Fitting Binary Black Hole Populations with Phenomenological Models

Calley Tinsman[1], Colm Talbot[2], and Simon Stevenson[3]
[1] *Department of Physics, Embry-Riddle Aeronautical University, Prescott, Arizona 86301, USA*
[2] *School of Physics and Astronomy, Monash University, Clayton, Victoria 3800, Australia*
[2,3] *OzGrav: The ARC Centre of Excellence for Gravitational-wave Discovery, Clayton, Victoria 3122, Australia and*
[3] *Centre for Astrophysics and Supercomputing, Swinburne University of Technology, Hawthorne, Victoria 3800, Australia*
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Gravitational wave observatories LIGO and VIRGO are beginning to detect a population of merging binary black holes, allowing researchers to perform basic inferences about the distribution of black holes in the universe. As an increasing number of mergers are detected, more sophisticated models can be used. We investigate how well the physics of pulsational pair-instability supernovae can be inferred with a simple model of the binary black hole mass distribution. By performing a Bayesian statistical analysis of the results of simulations from the population synthesis code COMPAS, we find that a pulsational pair-instability supernovae motivated model is a better fit to the binary black hole mass distribution compared to a simple power law model, presenting KL-divergences of 0.05 and 0.41, respectively. However, the model parameters intended to describe a pile-up of black holes due to pulsational pair-instability supernova instead fit to an abundance of black holes caused by the treatment of mass transfer stability in COMPAS simulations.

I. INTRODUCTION

With the growing number of merging binary black hole observations being detected by gravitational wave observatories such as the Laser Interferometer Gravitational-Wave Observatory (LIGO) and Virgo, we are able to learn an increasing amount about the mass distribution of binary black holes in the universe. This information can help researchers understand the evolution of these black hole systems. There are three primary channels of binary black hole evolution: classical isolated binary evolution, chemically homogeneous evolution, and dynamical formation, which are all shown in Figure 1.

Classical isolated binary evolution occurs when a binary star system with a wide orbit undergoes mass transfer, resulting in a common envelope of gas that creates friction within the system. This brings the binaries closer together as they become black holes. In chemically homogeneous evolution, a binary pair with a tighter orbit is tidally locked and rapidly spinning, preventing the stars from expanding as they die. This allows them to evolve and become black holes despite their tight orbit. Lastly, dynamical formation occurs when black holes in dense areas of space such as star clusters are brought together by interactions with other bodies such as stars. This forms a binary black hole system [1].

The question we now ask is how can we make accurate models of the distribution of binary black holes in the universe? It is impossible to study every single star in the sky. Therefore, we depend on different methods to help predict the distributions of astrophysical bodies in the universe. Among these methods are population synthesis, which uses the real observations of stars made by scientists, and population inference, which uses astrophysical theories such as the channels of binary black hole evolution described in the previous paragraph.

Population synthesis combines observations of nearby stars and stellar evolution theories to develop models for astrophysical populations in the universe. Compact Object Mergers: Population Astrophysics and Statistics (COMPAS) is a rapid Monte-Carlo code that uses population synthesis to simulate the evolution of binary systems [2]. This code allows for the simulation of millions of stars with different initial conditions to see how they and their remnants evolve. In particular, we can use the results from COMPAS simulations to analyze the mass distribution of remnant black holes that become binary black hole mergers.

Another method for modeling black hole distributions is population inference. To describe a distribution of binary black hole mergers in this way, we choose a phenomenological model based on astrophysics theory, population synthesis models, and real, physical observations. Then we apply Bayesian inference methods to infer the hyperparameters of the model, providing insight into the physics driving the shape of the distribution [3].

In this paper we explore how the binary black hole mass distributions produced via population synthesis in

