matter.

Accurate theoretical models of gravitational waves are critical for interpreting gravitationalwave observations—specifically, for inferring the nature and behavior of their sources. Long before the time of coalescence, the gravitational waves from merging black holes and neutron stars can be well modeled using the post-Newtonian approximation, which approximates general relativity in the limit of weak gravity and small velocities. Long after the time of coalescence, the gravitational waves from a black hole remnant resulting from merging black holes and neutron stars can be well approximated using perturbation theory. But near the time of coalescence, when the spacetime curvature and (if present) neutron-star matter are the most nonlinear and dynamic, all known analytic approximations break down: the emitted gravitational waves and the strong-gravity dynamics of their source can only be calculated with numerical relativity.

Numerical relativity amounts to numerically solving the equations of general relativity or, for simulations involving neutron stars, the equations of general relativistic radiation magnetohydrodynamics (fluid dynamics, magnetic fields, and radiation transport); the techniques of numerical relativity are reviewed, e.g., in Refs. [16–20], and briefly discussed in Sec. 2. Numerical-relativity calculations are technically challenging, in part because the equations are strongly nonlinear and, in the presence of neutron-star matter, because the solutions contain small scale features that are especially challenging to resolve, such as shocks, neutron-star surfaces, and turbulence. These cal-

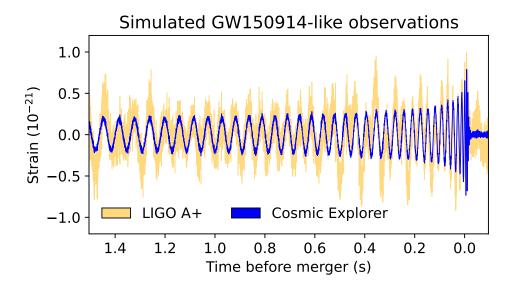


Figure 1: Simulated gravitational-wave detector strain measurements of gravitational waves from two merging black holes. The signal is similar to GW150914 [1], the first directly detected gravitational waves. The strain is shown as a function of time for the signal superimposed on both simulated Cosmic Explorer noise (blue) and simulated LIGO A+ noise (yellow). Taken from Fig. 5.2 of Ref. [21].

culations are also computationally expensive, requiring high-performance computing to achieve the necessary accuracy.

How much accuracy is enough? The answer depends on the signal-to-noise ratio of an observation: roughly speaking, avoiding any bias in gravitational-wave interpretation requires numerical uncertainties smaller than the observation's measurement uncertainty. The observations with the most potential to reveal new fundamental physics are those with the highest signal-to-noise ratios precisely those observations that demand the most accuracy from numerical-relativity models. And the observations with the highest signal-to-noise ratios will come from next-generation detectors: their loudest observations will have signal-to-noise ratios in the thousands, more than an order of magnitude beyond the strongest signals observed to date. Figure 1 illustrates this gain in sensitivity by showing two simulated gravitational-wave detections of the same gravitational-wave source, one using an upgraded LIGO detector, and the other using Cosmic Explorer, a next-generation detector.

Extracting information from such high-fidelity signals while limiting systematic biases will require models with an order of magnitude increase in accuracy over today's state of the art. Achieving this accuracy will require a new generation of numerical-relativity software, designed to run at scale on the exascale supercomputers that will be available in the 2030s. New (typically opensource) numerical-relativity codes under development today will help meet this goal by producing publicly available catalogs of simulated gravitational waveforms for coalescing compact binaries (i.e., binary black holes, binary neutron stars, and black-hole/neutron-star binaries).

