GWSurrogate: A Python package for gravitational wave surrogate models

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1 Department of Mathematics and Center for Scientific Computing & Data Science Research, University of Massachusetts, Dartmouth, MA 02747, USA **2** Theoretical Astrophysics 350-17, California Institute of Technology, Pasadena, California 91125, USA **3** Institute for Gravitational and Subatomic Physics (GRASP), Utrecht University, 3584 CC Utrecht, The Netherlands **4** Kavli Institute for Theoretical Physics, University of California Santa Barbara, CA 93106, USA **5** Department of Physics and Center for Computational Research, East Hall, University of Rhode Island, Kingston, RI 02881, USA **6** Department of Physics and Astronomy, The University of Mississippi, University, MS 38677, USA **7** Cornell Center for Astrophysics and Planetary Science, Cornell University, Ithaca, New York 14853, USA ***** These authors contributed equally.

Summary

Gravitational waves are ripples in space-time caused by the motion of massive objects. One of the most astrophysically important sources of gravitational radiation is caused by two orbiting compact objects, such as black holes and neutron stars, that slowly inspiral and merge. The motion of these massive objects generates gravitational waves that radiate to the far field where gravitational-wave detectors can observe them. Complicated partial or ordinary differential equations govern the entire process.

Traditionally, the dynamics of compact binary systems and the emitted gravitational waves have been computed by expensive simulation codes that can take days to months to run. A key simulation output is the gravitational wave signal for a particular set of parameter values describing the system, such as the black holes' masses and spins. The computed signal is required for a diverse range of multiple-query applications, such as template bank generation for searches, parameter estimation, mock data analysis, studies of model bias, and tests of general relativity, to name a few. In such settings, the high-fidelity signal computed from differential equations is often too slow to be directly used.

Surrogate models offer a practical way to dramatically accelerate model evaluation while retaining the high-fidelity accuracy of the expensive simulation code; an example is shown in Fig. 1. Surrogate models can be constructed in various ways, but what separates these models from other modeling frameworks is that they are primarily data-driven. Given a training set of gravitational waveform data sampling the parameter space, a model is built by following three steps:

1. Feature extraction: the waveform is decomposed into *data pieces* that are simple to model,
2. Dimensionality reduction: each data piece is approximated by a low-dimensional vector space, which reduces the degrees of freedom we need to model, and
3. Regression: fitting and regression techniques are applied to the low-dimensional representation of each data piece over the parameter space defining the model.
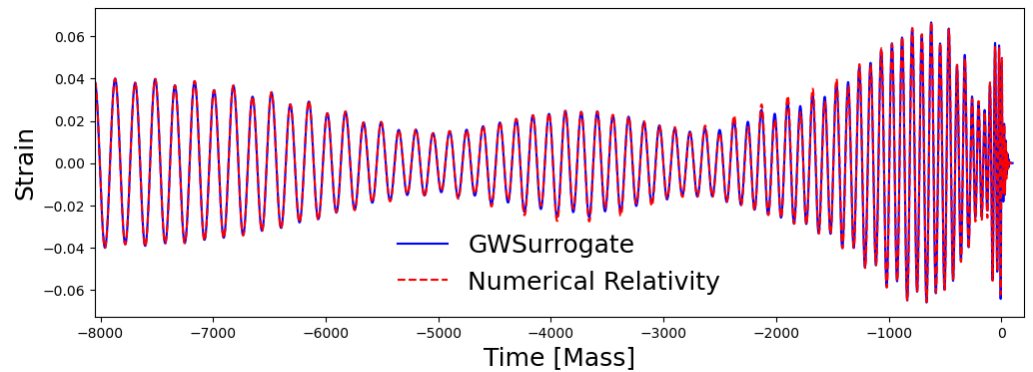

Figure 1: Example gravitational wave prediction from a surrogate model compared with numerical relativity for a precessing binary black hole system. This particular numerical relativity simulation took 70,881 CPU-hours (about 1.75 months using 56 cores on the supercomputer Frontera), while the surrogate model can be evaluated in about 100 milliseconds.