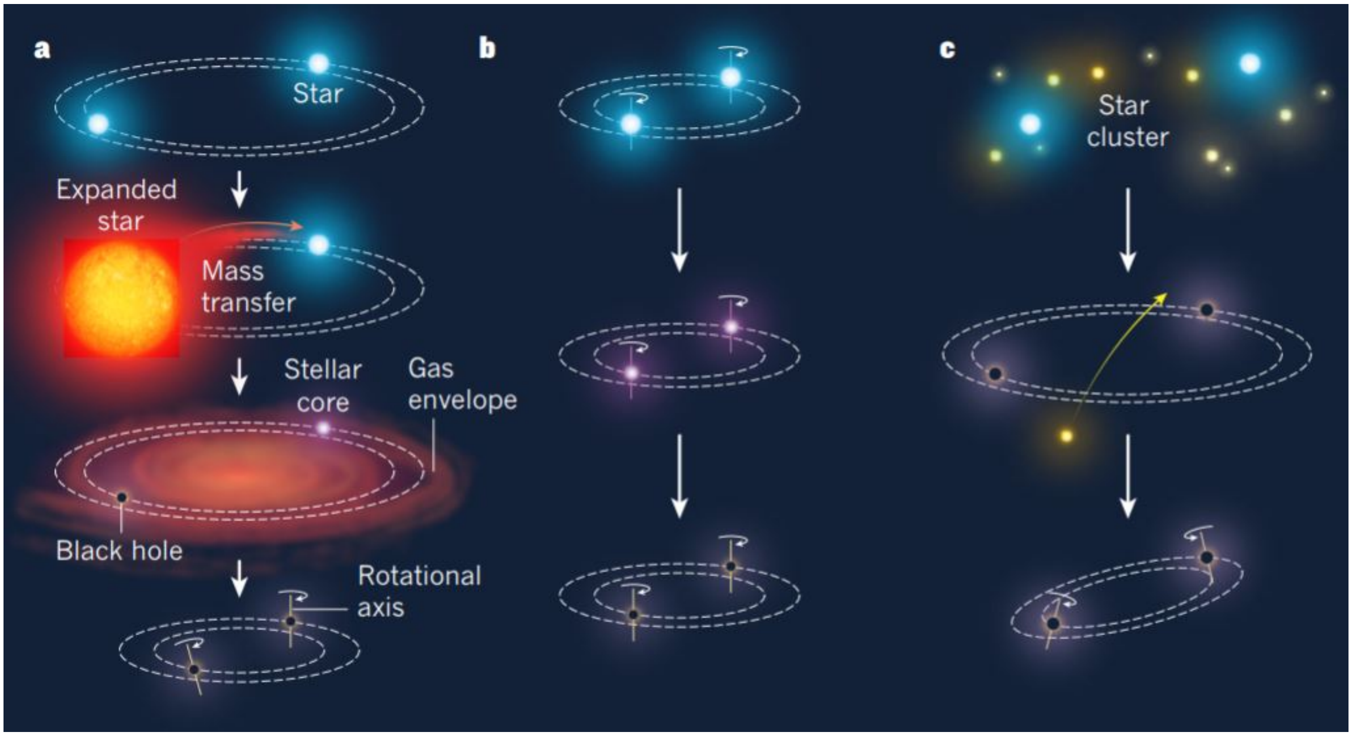

FIG. 1. **a) Classical isolated binary evolution. b) Chemically homogeneous evolution. c) Dynamical formation.** This picture, from Mandel and Farmer [1], shows the three primary evolutionary channels for binary black hole systems and visually describes the main stages of each one.

COMPAS simulations compare to astrophysically motivated models generated with population inference. This is done by fitting a phenomenological model to the binary black hole mass distribution from COMPAS and using the Kullback-Leibler (KL) divergence as a measure of how much the two probability distributions diverge. In addition, we see how well a simple power law compares.

II. METHODS

A. Building a Binary Black Hole Population with COMPAS

We use COMPAS to simulate the evolution of 12 million binary star systems with 12 different metallicities. For this analysis, we take only the results that describe systems that produce binary black hole systems that merge within the age of the universe. Figure 2 shows the primary mass distribution from these results.

Next, we process the data to convert the histogram shown in Figure 2 to a probability distribution weighted by both metallicity and cosmic history in order to obtain a more representative binary black hole population. Using Eq. 9 in Barrett *et al.* [4] as a basis, we find the distribution of merging binary black holes as a function of redshift:

$$\frac{\mathrm{d}^3 N_{\mathrm{merge}}}{\mathrm{d}t_{\mathrm{s}}\,\mathrm{d}V_{\mathrm{c}}\,\mathrm{d}M}(z) = \int \mathrm{d}Z \int \mathrm{d}\tau_{\mathrm{delay}} \left[\frac{\mathrm{d}^3 N_{\mathrm{form}}}{\mathrm{d}M_{\mathrm{form}}\mathrm{d}\tau_{\mathrm{delay}}\mathrm{d}M}(Z) \times \frac{\mathrm{d}^3 M_{\mathrm{form}}}{\mathrm{d}t_{\mathrm{s}}\mathrm{d}V_{\mathrm{c}}\mathrm{d}Z}(Z, t_{\mathrm{form}} = t_{\mathrm{merge}}(z) - \tau_{\mathrm{delay}}) \right] \quad (1)$$