The rest of this whitepaper is organized as follows. Sec. 2 briefly summarizes the methods of gravitational waveform modeling, especially numerical relativity. Then, Sec. 3 discusses progress and challenges in applying numerical relativity to probe nuclear physics and the nature of neutron

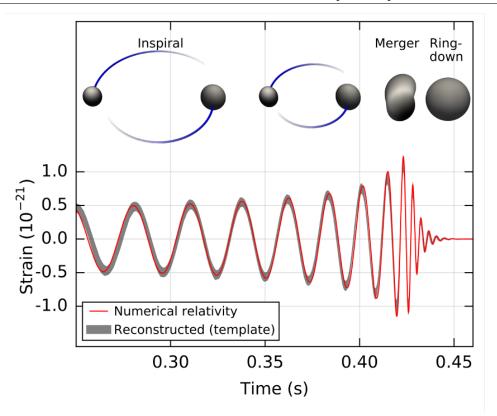


Figure 2: Numerical relativity waveform modeling GW150914, the first gravitational wave signal detected by LIGO. The inset shows the black holes' horizons during the inspiral, merger and ringdown. Taken from Fig. 2 of Ref. [1].

stars. Sec. 4 explains in more quantitative detail the challenge that high-precision gravitationalwave observations pose to numerical-relativity waveform modeling. In Sec. 5, we discuss the importance of numerical-relativity waveform modeling in using gravitational-wave observations to seek physics beyond general relativity, and in Sec. 6 we discuss numerical relativity's role in the possibility of using black holes as cosmic particle detectors. Finally, in Sec. 7 we present a brief summary and discuss the future work needed to fully realize the potential of gravitational waves as probes of fundamental physics.

# 2 Gravitational waveform modeling

A gravitational wave signal encodes vital information about its sources, such as the masses and spins of the companions in a compact binary, the equation of state of dense matter if one of them is a neutron star, and the underlying theory of gravity. These parameters are identified by using matched filtering techniques, in which the observed signal is compared against a catalog of theoretical gravitational waveform models, called templates. The templates need to accurately cover the different phases of a binary's evolution consisting of the inspiral, merger and ringdown illustrated in Fig. 2.

Models of a binary's evolution typically rely on two core methods: (i) approximations, such

as Post-Newtonian (PN) or Post-Minkowskian expansions, that are suitable for modeling the early inspiral of a compact binary using a weak-field and small velocity expansion; and (ii) numerical relativity, which numerically calculates a binary's late inspiral, merger and ringdown by solving Einstein's equations (or extensions of them) in the nonlinear regime. Both core methods feed into the production of full inspiral-merger-ringdown templates using either phenomenological models that directly combine PN and numerical relativity waveforms (e.g. [22]), effective-one-body models (e.g. [23]) that are a resummation of the PN expansion and are calibrated against numerical relativity, or surrogate models (e.g. [24]) that directly interpolate numerical-relativity waveforms. To ensure that the gravitational-wave interpretation is not limited by modeling errors, even as future gravitational wave detectors achieve ten to hundred times better sensitivity than today's detectors, highly accurate waveform templates are crucial. In this white paper, new advances and challenges in numerical relativity are discussed, while new developments in using scattering amplitudes and effective field theory for gravitational-wave modeling are presented in a separate Snowmass White Paper [25]. A more extensive review on waveform modeling for future gravitational wave detectors can be found in the LISA Waveform Working Group White Paper [26].

Before outlining new physical applications and computational challenges below, we here give a brief summary of the current status of numerical relativity. Numerical relativity refers to solving Einstein's equations, or extensions of them, possibly coupled to matter or additional fundamental fields, in four spacetime dimensions. This typically requires high-performance computing, because the equations form a system of more than ten coupled, nonlinear, partial differential equations (PDEs) of mixed character. By applying a spacetime decomposition into three dimensional, spatial hypersurfaces that are then propagated in time, the equations can be formulated as a time-evolution problem, subject to a set of constraints. Using this approach, a numerical-relativity calculation is divided into three stages:

