# White Paper: “Mathematical and Computational Challenges in the Era of Gravitational-wave Astronomy” (IPAM Long Program, Fall 2021)

S. Albanesi
*Dipartimento di Fisica, Università di Torino, and INFN Sezione di Torino, via P. Giuria 1, 10125 Torino, Italy*

M. Berbel and S. Serna
*Departament de Matemàtiques, Universitat Autònoma de Barcelona, 08193 Bellaterra, Spain*

P. Cameron
*Department of Applied Mathematics and Theoretical Physics,*
*University of Cambridge, Wilberforce Road, Cambridge CB3 0WA, UK*

M. Cavaglià, R. Quitzow-James, and Y. Zheng
*Institute of Multi-messenger Astrophysics and Cosmology, Physics Department,*
*Missouri University of Science and Technology, Rolla, MO 65409, USA*

C.K. Chien
*Department of Mathematics, University of Washington, Seattle, WA 98195, USA*

J.A. Font
*Departament d’Astronomia i Astrofísica, Universitat de València,*
*Dr. Moliner 50, 46100, Burjassot (València), Spain*
*Observatori Astronòmic, Universitat de València,*
*Catedrático José Beltrán 2, 46980, Paterna (València), Spain*

F. Di Giovanni, D. Guerra, and M. Miravet-Tenés
*Departament d’Astronomia i Astrofísica, Universitat de València,*
*Dr. Moliner 50, 46100, Burjassot (València), Spain*

C-Y Kao
*Department of Mathematical Sciences, Claremont McKenna College,*
*850 Columbia Ave, Claremont, CA 91711, USA*

Y-H Kung
*Physics Division, National Center for Theoretical Sciences, Taipei 10617, Taiwan*

L. Magaña Zertuche
*Department of Physics and Astronomy, University of Mississippi, University, MS 38655-1848, USA*

A. Marquina
*Departamento de Matemáticas, Universitat de València,*
*Dr. Moliner 50, 46100, Burjassot (València), Spain*

M. Sakellariadou
*Department of Physics, King’s College London, University of London, Strand London WC2R 2LS, UK*

J. Teixeira
*Mullard Space Science Laboratory, University College London, Holmbury St Mary, Surrey RH5 6NT, UK*

D. Tseneklidou
*Theoretical Astrophysics, Eberhard-Karls University of Tübingen, Tübingen 72076, Germany*

G. Uhlmann
*Department of Mathematics, University of Washington, Seattle, WA 98195, USA*
*Institute for Advanced Study of HKUST*

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## I. EXECUTIVE SUMMARY

This document summarizes the activities and outcomes of the long program “Mathematical and Computational Challenges in the Era of Gravitational-wave Astronomy” which was held at the Institute of Pure and Applied Mathematics (IPAM) from September 12 to December 17, 2021. It also briefly explores some of the current open questions and future directions in the field of gravitational-wave (GW) astronomy and related fields that were discussed during the program.

On September 14, 2015, a worldwide effort of countless of scientists that had started one hundred years earlier with Einstein’s formulation of the Theory of General Relativity (GR) came to a climax with the LIGO and Virgo’s historic detection of GWs from a pair of colliding black holes (BHs) [1]. GWs are dynamical changes in the curvature of spacetime. Their astrophysical and cosmological sources are cataclysmic events, such as coalescing binary systems of BHs and supernovae explosions. Less than two years after the first detection, LIGO and Virgo observed GWs from a pair of neutron stars (NSs), ushering a new era of multi-messenger astrophysics (MMA) [2]. The most recent LIGO-Virgo-KAGRA (LVK) GW transient catalog [3] includes a total of 90 detections of compact binary coalescences (CBCs). These observations provide physicists with a plethora of new physical information, from testing GR in the strong field regime to using new ways of measuring the expansion of the universe to exploring the properties and dynamics of matter in extreme densities.

Because of the extreme sensitivity of the detectors and the complexity of the physics involved, the extraction of physical information from the data is very challenging. The process that leads from signal detection to their physical interpretation requires a synergy of expertise encompassing instrumental science, mathematics, fundamental physics, astrophysics, and computer science.