where N_{merge} is the number of mergers, t_s is the source time, V_c is the comoving volume, M is the primary black hole mass, z is redshift, Z is metallicity, τ_{delay} is the time delay between the formation time t_{form} of the star and the merger time t_{merge} of the binary black hole system, N_{form} is the number of mergers formed, and M_{form} is the star formation mass.

The first term in the integrand in Eq. 1 represents the rate of binary black hole formation per unit star formation mass (which is obtained from COMPAS simulations), while the second term represents the metallicity

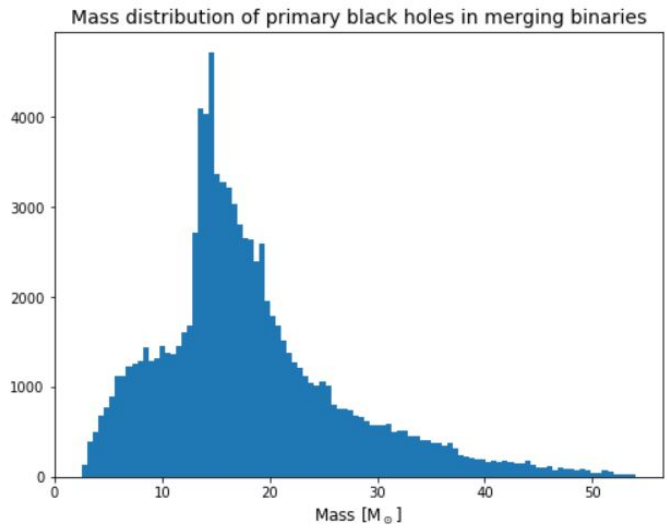

FIG. 2. **Mass distribution of primary black holes in merging binaries.** This histogram shows the distribution of primary black holes that were created by evolving 12 million binary star systems in the population synthesis code COMPAS. An abundance of black holes are formed around 15 solar masses due to the treatment of mass transfer stability in COMPAS. At the time of writing, a paper investigating this theory is in prep.

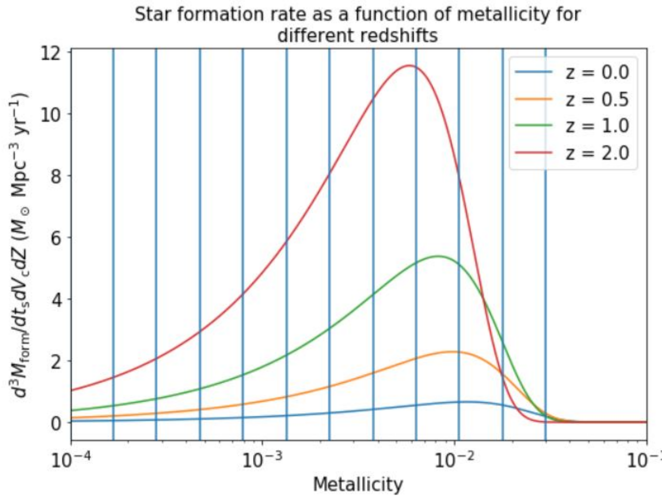

FIG. 3. **Metallicity specific star formation rate.** Each curve in the figure above is a probability distribution showing the amount of mass being formed into stars per unit volume per unit time as a function of metallicity for a different redshift. The vertical blue lines indicate the metallicities of the binary systems that were simulated in COMPAS. These curves are used to weigh the binary black hole mass distribution that is output by COMPAS.

specific star formation rate. We use the star formation rate as a function of redshift z by Madau and Dickinson [5] and the star formation rate as a function of metallicity from Langer and Norman [6] given by Eqn. 8 in Mandel and de Mink [7]. A visual representation of the second term is shown in Figure 3.