- 1. Construction of initial data that represents the initial configuration (e.g., two compact objects orbiting each other in equilibrium). This requires solving the constraint equations, a set of coupled, elliptic-type PDEs in three dimensions. The bulk of contemporary numerical relativity software uses either the Bowen-York conformal approach or the conformal thin-sandwich method.
- 2. Time evolution, i.e., a binary's development in time that is encoded in a set of coupled, hyperbolic-type PDEs and must be complemented by suitable gauge conditions. The majority of the numerical relativity codes uses either a variant of the generalized harmonic formulation of Einstein's equations together with the damped harmonic gauge [27–29] or a variant of the Z4 [30–34] or Baumgarte-Shapiro-Shibata-Nakumara (BSSN) formulations [35, 36] that are complemented by the moving puncture approach [37, 38].
- 3. Extraction of physical information such as the gravitational and additional radiation or, in case of black hole spacetimes, the apparent horizons. Note that for modeling observations in distant gravitational-wave detectors, the gravitational radiation must be propagated to future null infinity (see Ref. [39] for a review), either by extrapolation [40], by evolving it, e.g. Cauchy-Characteristic Evolution (CCE) [41], or through perturbative techniques [42], and gauge conditions and transformations at future null infinity must be treated with care to yield well-behaved numerical waveforms.

Since the breakthroughs in numerical relativity in 2005 [27] and 2006 [37, 38], that saw the

Code	Open Source	Catalog	Formulation	Hydro	Beyond GR
AMSS-NCKU [43–46]	Yes	No	BSSN/Z4c	No	Yes
BAM [47–49]	No	[18]	BSSN/Z4c	Yes	No
BAMPS [50, 51]	No	No	GHG	Yes	No
COFFEE[52, 53]	Yes	No	GCFE	No	Yes
Dendro-GR [54–56]	Yes	No	BSSN/CCZ4	No	Yes
Einstein Toolkit [57, 58]	Yes	No	BSSN/Z4c	Yes	Yes
*Canuda [59–62]	Yes	No	BSSN	No	Yes
*IllinoisGRMHD [63]	Yes	No	BSSN	Yes	No
*LazEv [37, 64]	No	[65–68]	BSSN+CCZ4	No	No
*Lean [69, 70]	Partially	No	BSSN	No	Yes
*MAYA [71]	No	[71]	BSSN	No	Yes
*NRPy+ [72]	Yes	No	BSSN	Yes	No
*SphericalNR [73, 74]	No	No	spherical BSSN	Yes	No
*THC [75–77]	Yes	[18]	BSSN/Z4c	Yes	No
ExaHyPE [78]	Yes	No	CCZ4	Yes	No
FIL[79]	No	No	BSSN/Z4c/CCZ4	Yes	No
FUKA [80, 81]	Yes	No	XCTS	Yes	No
GR-Athena++ [82]	Yes	No	Z4c	Yes	No
GRChombo [83–85]	Yes	No	BSSN+CCZ4	No	Yes
HAD [86–88]	No	No	CCZ4	Yes	Yes
Illinois GRMHD [89, 90]	No	Yes	BSSN	Yes	No
MANGA/NRPy+ [91]	Partially	No	BSSN	Yes	No
MHDuet [92, 93]	No	No	CCZ4	Yes	Yes
SACRA-MPI [94]	No		BSSN+Z4c	Yes	No
SpEC [95, 96]	No	[96, 97]	GHG	Yes	Yes
SpECTRE [98, 99]	Yes	No	GHG	Yes	No
SPHINCS_BSSN [100]		No	BSSN	SPH	No

Table 1: List of numerical relativity codes. We indicate if a code is open-source, if it has been used to produce gravitational waveform catalogs, the formulation of Einstein's equation used (GHG: generalized harmonic, BSSN: Baumgarte-Shapiro-Shibata-Nakamura, CCZ4 / Z4c variants of the Z4 formulation, GCFE: generalised conformal field equations ), if a code implements general relativistic hydrodynamics, and if it is capable to simulate compact binaries beyond general relativity. An asterisk indicates codes that are either (partially) based on the open-source Einstein Toolkit or are co-funded by its grant. Credit: Deidre Shoemaker; taken from Ref. [26].