Construction of accurate theoretical models is one of the main requirements to identify and interpret the observed GW signals. This involves a deep mathematical knowledge and a synergy between analytic and numerical techniques to solve the field equations of GR. In the presence of matter, such as in NSs, GR must be combined with additional physics, such as magnetohydrodynamics (MHD).

Confident detection of GW signals and the extraction of their physical information are computationally intensive. Therefore, the development of fast and robust tools to increase the speed of these processes is crucial for the GW community and bound to become even more critical as the sensitivity of current detectors improves and next-generation detectors come online.

Machine learning (ML) is a common tool for all these topics.

The aim of this IPAM long program was to connect these many facets of GW science and MMA by bringing together some of the foremost mathematicians, physicists and computer scientists working in the GW community. The program was designed with a structure mimicking the complex process that leads from first mathematical principles in GR to the physical interpretation of GW observations. Thus the program consisted of four workshops (WSs), each addressing one of the main aspects of the GW science:

- WS I “Computational Challenges in Multi-Messenger Astrophysics” focused on the physics of source dynamics of future detections of GW signals and the generation of accurate GW templates.
- WS II “Mathematical and Numerical Aspects of Gravitation” focused on the mathematics of the equations governing relativistic systems.
- WS III “Source Inference and Parameter Estimation in Gravitational-Wave Astronomy” focused on current, state-of-the-art approaches for parameter estimation in MMA.
- WS IV “Big Data in Multi-Messenger Astrophysics” focused on the development of ML techniques for a more efficient handling of GW data sets, reduction of detector noise, identification of astrophysical signals, and increase in detection confidence.

Given the interconnection between the topics covered in the four WSs, this document has been organized into the following sections: Mathematics of spacetime, numerical relativity (NR), GW data analysis, and physical interpretation of GW observations.

## II. MATHEMATICS OF SPACETIME

GR has so far proved to be a successful theory. In 2020, Penrose shared the Nobel Prize for his prediction that BHs occur generically in nature, as has been observed in a number of experiments. But despite the successes of GR, there are still a number of important aspects that are not fully understood. Topics such as BH stability, cosmic censorship, inverse problems, gluing and memory were discussed in WS II: “Mathematical and Numerical Aspects of Gravitation”.

One of the unresolved issues in the mathematical theory of GR is the question of stability of BHs. WS II featured a presentation on the recent work of Hintz and Vasy in which they prove the global nonlinear stability of slowly rotating Kerr-de Sitter BHs. If one perturbs such a BH, it will settle down to a BH of the same type, emitting GWs in the process. A potential application of this is the determination of properties of BHs by the measurement of GWs. The result of Hintz and Vasy assumes a positive cosmological constant. The case of negative cosmological constant was also considered. It was shown that there are arbitrarily small perturbations to the initial data of Anti-de Sitter spacetime which lead to the formation of BHs after sufficiently long time.

Another major topic covered in WS II was the cosmic censorship conjectures. These concern the structure of gravitational singularities arising in GR. The strong cosmic censorship conjecture asserts that GR is generically a deterministic theory: The classical fate of all observers should be predictable from initial data. Mathematically, the conjecture states that the maximal Cauchy development of generic asymptotically flat initial data is locally inextendible as a regular Lorentzian manifold. The weak cosmic censorship conjecture proposes that singularities must be hidden from observers at infinity by the event horizon of a BH.

Lovelock's theorem states that GR is the unique four-dimensional theory of gravity which includes only second derivatives of the metric. However, under different assumptions, it is possible to construct alternative theories, for example by including additional fields. These theories should yield a well-posed initial value problem that can be solved to give predictions which can be compared to experiment. Although GR has so far agreed with all observations, there are still regimes where it has not been tested. Any alternative theory must agree with current observations, but may yield different results in other scenarios. Numerical attempts to test the validity of GR and alternative theories of gravity were discussed.