These model-building steps result in an HDF5 file defining the surrogate model's data and structure, which is stored on Zenodo. The GWSurrogate package provides access to these models through its catalog interface, and all available models and their associated HDF5 files can be found in `gwsurrogate.catalog.list()`. For a recent overview of surrogate modeling as used in gravitational wave astrophysics, please see Section 5 of Afshordi et al. (2023).

The development of GWSurrogate is hosted on GitHub and distributed through both PyPI and Conda. Quick start guides are found on the project's homepage while model-specific documentation is described through a collection of model-specific Jupyter notebooks. Automated testing is run on GitHub Actions.

Statement of need

GWSurrogate is a Python package first introduced in 2013 to provide an intuitive interface for working with gravitational wave surrogate models. Specifically, GWSurrogate gravitational wave models provide evaluation of

$$h_{\mathrm{S}}(t, \theta, \phi; \Lambda) = \sum_{\ell=2}^{\infty} \sum_{m=-\ell}^{\ell} h_{\mathrm{S}}^{\ell m}(t; \Lambda) \, ^{-2}Y_{\ell m}(\theta, \phi),$$

where $^{-2}Y_{\ell m}$ are the spin$= -2$ weighted spherical harmonics and Λ describes the model's parameterization. The surrogate model provides fast evaluations for the modes, $h_{\mathrm{S}}^{\ell m}$. As described more fully in the documentation, the high-level API allows users direct access to the modes $\{h_{\mathrm{S}}^{\ell m}(t)\}$ (as a Python dictionary) or assembles the sum $h_{\mathrm{S}}(t, \theta, \phi)$ at a particular location (θ, ϕ). The models implemented in GWSurrogate are intended to be used in production data analysis efforts. As such,

- computationally expensive operations (e.g., interpolation onto uniform time grids) are implemented by wrapping low-level C code for speed, whereas GWSurrogate provides a user-friendly interface to the high-level waveform evaluation API,
- models implemented in GWSurrogate follow the waveform convention choices of the LIGO-Virgo-Kagra collaboration, thus ensuring that downstream data analysis codes can use GWSurrogate models without needing to worry about different conventions, and
- GWSurrogate models can be directly evaluated in either physical units (often used in data analysis studies) and dimensionless units (often used in theoretical studies) where all dimensioned quantities are expressed in terms of the system's total mass.

Currently, there are 16 supported surrogate models (Barkett et al., 2020; Blackman et al., 2015, 2017; Field et al., 2014; Gadre et al., 2024; Islam et al., 2022; O'Shaughnessy et al., 2017; Rifat et al., 2020; Varma, Field, Scheel, Blackman, Kidder, et al., 2019; Varma, Field, Scheel, Blackman, Gerosa, et al., 2019; Yoo et al., 2022, 2023), with additional models under development (Islam et al., 2021; Rink et al., 2024). These models vary in their duration, included physical effects (e.g. nonlinear memory, tidal forces, harmonic modes retained, eccentricity, mass ratio extent, precession effects, etc), and underlying solution method (e.g. Effective One Body, numerical relativity, and black hole perturbation theory). Details about all models can be found by doing `gwsurrogate.catalog.list(verbose=True)`, while the GWSurrogate homepage summarizes the state-of-the-art models for each particular problem. Certain models allow for additional functionality such as returning the dynamics of the binary black hole. These special features are described further in model-specific example notebooks.

Several other software packages are available for waveform generation, including tools for effective-one-body models (Mihaylov et al., 2023; Nagar et al., 2020), ringdown signals (Carullo et al., 2023; Isi & Farr, 2021; Nitz et al., 2024), extreme-mass-ratio inspiral systems through the Black Hole Perturbation Toolkit's `FastEMRIWaveforms` and `BHPTNRSurrogate` packages (*Black Hole Perturbation Toolkit*, n.d.), and the `Ripple` framework that enables specialized acceleration techniques using JAX (Edwards et al., 2024). Among these, LALSuite (LIGO Scientific Collaboration et al., 2018) stands out as the most comprehensive, offering the largest collection of waveform models via its LALSimulation subpackage, which includes Python bindings and the new Python-based gwsignal waveform generator. While GWSurrogate shares similarities with LALSuite in providing a variety of models, it differs by exclusively focusing on surrogate models. Notably, GWSurrogate includes many state-of-the-art numerical relativity models that are only available through its library, whereas LALSuite offers a broader but less specialized collection.

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