very first simulations of the last orbits of a black hole binary and its merger, the field has matured into a state-of-the-art tool to investigate extreme gravity. A large variety of numerical relativity cyberinfrastructures for computational astrophysics is available. In Table 1, we present a list of currently available numerical-relativity software, indicating for each if it is open-source, the formulation of Einstein's equations used, if it is capable of performing general relativistic hydrodynamics simulations (and not just vacuum simulations), and if it is capable to perform simulations in alternative theories of gravity. This list is adapted from the LISA Waveform Working Group White Paper [26].

A number of the numerical relativity codes (collaborations) have constructed catalogs of simulated gravitational waveforms as indicated in Table 1. For black-hole binaries, the combined catalogs contain more than 5,700 waveforms that cover mass ratios  $q = m_1/m_2 = 1, ..., 15$  up to q = 128, where  $m_1$  ( $m_2$ ) is the mass of the heavier (lighter) black hole, and spins magnitudes up to 0.998 [65–68, 71, 96, 101, 102]. There are also the first numerical relativity waveform catalogs for binary neutron stars [18], and a recent study [103] used head-on collisions (in which the black holes begin at rest) to demonstrate that numerical-relativity techniques can in principle model gravitational-wave emission at mass ratios as high as 1000.

Given the wealth of available simulations, what future development is needed? The answer is two-fold and concerns the waveform accuracy as well as the physics included in the models. Each of these items will be discussed in detail in the following sections.

### **3** Nuclear physics and neutron stars

When two neutron stars, or a black hole and a neutron star, coalesce, they emit gravitational waves that encode the behavior of the densest matter in the universe. The cold cores of neutron stars are expected to have densities  $\rho \sim 10^{15} \,\mathrm{g/cm^3}$ . In that regime, the strength of nuclear interactions between densely packed particles is uncertain, and even the composition of the core is unknown. The properties of dense matter are however tightly correlated with the size of neutron stars, their maximum mass, and their response to external gravitational fields. Dense matter's presence in a merging binary, as a finite size object distorted by the gravitational field of its companion, leads to more gravitational wave emission than for black hole binaries and a faster evolution towards merger [104–111]. The size of a neutron star also determines if and when it can be tidally disrupted by a black hole companion (for black hole-neutron star binaries) and when two neutron stars collide and merge (for neutron star-neutron star binaries) [112–115]. Finally, the post-merger evolution of a neutron star-neutron star binary is strongly impacted by the properties of dense matter: unknown nuclear physics determines whether the remnant collapses to a black hole, as well as the frequency of post-merger gravitational waves driven by oscillations in the remnant [116–132]. Recovering this information from gravitational-wave observations requires an accurate theoretical understanding of the emitted waves and thus high-accuracy numerical relativity simulations.

These simulations are challenging and expensive, yet they must be sufficiently accurate to avoid introducing systematic biases into the interpretation of gravitational-wave observations. The accuracy required (cf. Sec. 4) increases with the square of the observation's signal-to-noise ratio [133]. The first (and loudest) gravitational wave observation from coalescing binary neutron stars to date, GW170817 [2], had a signal-to-noise ratio (SNR)  $\sim 30$ . Recent studies [134–136] find that systematic uncertainties from inaccurate waveform models would be substantial at SNRs  $\gtrsim 70$ ,

which could be achieved if a signal as loud as GW170817 were observed in current-generation detectors when they achieve their design sensitivities. The tremendous sensitivity gains that future gravitational-wave detector concepts [8–10] would achieve means that they would observe a GW170817-like signal with an SNR in the thousands [137], requiring vastly more accurate theoretical waveform models.