WS II also covered progress made in inverse problems arising in GR. This field seeks to address the question of whether one can determine the structure of spacetime in the past by making observations in the present. Recent work includes methods to generate GWs from electromagnetic (EM) waves near an observer's worldline. This is then used to recover the local vacuum spacetime metric. Another development concerns the local recovery of the topology, smooth structure and conformal class of a globally hyperbolic metric from data that includes active measurements made near the worldline. These methods exploit the nonlinearity of the hyperbolic partial differential equations (PDEs) in question, producing new singularities from interacting ones. These can then be analyzed using tools from microlocal theory.

This WS displayed some of the progress made in mathematical GR. Future work will aim to prove the cosmic censorship conjectures and the stability of Kerr-de-Sitter BHs in vacuum with zero cosmological constant.

### A. Projects and future directions

During the long program, a collaboration was formed to work on mathematical GR, focusing primarily on the asymptotic structure of spacetime. A useful method for studying this asymptotic structure was proposed by Penrose [4] and involves conformally mapping spacetime onto a compact manifold and attaching a boundary representing points "at infinity". The work done during the program investigated the regularity of this conformal metric at the boundary. In particular it was observed that a non-zero global mass presents an obstruction to differentiability, while higher dimensional spacetimes will in general admit conformal metrics of greater regularity.

The effect of mass on spacetime was also investigated through the positive mass theorem. The mathematical structure of GR means that it is not obvious how mass should be defined and a number of definitions of global mass are currently in use. Indeed, Penrose's list of unsolved problems in GR [5] includes finding a reasonable definition of quasi-local mass. The positive mass theorem supports the definition of global mass proposed by Arnowitt, Deser and Misner [6] by proving that this quantity is non-negative under certain physically reasonable assumptions. Work done during the program led to a proof of this theorem using methods which are more closely related to features we expect of positive mass spacetimes, in particular the focusing of light rays. This proof also used significantly weaker assumptions than previous versions, leading to a stronger result.

A group was also formed to work on inverse problems using methods from mathematical theory, numerical analysis and ML. This was motivated by recent work which proposed a convolutional neural network (CNN) structure that concretely applies the interactions of singularities in Lorentzian backgrounds to inverse problems for a nonlinear wave equation given actively measured data. Gravitational astrophysicists are interested in learning about the structure of spacetime based on local measurements. However, the utility of these inverse problem results to physicists is contingent on translating theorems into a usable format. Building this neural network (NN) for the toy case of a nonlinear acoustic wave equation would be a first step towards implementing a similar CNN for Einstein's equations.

The group worked towards building such a network to learn the local source-to-solution map, from which one can subsequently recover the wave speed and nonlinearity of the PDE. In particular, the focus was on understanding the structure of the network in terms of convolutional and dense layers, the data necessary for training, and methods to generate such data. This involved solving the PDE numerically for different source terms using a physics-informed NN, so that the source-solution pairs could then be input into the CNN. The group's future work will involve building the CNN and producing the data required to train the network. A new direction would be to design a NN adapted to Einstein's equations.

## III. NUMERICAL RELATIVITY

The birth of NR as an independent research area dates back to the 1960s when pioneering work foresaw the importance of numerical simulations as theoretical laboratories for GR. The field has improved significantly during the 1980s-1990s and culminated with the "2005/2006 breakthrough" in NR. (For a detailed overview on the topic, see for example Ref. [7].) Nowadays, NR has reached a state of maturity: It is applied regularly for waveform modeling of compact binaries, core-collapse supernovae (CCSNe) and isolated systems, and finds new applications in high-energy physics and cosmology, as well as simulations of compact binaries in extensions of GR. The tremendous improvements in NR occurred in parallel to the developments of advanced interferometric GW detectors. Nowadays, NR plays an important role in the analysis of GW signals by providing LVK researchers with accurate waveforms. This long program brought together experts in mathematical relativity, NR and astrophysics to discuss open issues and improving waveform modeling.