Next, following Eq. 16 from Barrett *et al.* [4], we multiply by the rate of change of comoving volume with redshift, as well as the rate of change of the source time with observer time and integrate over the merger redshift:

$$\frac{\mathrm{d}N}{\mathrm{d}t_{\mathrm{obs}}\mathrm{d}M} = \int \mathrm{d}z \left[\frac{\mathrm{d}^3 N_{\mathrm{merge}}}{\mathrm{d}t_{\mathrm{s}}\mathrm{d}V_{\mathrm{c}}\mathrm{d}M} \frac{\mathrm{d}V_{\mathrm{c}}}{\mathrm{d}t_{\mathrm{obs}}} \right] \quad (2)$$

where N is the number of binary black holes, t_s is the time in the source frame, and $t_{obs} = (1+z)t_s$ is the time in the observer's frame. The result is the probability distribution for binary black hole mergers in the universe as exists today, accounting for metallicity and cosmic history. This result is shown in Figure 4.

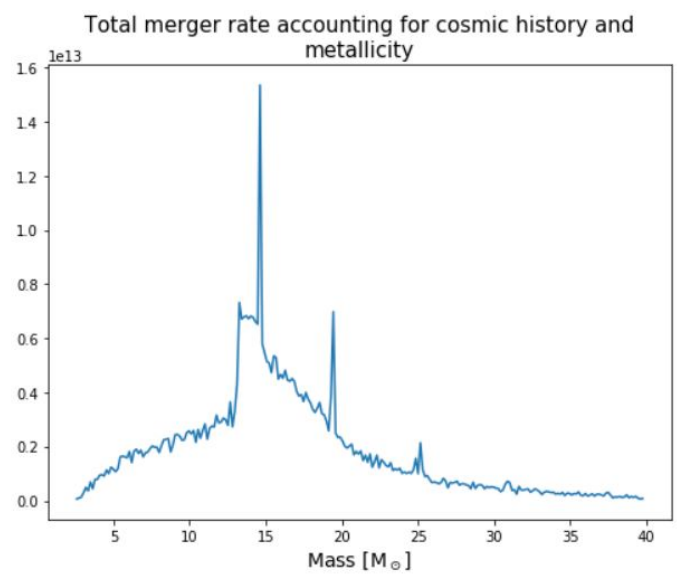

FIG. 4. **Total merger rate considering cosmic history and metallicity.** The spikes at masses of approximately 15, 20, 25, and 31 solar masses are artificial and are due to the discrete grid of metallicities used in COMPAS simulations. The wider peak around approximately 15 solar masses is due to the treatment of mass transfer stability in COMPAS. At the time of writing, papers investigating these features are in prep.

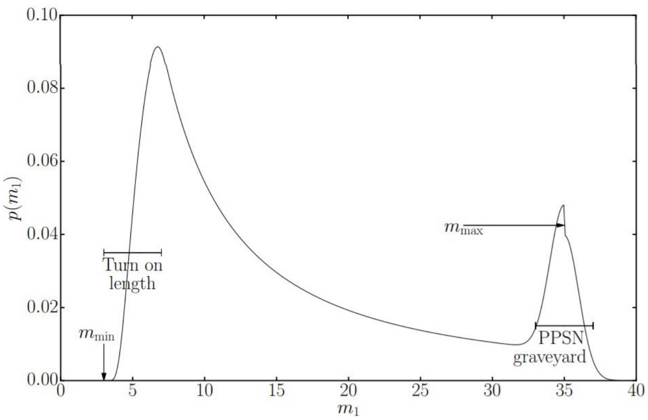

FIG. 5. **Astrophysically motivated model for the binary black hole primary mass distribution with (hyper)parameters as specified in Talbot and Thrane [3].** In this model we see a pile-up of binary black holes at around 35 solar masses due to pulsational pair-instability supernovae. We note a cutoff at 40 solar masses, which is due to typical pair-instability supernovae.