Simulations modeling the tidal response of the neutron stars during the last stages of the inspiral need to decrease their phase errors by more than two orders of magnitude. With current simulation technology, this is expected to require the grid resolution to be decreased by at least a factor 10 compared to the highest resolution simulations available to date [138, 139] (assuming second order convergence), leading to a  $\sim 10^4$  increase in computational cost. Even if numerical relativity codes could scale efficiently to millions of CPU cores, a single simulation would still require several years to complete and tens of billions of CPU hours.

Neutron star mergers also power bright electromagnetic counterparts that carry additional information about the merging objects, including the properties of dense matter. Neutron-rich matter ejected during and after merger undergoes r-process nucleosynthesis, making neutron star mergers one of the lead candidates for the production site of r-process elements [140]. The radioactive decay of the ashes of the r-process powers *kilonovae*, UV/optical/infrared transients observable days to weeks after the merger [141–143]. Some neutron star mergers also result in the formation of massive accretion disks around a compact object that power narrow jets of highly-relativistic material observed from Earth as *short gamma-ray bursts* [144–146]. Both types of signals were observed following the first neutron star mergers detection (GW170817) [147]. Numerical simulations are required to understand which mergers power electromagnetic signals and to connect the observable properties of these signals to the properties of the merging compact objects and to the equation of state of dense matter.

Simulations aiming to model the post-merger gravitational wave signal of neutron star binaries and to study their electromagnetic counterparts face the additional challenge of having to resolve high Reynolds number magneto-hydrodynamics turbulence and to model complex neutrinoradiation effects, which might impact the postmerger gravitational wave signal and will certainly impact the electromagnetic counterparts and nucleosynthesis yields of these events [125]. Extremely strong magnetic fields ( $\sim 10^{16}$  G) are likely grown from small scale magneto-hydrodynamics instabilities in neutron star mergers, and even the highest resolution simulations performed to date (with grid spacing an order of magnitude smaller than what is typically affordable with current codes) have not been able to converge to a well-defined answer for the post-merger magnetic field [148]. As magnetic fields are likely a crucial ingredient in the production of short gamma-ray bursts [149-151] and in the ejection of the material producing r-process elements and kilonovae [151, 152], this represents a major limitation in our ability to model these systems. Neutrinomatter interactions are less important to the dynamics of the post-merger remnant, but they play a major role in setting the composition (neutron-richness) of matter outflows, which largely determines the outcome of r-process nucleosynthesis [153]. Properly including all relevant neutrino processes is a daunting challenge. At the very least, we will need to solve the 7-dimensional transport equations; but even that may not be enough. For example, neutrino oscillations due to fast-flavor instabilities may significantly impact the composition of matter outflows [154] and can only be captured by evolving the quantum kinetics equations with grid resolution orders of magnitude smaller than what is used in merger simulations.

A direct approach using current codes and numerical methods cannot be successful. Instead,

the numerical relativity community will need to develop more accurate numerical schemes to model tidally interacting neutron stars, sophisticated algorithms for neutrino-radiation hydrodynamics, and subgrid turbulence models. First steps in these directions have been made [76, 98, 155–157], but significant more work needs to be done in preparation for next-generation gravitational wave experiments. Several next-generation numerical relativity code are currently in development, employing novel methods that will enable high accuracy and performance on the supercomputers that will be available in the next decade (e.g. [82, 98, 155]), but none of them have yet matured to the point where they can calculate gravitational waves or electromagnetic signals from merging neutron-star binaries.

### 4 Modeling high-precision gravitational-wave observations

The next generation of gravitational-wave detectors on Earth and in space will yield observations of coalescing binary black holes with signal-to-noise ratios in the thousands, enabling high-fidelity observation of the behavior of the curved spacetime near stellar-mass black-hole horizons, the most strongly curved spacetime known. Gravitational wave signals will be so plentiful they will sometimes overlap.