### A. Research topics

**Binary neutron stars and equations of state.** The equation of state (EOS) of matter above nuclear density is one of the open problems in physics. Fortunately, NSs provide an ideal laboratory for studying high-density matter. Information about the EOS is encoded in the GW strain of isolated NS, BNS and NSBH systems. NR simulations provide templates for observed signals allowing to check the accuracy of physical models, e.g., by defining constraints on the EOS for matter at nuclear densities (WS I, WS III). More accurate simulations will be achieved with more realistic EOSs. Thermodynamics and particle composition are being explored within the community to efficiently extract waveforms from NR simulations.

**Magnetic field amplification.** In astrophysical systems involving matter, such as BNS mergers and CCSN explosions, direct numerical general-relativistic magnetohydrodynamic (GRMHD) simulations are needed in order to accurately model the GW signal generated in these events. One open issue which was discussed in WS I is the amplification of large-scale magnetic fields due to MHD instabilities driven by small-scale turbulence. Numerical simulations with very high resolution seem to capture the effects of the dynamics at small scales, but the amount of computational resources required to perform a systematic study is prohibitively large. The presence of such intense magnetic fields has important consequences for the dynamics and the stability of the merger remnant and might leave an imprint in the emitted GWs. If the turbulence is not properly captured by the simulations, the ensuing GWs might be inaccurate.

**Core-collapse supernovae.** GW signals from CCSNe explosions are among the most promising multi-messenger signals yet to be detected. They are expected to be observed electromagnetically, as well as with GWs and neutrinos. In most scenarios, a proto neutron star (PNS) is created and surrounded by a standing accretion shock during the explosion. In the shock region, instabilities develope due to convection and standing accretion shock instability (SASI), leading to emission of neutrinos and GWs. The latter emission is mainly the result of the excitation of PNS oscillation modes. Asteroseismology of PNSs may give us insights about the explosion mechanism, the birth of NSs and their EOS. The signal of CCSNe is highly stochastic, imposing challenges on numerical simulations, identification of the modes, and estimation of the source parameters. CCSNe models require a broad variety of physical parameters stemming from sophisticated microphysics, GRMHD, nuclear-physics EOS, and neutrino kinetics, among others. Consequently, numerical simulations are computationally expensive. Furthermore, traditional techniques of matched filtering cannot be applied due to the complexity of the waveforms.

**Accuracy and parameter space of binary black hole simulations.** Improving the accuracy of BBH simulations is essential to fully exploit the potentials of future ground- or space-based GW detectors. This may be achieved, for example, through better gauge conditions, new waveform-extraction methods, improved initial data, and numerical techniques. Modeling the BBH GW sources seen by next-generation instruments will also require extendeding the simulation parameter space, for example by computing templates for high mass-ratio binaries, highly spinning BHs, eccentric/hyperbolic systems and dynamical captures. A better coverage of the intrinsic-parameter space of BBHs would also help in decreasing the systematics in the parameter estimation of GW detections. These topics were discussed in WS I and II.

**Testing general relativity and the nature of dark matter.** GW astronomy opened a path for testing GR in its strong-field, nonlinear regime which unfolds in the late inspiral and merger of compact binaries. GWs also provide a new way to probe the nature of dark matter. Theories of gravity that go beyond GR may leave a distinct imprint in the waveforms that could be detectable with current and future GW interferometers. Moreover, exotic matter can give rise to new classes of compact objects and alter the physical properties of known GW sources, such as BHs and NSs. NR simulations may be necessary to understand how modifications to GR or the presence of exotic matter may affect the GWs produced in different astrophysical scenarios.

**Relation with machine learning.** Numerical simulations of BBHs can also be used to build surrogate models with ML techniques. Another particular application of ML to numerical modeling is the classification of CCSNe signals from noise and a more efficient identification of these signals by creating spectrograms from phenomenological waveforms and analyzing the images through NNs.