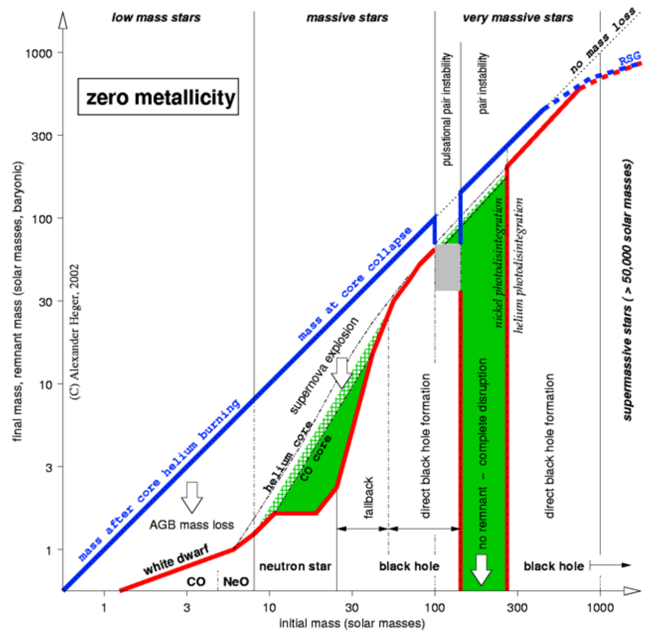

FIG. 6. **Singular stellar evolution at zero metallicity.** This figure shows the mass of the remnant left behind when a star dies as a function of the star's initial mass. The model in Figure 5 incorporates the astrophysical phenomena displayed by this plot; specifically, pair-instability and pulsational pair-instability supernovae.

B. The Phenomenological Model

The method used to develop the probability distribution for the binary black hole mass spectrum for our phenomenological model is that as described in detail in Talbot and Thrane [3] and shown in Figure 5. In this study, we generate only a one-dimensional probability distribution that will only consider the primary black holes. This is the model to be fit to the COMPAS distribution.

The model is motivated by the presence of pulsational pair-instability supernovae, a supernova imposter event. This event occurs when a star appears to undergo a typical pair-instability supernova where energy is lost through electron-positron pair production. However, rather than entirely explode, the star sheds only some of its mass and continues to undergo a core collapse, resulting in a pulsational pair-instability supernova. These stars range in mass of between 100 and 130 solar masses and their remnants are black holes expected to be between 30 and 40 solar masses [8]. The cut-off in the model at approximately 40 solar masses is due to the pair-instability supernovae which do not leave remnants behind, as shown in Figure 6 from Heger and Woosley [9].

This model has free (hyper)parameters α, β, m_{max}, m_{min}, λ, m_{pp}, σ_{pp}, and δm, which describe the spectral index of the primary mass for the power-law distributed component as the mass spectrum, the spectral index of the secondary mass, the maximum mass of the power-law distributed component as the mass spectrum, the minimum mass, the proportion of primary black holes formed via pulsational pair-instability supernovae, the mean mass of black holes formed via pulsational pair-instability supernovae, the standard deviation of masses of black holes formed via pulsational pair-instability supernovae, and the mass range over which the black hole mass spectrum turns on, respectively.

C. Fitting Methods

We perform a best-fit of the one-dimensional phenomenological model and a best-fit for a simple power law to the COMPAS distribution. The parameters of the phenomenological model are discussed in Section II C. In the power law model, the only free parameters are α, m_{max}, and m_{min}. The other parameters are fixed to be $\lambda = 0$, $m_{pp} = 35$, $\sigma_{pp} = 1$, $\beta = 0$, and $\delta m = 0$. The free parameters are not bounded. The optimization algorithm `basinhopping` in Python is used to identify the

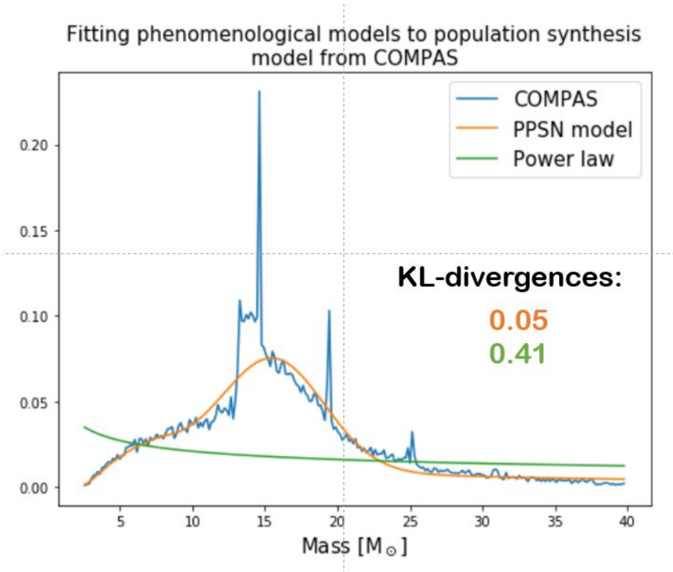

FIG. 7. **Fitting phenomenological models to a binary black hole mass distribution from the population synthesis code COMPAS.** The blue curve represents the mass distribution from COMPAS, the orange curve the phenomenological model motivated by pulsational pair-instability supernovae, and the green curve a power law fit. Visually, we can see that the orange curve seems to fit the distribution very well, whereas the green curve does not.