As they have for current observations [2, 158, 159], numerical-relativity simulations will play crucial roles in the detection and interpretation of gravitational waves from merging black holes and neutron stars. In particular, waveforms from these simulations have been used to construct and validate approximate, phenomenological models necessary for interpreting observations (since numerical relativity is too costly to produce every model waveform needed) [158, 160–164], have featured in direct analysis of observations [165], and have helped validate our methods for detecting faint gravitational waves in detector data [166].

But to model high-precision observations, numerical-relativity calculations will have to be significantly more accurate than today's state of the art. Qualitatively, the increase in accuracy is necessary to ensure that numerical errors are smaller than experimental uncertainty given the much lower noise level that next-generation gravitational-wave detectors will achieve (cf. Fig. 3). Section 4 of Ref. [96] gives a quantitative estimate of how much the accuracy must improve in terms of the improvement in signal to noise ratio, based on a sufficient condition [133, 167–169] for a model waveform and an observed gravitational waveform to be indistinguishable. Specifically, two gravitational waveforms are indistinguishable if their mismatch  $\mathcal{M}$  (a noise-weighted inner product, defined, e.g., by Eq. (24) of Ref. [96]) is no larger than an amount proportional to the inverse square of the signal-to-noise ratio  $\rho: \mathcal{M} < D/(2\rho^2)$ , where D is a constant that depends on the number of parameters needed to specify the gravitational waveform (e.g., in Ref. [96], for binary-black-hole waveforms, D = 8). Thus the accuracy required scales as the square of the signal-to-noise ratio  $\rho$ .

With today's detectors, the loudest gravitational waves from binary black holes have  $\rho \sim 24$ , whereas future detectors will observe binary black holes with  $\rho$  in the thousands. The estimate in the previous paragraph suggests that future detectors will demand more than an order of magnitude more accuracy from numerical-relativity codes, even for modeling binary black holes (a less challenging case than the case of simulations involving dense matter, cf. Sec. 3). Studies using more sophisticated variants of the estimate sketched in the previous paragraph [170, 171] give comparable conclusions: numerical-relativity waveforms will need to be significantly more sensitive to

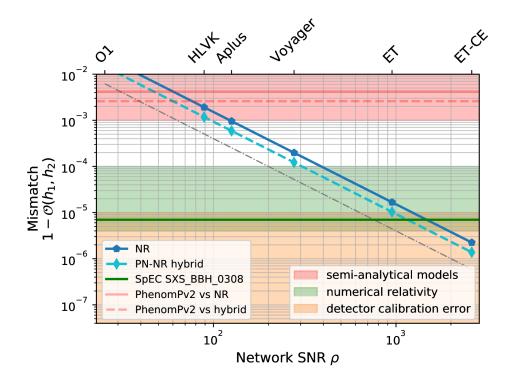


Figure 3: Predicted waveform accuracy for current second generation and future third generation detectors. The mismatch between the waveform models is shown as a function of the detector signal-to-noise ratio (SNR). Solid lines indicate results for pure numerical-relativity simulated signals, while dashed lines come from numerical-relativity signals extended ("hybridized") with post-Newtonian (PN) waveforms in the inspiral. The blue lines and data points show how the mismatch falls with rising SNR. Horizontal red lines show the mismatch of the signal against the IMRPhenomPv2 phenomenological template waveform at the signal parameters for LIGO's design sensitivity. Taken from Fig. 2 of Ref. [170].

avoid introducing bias into interpretation of high-precision gravitational-wave observations.

## **5** Testing gravity in the nonlinear regime

A consistent theory of quantum gravity is a major goal of modern physics. General relativity (GR) itself is not consistent with quantum mechanics, because it breaks down at high-energy scales: it is non-renormalizable and exhibits physical singularities, such as those inside black holes and at the big bang. Candidate quantum-gravity theories include well-motivated extensions of GR, typically involving additional fields, higher curvature corrections, or symmetry breaking [172–176].