### B. Activities and projects

During the program some of the core participants formed a working group on NR. The members of the group discussed topics presented during WS I and shared their knowledge on different aspects of NR in weekly meetings. The group (with contributions from some of the invited speakers) organized specialized lectures and practical tutorials on some of the numerical tools which are used within the NR community. These activities led to the start of a project on exotic compact objects. Fermionic compact objects, such as NSs and white dwarfs, may accrete dark matter during their life. The idea behind this project is to consider axion-like particles as a potential candidate for dark matter and construct models of NSs with an axionic core, and investigate their stability and possible implications for the physical properties of NSs. During the long program, the group worked on building the existence 2D-plane domain for a particular fermion-axion model. Future developments are to explore the parameter space and to verify the stability of the equilibrium configurations via NR simulations.

### C. Future research directions

Additional discussions held during the program focused on the development of new sub-grid models which could be used to accurately describe the magnetic field amplification due to MHD instabilities with an affordable computational cost. Future steps in this area will involve the improvement of current sub-grid models for actual binary merger simulations.

Another new project that started at IPAM concerns the asteroseismology of PNS and their mode classification. Here the target is to extend and refine previous analyses to study the SASI, its interaction with the fluid modes, and its imprint on the GW signals from CCSNe.

Finally, NR simulations of compact objects may be used to create phenomenological models and tune parameters of Effective One-Body (EOB) models to have more accurate semi-analytical models.

## IV. DATA ANALYSIS

The detection of GWs involves large amounts of data and requires a comprehensive understanding of the detectors, detailed knowledge of a myriad of noise sources, and development and implementation of different analysis techniques to search for both modeled and unmodeled GW signals. A major challenge in GW data analysis is managing and analyzing the large amount of data from the detectors. This includes many thousands of auxiliary data streams monitoring various aspects of the detectors as well as the output data from the detectors. In addition to analyzing data and searching for GWs, another challenge is to produce accurate sky localizations of potential signals. These can then be sent to astronomers for EM follow-up observations, adding GWs to MMA.

### A. Research topics

**Data characterization.** One of the challenges in detecting GWs is distinguishing astrophysical signals from instrumental or environmental noise triggers produced by non-linear couplings between the detector subsystems and their environment. Auxiliary data streams providing information on the state of various components of the detectors as well as the surrounding environment can be used to help mitigate the effects of noise on the detector output. These data can also guide improvements to the detector sensitivity by helping identify noise sources that can be mitigated through changes to the hardware or software. ML techniques, such as CNNs, dictionary learning, and k-nearest neighbors, are being developed to reduce the background of GW searches, improve the quality of detector data, and aid with low-latency analyses. Several talks related to data characterization and ML applications were given during the tutorial and WS IV.

**Gravitational-wave searches.** During the program, searches for GWs from different astrophysical sources were discussed, including CBC and burst searches. GW sources may have EM counterparts, lending themselves to potential multi-messenger analyses. CCSNe emitting neutrinos and EM radiation are an example of multi-messenger sources difficult to model since different explosion mechanisms lead to different waveforms. Many search techniques relying on ML were presented in WS I, III, and IV. Other potential multi-messenger GW sources are soft gamma repeaters, anomalous X-ray pulsars, cosmic strings, and asymmetric isolated spinning NSs. The long program included discussions of MMA searches targeting these sources and the stochastic GW background, defined as the superposition of GWs from all unresolved sources of astrophysical or cosmological origin.

**Computational challenges.** Searches for GWs require significant computational resources. An overview of the computational challenges faced by the LVK collaborations in GW science was discussed in the tutorial. The distributed computing architecture and global cyberinfrastructure of the Open Science Grid and how it can be used to support MMA and other scientific efforts were presented in the WS IV.

### B. Activities and projects

**Classification of electromagnetically bright events.** MMA research provides constraints on models from several perspectives and requires communication between scientists in different facilities and disciplines. One important aspect is to be able to treat the data from the detectors in real time. However, achieving the required computational speed and accuracy is challenging. At IPAM, a ML working group was created aiming to improve the recovery of parameters in low latency. The method relies on two steps. The first one involves regression to improve the parameters recovered by the detection pipelines at runtime. The goal is to remove as much systematic error as possible. The second step is to use the improved parameters and perform classification to assign a probability to the event of being electromagnetically bright.