Parameters	Phenomenological model	Power law model
α	1.05	0.38
β	54.78	70.16
m_{max}	0.89	2.10
m_{min}	0.55	**0**
λ	15.62	**35**
m_{pp}	3.50	**1**
σ_{pp}	3.73	**0**
δ_m	8.77	**0**

TABLE I. **Best-fit parameters for the phenomenological and power law models.** The fixed parameters are in bold. Note that these parameters were not bounded and may not be consistent with the astrophysical limits understood by current observational data and theoretical predictions of pulsational pair-instability supernovae and population synthesis modeling.

optimal values of these parameters for the best-fit to the COMPAS distribution.

The KL divergence is used to determine the goodness of fit. The KL divergence describes the divergence, or deviation, between two probability distributions and is given by the following equation [10]:

$$D(p(x), q(x)) = \int_{-\infty}^{\infty} p(x) \log \left(\frac{p(x)}{q(x)} \right) dx \qquad (3)$$

where $p(x)$ and $q(x)$ represent our distributions from population synthesis (COMPAS) and our phenomenological model, respectively. The less the probability distributions deviate from one another, the closer to zero the KL divergence becomes, implying that a small KL divergence represents a better fit.

III. CONCLUSION

A. Results

Figure 7 shows the fits of our phenomenological models to the binary black hole mass distribution from COMPAS. In blue is the COMPAS distribution, in orange is our model motivated by pulsational pair-instability supernovae, and in green is the power law fit. Visually, we can see that the orange curve appears to represent the mass distribution very well, whereas the green curve fails to do so. This is also evident by the KL divergences; the pulsational pair-instability supernovae fit and power law fit have KL divergences of 0.05 and 0.41, respectively. The best-fit parameter values are listed in Table III A.

Physically, however, the phenomenological model does not describe the distribution anticipated. The parameters that allow for the model to fit the peak at around 15 solar masses were intended to describe the theoretical pile-up of black holes at approximately 35 solar masses due to pulsational pair-instability supernovae. It is clear that there is no evidence of this pile-up in the binary black hole mass distribution from COMPAS; but, there is an abundance of black holes around 15 solar masses due to the treatment of mass transfer stability in the COMPAS code. Therefore, the parameters fit to this peak instead.

In conclusion, the phenomenological model developed by Talbot and Thrane [3] is a good description of the binary black hole primary mass distribution produced by the population synthesis code COMPAS. A simple power law does not provide a good representation.

B. Future Work

There are many ways to expand this research. In the analysis presented here, the parameters of the models were not bounded, meaning that the best-fit parameters may not be consistent with the astrophysical limits understood by current observational data and theoretical predictions of pulsational pair-instability supernovae and population synthesis modeling. One should repeat the analysis, but impose limits on the free parameters. Also, one may extend the one-dimensional probability distribution into a two-dimensional one in order to take into account both primary and secondary black hole masses.

One may in addition explore other models and how well they describe the mass distribution from COMPAS. The analysis with the models presented here show the binary black hole mass distribution as existing in the universe. The analysis may be repeated for the binary black hole mass distribution observable by LIGO, which can be done by multiplying the distributions by an observational bias factor before determining the best-fits. This would allow one to compare the models to real LIGO and Virgo observations.

Lastly, it would be interesting to investigate how changing parameters in COMPAS may affect the mass distribution it outputs. One could change the specifications in the COMPAS code in an attempt to turn off the special treatment of mass transfer stability in order to see how the mass distributions would change, and then perform the analysis as described in this paper. One may also experiment with the COMPAS specifications that affect the treatment of pulsational pair-instability supernovae, and adjust these parameters (within astrophysical limits) in an attempt to induce a pile-up of black holes from this phenomenon in order to see if it is possible to ever see an abundance of black holes from pulsational pair-instability supernovae, or if the amount is always insignificant.

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