Studies focusing on the formation or evolution of single black holes were considered in Lorentzviolating theories [177, 178], massive gravity [179–184], quadratic gravity [185–194], or higher curvature effective theories [195]. These have shown that black holes may develop scalar hair during their collapse, e.g., if described in quadratic and higher derivative gravity. In contrast, in scalar-tensor theories it is neutron stars that can develop a scalar hair, while black holes may remain the same as their general-relativistic counterparts. Given the extended phase-space of allowed, possibly hairy solutions one might expect new signatures during the inspiral, merger and ringdown such as additional (scalar) radiation channels, a phase-shift of the gravitational wave emission as compared to the GR signal or new nonlinear effects during the merger.

The nonlinear regime of gravity that unfolds during the collision of compact objects is a particularly promising target to probe for extensions of GR, both because new phenomena are expected to be most prominent in that case [196] and because candidate theories can be confronted with gravitational-wave observations [172, 175, 197–199]. However, current gravitational-wave based tests of gravity have either been limited to the weak-field regime or to null-tests against GR, because complete inspiral-merger-ringdown waveform models that capture these truly nonlinear beyond-GR effects are lacking. Numerical relativity has produced first proof-of-principle simulations beyond GR in scalar-tensor theories [70, 200–203], Einstein-Maxwell-Dilaton models [204, 205], cubic Horndeski theories [206], effect field theories for dark energy, namely kessence [207–209], dynamical Chern-Simons gravity [210–212], or scalar Gauss-Bonnet gravity [62, 213–216]. A second body of work has studied the nonlinear dynamics of black-hole mimickers such as boson stars [217–227]. The effect of fluctuations near black holes' horizons, mimicking for example microstate geometries, was modelled in Ref. [228].

An important difficulty when attempting simulations of binary mergers in beyond-GR theories is to devise mathematically well-posed and numerically stable formulations of the evolution equations. The development of formulations of Einstein's equations amenable to numerical simulations took decades to come to fruition [27, 35, 36, 229–231], and repeating that work for every possible theory of gravity beyond general relativity is a daunting task. For Brans-Dicke type scalar tensor theories it was proven that the resulting time evolution equations are indeed well-posed [232]. More general scalar tensor theories of the Horndeski class can be cast in well-posed form if they are complemented with a modified generalized harmonic gauge as long as coupling parameters remain small [233]. Other theories for which hyperbolic formulations are available include f(R)gravity [234], or Einstein-Aether theory [235]. On the other hand, there are a number of gravity theories that involve higher derivative terms that lead to (Ostrogradski) ghost instabilities and ill-posed evolution equations if they are treated as a complete theory. For example, this has been shown for dynamical Chern-Simons gravity, and one "cure" is to treat it as an effective field theory [236]. Another remedy, proposed in Refs. [237, 238], and tested for a sixth-order model in [239], is a reformulation of the evolution equations in the spirit of Israel-Stewart theory for hydrodynamics.

Therefore, existing beyond-GR simulations have so far mainly focused on theories that can be recast as the evolution of a scalar or vector field coupled to the usual equations of general relativity (scalar-tensor, Maxwell-dilaton, boson stars), or on treating beyond-GR effects perturbatively [62, 210, 212–214]. That said, the calculations in the decoupling limit have already identified new dynamical effects that have been missed with weak-field approximations. This includes burst of scalar radiation during the merger of black holes in dynamical Chern-Simons gravity [210] or dynamical scalarization and descalarization of black holes in scalar Gauss-Bonnet gravity [214]. The gravitational waveform typically exhibits a phase-shift, compared to the vacuum GR case, due to additional radiation channels [62, 213, 216].

Enabling high precision tests of gravity and searches for signatures of new physics will likely require innovative theoretical avenues to devise well-posed formulations of beyond-GR theories, and their application to creating high-precision catalogs of simulated waveforms.