As a proof of concept, Program participants generated artificial events and applied a nonlinear transformation to the parameters to mimic the recovery error of the real pipeline. Three different algorithms were used for each part of the project. For the regression step, it was found that a NN constraining the final output to physical values with a different activation function is a promising approach. The group also explored the possibility of training Gaussian Process Regression (GPR) in mini batches to produce a predicted value for the parameters, as well as an estimation of the error of the prediction. In classification, up to now, the best results were obtained with a fine-tuned random forest, as compared with the K-nearest neighbors or Support Vector Machine algorithms. Even with preliminary results from regression, it was observed a slightly improved classification score compared to the data straight from the artificial pipeline. Next steps include improving control of the algorithms used, designing better cross validation for fine tuning, building a working pipeline that could be integrated into current infrastructure, and applying the methods to real data.

**Gravitational-wave detection with convolutional neural networks.** Approximately one hundred CBC events have been detected since 2015. Search methods are computationally expensive. Thus, they may benefit from the implementation of ML algorithms. One particular example of the application of ML for classification and regression is CNNs, which have a very low computational cost for training compared to other alternatives such as dense NNs. CNNs learn local features of the data very fast by means of convolutional kernels and incrementally learn from data structures with simple features or complex ones through the hidden layers. During the program, a new project applying CNNs to LIGO-Virgo data emerged. The project involved creating datasets by injecting CBC signals into the GW data stream. To avoid overfitting, the dataset was split into a training dataset and a testing dataset. Once the model is trained, it can be used to identify and detect GW signals in low-latency.

### C. Future research directions

During the first two LV observing runs and the latest LVK observing run, the rate of observed GW events has progressively increased. The detection rate is expected to further increase in the next observing runs. Analysis of GW signals has required large amounts of computational and human power. As the amount of data to be analyzed will quickly surpass the capability of current methods, more sophisticated and automated methods need to be developed and deployed. The implementation of ML algorithms is a promising strategy.

## V. PHYSICAL INTERPRETATION

With the beginning of GW astronomy, the study of astrophysical and cosmological sources which are difficult to observe through traditional EM techniques has now become feasible. Inferring the properties of the sources from their GW signals is one of the key objectives of GW data analysis. The planned improvements in the sensitivity of the ground-based detectors and future space-based observatories bring unique computational and mathematical challenges to the source inference problem. These challenges include interpreting a variety of signals with different features, increased parameter dimensionality, and a high rate of signals. Most of the topics related with the physical interpretation of GWs were discussed during WS III.

### A. Research topics

**Bayesian inference.** One of the main topics of WS III was parameter estimation of compact objects binaries using Bayesian inference. Since this process is computationally expensive and can take up to several weeks for a single event, many discussions were dedicated to likelihood-free inference, such as simulation-based inference. Recent attempts for conducting such types of inference were examined, showing their potential for the upcoming LVK observing runs. Nested sampling and probabilistic inference were also discussed.

**Waveform modeling for compact binaries.** Identification of the source properties strongly relies on accurate waveform models incorporating all parameters of astrophysical systems. Some categories of the semi-analytical models used for parameter estimation are: Post-Newtonian, phenomenological, and EOB models. Although these sophisticated models are able to faithfully describe highly symmetric systems, many efforts are dedicated to the accurate modeling of the full parameter space. An example of this is the generalization of current models to describe precessing and noncircular BBHs. Furthermore, high-precision surrogate models using ML methods, such as GPR, are being developed to alleviate the problem of a sparsely populated parameter space. However, the lack of physical information, and the approximations adopted in these models introduce “waveform systematics” which must be identified and mitigated. WS III included a deep overview of waveform systematics for BBH and BNS systems. For BNS systems, the focus was mainly on systematics associated with the inference of tidal parameters and the EOS.

**Population studies and cosmological implications.** The LVK network of detectors is sensitive to stellar-mass BHs allowing scientists to perform population studies, such as inferring formation channels and merger rates. Issues about accurate population inference were thoroughly covered in WS III. Population studies are relevant to infer key cosmological parameters such as the Hubble constant using the BBH signals as dark sirens. Moreover, these studies are applied to searches for the stochastic GW background.

**Inference of CCSNe signals.** A recent method was built upon PNS asteroseismology that universally relates the time-frequency evolution of the oscillation modes of the star with its intrinsic properties. This allows for a detectability study for current and third-generation GW detectors. Additionally, inference of rapidly-rotating progenitors using the early core bounce part of the CCSN signal suggests it may be possible to infer rotational properties of newly formed PNSs.

**Inference of neutron star properties.** Inference of compact objects involving NSs was discussed in several talks during WS III. One of the main topics was the inference of the EOS from observations of BNS mergers and its many challenges and uncertainties. The WS also covered Hidden Markov processes to track continuous GW signals from rotating NSs.

**Inference of exotic sources.** The detection of ultralight bosons through GW observations is an intriguing possibility. Searches of these particles (focusing on the QCD axion) are undertaken by analyzing the quasi-monochromatic GW emission from scalar field clouds surrounding BHs. Some of the presentations proposed alternative interpretations of the most massive sources observed by the LVK. Proposed scenarios suggest that these events could be produced by collisions of a class of bosonic exotic compact objects made up of vector bosons.

### B. Future research directions

Once a GW signal is detected, several steps are needed to accurately perform parameter estimation, which predominantly relies on accurate waveforms. Better models will be crucial to fully exploit the potential of third-generation ground- and space-based detectors. As in NR, this will require exploring the regions of parameter space with higher mass ratios and spins, as well as including the effects of eccentricity, higher order modes, and spin-precession. Further developments in waveform modeling will also be needed to deal with systems where matter is present, such as BNSs and CCSNe. This will require taking into account additional physics, such as MHD, neutrino leakage, and different EOSs.

## VI. CONCLUSIONS

The direct detection of GWs has marked the beginning of a new era in astrophysics. Strong, dynamical relativistic gravitational fields can now be used to map the dark universe and prove fundamental physics. The next decade will see this new branch of scientific research expand to a mature field. Routine detections will spur a plethora of astrophysical and theoretical investigations. The LVK collaborations will strive to bring the instruments to design sensitivity and interpret new and more varied observations. Further instrumental research and development will focus on the design and realization of the next generation of GW interferometric detectors on Earth and in space.

This IPAM program touched on many aspects of this new branch of physics from the mathematics of the equations governing GW sources to the current state-of-the-art approaches for the characterization and interpretation of the data. The program allowed participants to initiate new collaborations, explore new paths in the development of tools and techniques for MMA, and advance a number of innovative projects at the forefront of this new discipline. These accomplishments will have a significant impact in the field.

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## APPENDIX: LIST OF ACRONYMS

**BBH:** Binary Black Hole
**BH:** Black Hole
**BNS:** Binary Neutron Star
**CBC:** Compact Binary Coalescences
**CCSN:** Core-Collapse Supernova
**CNN:** Convolutional Neural Network
**EM:** Electromagnetic
**EOB:** Effective One-Body
**EOS:** Equation of State
**GPR:** Gaussian Process Regression
**GR:** General Relativity
**GRMHD:** General Relativistic Magnetohydrodynamics

**GW:** Gravitational Wave
**IPAM:** Institute of Pure and Applied Mathematics
**LIGO:** Laser Interferometer Gravitational-wave Observatory
**LVK:** LIGO-Virgo-KAGRA
**ML:** Machine Learning
**MMA:** Multi-messenger Astrophysics **NN:** Neural Network
**NR:** Numerical Relativity
**NS:** Neutron Star
**NSBH:** Neutron Star-Black Hole
**MHD:** Magnetohydrodynamics
**PDE:** Partial Differential Equation
**PNS:** Proto Neutron Star
**QCD:** Quantum Chromodynamics
**SASI:** Standing Accretion Shock Instability
**WS:** Workshop

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