#### 6 Black holes as cosmic particle detectors

Although dark matter makes up more than 80% of all matter in the universe, its nature, composition and properties have remained elusive. Black holes might shed light on the dark matter question and also ultralight beyond-standard model particles in general. Massive bosonic fields scattering off rotating black holes might form condensates around them if the fields' Compton wavelength is comparable to the black holes' size [240–242]. That is, astrophysical black holes in the mass range  $5M_{\odot} \dots 10^{10}M_{\odot}$  are sensitive to ultralight particles in the mass range  $10^{-21}$ eV  $\dots 10^{-8}$ eV [240, 241, 243]. This range includes popular dark matter candidates [244], the QCD axion [245] and axion-like particles of the string axiverse [246], as well as higher-spin fields such as vector fields [61, 243, 247–251] or massive spin-2 fields [252]; see also the companion Snowmass White Paper [7].

Because the underlying phenomenon of black hole superradiance only relies on gravitational interactions, it facilitates searches for new particles independently from their specific coupling to the standard model and thus complements traditional collider physics or direct detection experiments. The single black hole scenario has been studied extensively, and there are first computations of binary black-hole systems in the weak-field regime [253–255], for extreme mass ratio inspirals [256–258] and in the fully nonlinear regime modeling the last orbit before merger, the merger and ringdown [259]. How these light fields impact the nonlinear dynamics of the late inspiral and coalescence of black-hole binaries endowed with scalar condensates and what its observational signatures are remain open questions. Addressing them will enable gravitational-wave based searches for new particles but will require significant advances in numerical relativity.

# 7 Summary and future directions

The next generation of gravitational-wave detectors will probe fundamental physics with exquisite sensitivity. Observations with far higher signal-to-noise ratios than the loudest gravitational waves

observed to date will use neutron-star mergers to probe the nuclear physics of dense matter, use the loudest observations of binary black holes to seek physics beyond general relativity, and will perhaps enable a search for new particles that complements existing experimental searches.

Realizing these goals will require model waveforms that will rely on a new generation of numerical-relativity codes capable of achieving dramatically improved accuracy. These codes will need to use novel techniques (such as task-based parallelism) that enable them to scale to make effective use of the exascale computing resources expected to be available in the coming decade. Active development of such codes is already underway. Examples of next-generation numerical-relativity codes include NMesh [260], Dendro-GR [54], GR-Athena++ [82], bamps [50], GR-Chombo [83, 84] and SpECTRE [261].

Future studies will need to determine (more precisely than estimates such as in Refs. [170, 171]) how the challenges of extremely high signal-to-noise ratios and overlapping signals will impact the accuracy required to prevent numerical-relativity simulations from biasing the interpretation of next-generation gravitational-wave observations. One approach to such a study would be to use numerical-relativity simulations to create simulated gravitational-wave detections and then checking how much inaccuracies in model waveforms used to interpret those signals bias the inferred properties.

These calculations will require significant computational resources to complete. A typical numerical-relativity model waveform today typically require weeks to months of runtime on tens to thousands of compute cores. Future waveforms will require additional computational cost, in part because of higher accuracy requirements (which will require higher resolution) and in part because future detectors will have more sensitivity at lower frequencies, so that simulations will have to be much longer to span the detectors' sensitive frequency spaces. And many simulations will be necessary to span the parameter space of potential signals. Binary-black-hole waveforms, for instance, are characterized by at least 7 parameters (the mass ratio and the black-hole spin angular momenta); even spanning this space requires thousands of simulations (for instance, choosing 3 distinct possible values for each parameter would yield  $3^7 \approx 2,000$  simulations). Simulations involving neutron stars depend on even more parameters, including the parameters characterizing the (not yet well understood) neutron-star matter's equation of state. Simulations in theories beyond general relativity also introduce additional parameters.

By meeting the challenges ahead, numerical relativity will play a crucial role in realizing the science goals of future gravitational-wave observatories, by enabling accurate, unbiased interpretations of their high-fidelity observations.

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