Star Cluster Population of High Mass Black Hole Mergers in Gravitational Wave Data

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Stellar evolution theories predict a gap in the black hole birth mass spectrum as the result of pair instability processes in the cores of massive stars. This gap, however, is not seen in the binary black hole masses inferred from gravitational wave data. One explanation is that black holes form dynamically in dense star clusters where smaller black holes merge to form more massive black holes, populating the mass gap. We show that this model predicts a distribution of the effective and precessing spin parameters, χ_{eff} and χ_{p}, within the mass gap that is insensitive to assumptions about black hole natal spins and other astrophysical parameters. We analyze the distribution of χ_{eff} as a function of primary mass for the black hole binaries in the third gravitational wave transient catalog. We infer the presence of a high mass and isotropically spinning population of black holes that is consistent with hierarchical formation in dense star clusters and a pair-instability mass gap with a lower edge at $44^{+6}_{-4} M_{\odot}$. We compute a Bayes factor $\mathcal{B} > 10^4$ relative to models that do not allow for a high mass population with a distinct χ_{eff} distribution. Upcoming data will enable us to tightly constrain the hierarchical formation hypothesis and refine our understanding of binary black hole formation.

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Introduction—Observations of gravitational waves (GWs) from binary black hole (BH) mergers provides an unprecedented window into the astrophysics of massive stars [1–7]. However, our ability to learn from these detections is hindered by uncertainties in the theory of massive binary star evolution and BH formation and the dependence of model results on initial conditions and parameters (e.g., [8–11]). One of these uncertainties is the location (and presence) of a mass gap in the BH birth mass distribution due to (pulsational) pair instability supernovae [(P)PISN], estimated to begin in the ~ 40–$70 M_{\odot}$ range and ending at $\sim 130 M_{\odot}$ [12–15]. Such a gap is not seen in the BH mass distribution [6,16]. If such a gap exists, then the formation of BHs within the mass gap can be explained by scenarios involving dynamical interactions in dense star clusters or active galactic nucleus (AGN) disks, where BHs can grow through hierarchical mergers [17–24]. The detection of this high mass population will shed light on the origin of binary BH mergers as well as on the location of the (P)PISN mass gap.

The most precisely measured spin parameter from GW data is the effective inspiral spin χ_{eff}, a combination of the two component spins projected parallel to the orbital angular momentum [25]. Previous work has shown that the distribution of χ_{eff} can give important insights on the origin of the detected BH binary population [26–37]. The distribution of individual BH spins and of the precessing spin parameter χ_{p} [38] have also been leveraged in attempts to identify a dynamically-formed population in the data [32,39–45], and correlations between BH spins and binary mass ratio [6,28,46–49] and possibly redshift [49,50] have been inferred from the data. Other studies have examined possible relationships between BH mass and spin, as would be expected from a population of hierarchical mergers [34,37,42,43,47,50,51]; thus far, evidence for any correlation between BH masses and spins has been tentative, with different studies yielding different conclusions. A clear detection of the (P)PISN mass gap and a population of hierarchical mergers remains elusive.

Here, we consider the χ_{eff} and χ_{p} distributions as a function of primary BH mass m_1 to identify signatures of hierarchically formed BHs in the third gravitational wave transient catalog (GWTC-3).

Analytical model—We consider the spin parameters χ_{eff} and χ_{p} for a dynamically assembled BH merger population, in which the primary is a second-generation (2G) BH formed via an earlier merger and the secondary is a first-generation (1G) BH representing the direct end product of stellar evolution. The effective inspiral spin is defined as $\chi_{\mathrm{eff}} = (m_1 a_1 \cos\theta_1 + m_2 a_2 \cos\theta_2)/(m_1 + m_2)$ [52,53], and the effective precessing spin parameter is $\chi_{\rm p} = \max\{a_1 \sin\theta_1, [(3+4q)/(4+3q)]qa_2\sin\theta_2\}$ [54,55], where $q = m_2/m_1$ denotes the binary mass ratio, a_1 and a_2 are the dimensionless component spin magnitudes, and θ_1 and θ_2 are the angles between each spin vector and the orbital angular momentum.

For dynamical formation in a dense star cluster, we expect that (i) spin and orbital angular momenta are isotropically oriented [56]. For 1G + 2G mergers we also expect that (ii) $a_1 = \tilde{a} \simeq 0.69$, in line with predictions from numerical-relativity simulations [57], that (iii) $a_1 \gg a_2$, as a significant 1G + 2G merger rate requires that BHs are formed with small spin, allowing for a higher cluster retention probability of merger remnants [19,22]; and that [iv] $m_1 \simeq 2m_2$, based on dynamical selection favoring the high mass end of the BH mass function for both BH primary progenitors and for the secondary BH [58].

Given the above considerations, we expect that the most likely values of the spin parameters for a 1G + 2G mergers are $\chi_{\rm eff} \simeq (\tilde{a}/1.5)\cos\theta_1$ and $\chi_{\rm p} \simeq \tilde{a}\sin\theta_1$, leading to the mean relation $\chi_{\rm p} = \sqrt{\tilde{a}^2 - (1.5\chi_{\rm eff})^2}$. Isotropy then implies a uniform distribution for $\chi_{\rm eff}$ within $|\chi_{\rm eff}| < \tilde{a}/1.5 \simeq 0.47$, and $p(\chi_{\rm p}) \propto (\chi_{\rm p}/\sqrt{\tilde{a}^2 - \chi_{\rm p}^2})$. Integrating, we find the cumulative distribution functions (CDF)

$$N_{12}(\leq \chi_{\rm eff}) = 0.5 + 0.75\frac{\chi_{\rm eff}}{\tilde{a}} \tag{1}$$

and

$$N_{12}(\leq \chi_{\rm p}) = 1 - \sqrt{1 - \frac{\chi_{\rm p}^2}{\tilde{a}^2}}. \tag{2}$$

For 2G + 2G mergers, the probability density of $\chi_{\rm eff}$ is obtained from the convolution of two uniform distributions, which gives $p(\chi_{\rm eff}) \propto (\tilde{a} + \chi_{\rm eff})$ for $\chi_{\rm eff} \leq 0$ and $p(\chi_{\rm eff}) \propto (\tilde{a} - \chi_{\rm eff})$ for $\chi_{\rm eff} > 0$. The corresponding CDF is

$$N_{22}(\leq \chi_{\rm eff}) = \begin{cases} \frac{\chi_{\rm eff}}{\tilde{a}} + \frac{1}{2}\frac{\chi_{\rm eff}^2}{\tilde{a}^2} + \frac{1}{2} & \text{if } \chi_{\rm eff} \leq 0 \\ \frac{\chi_{\rm eff}}{\tilde{a}} - \frac{1}{2}\frac{\chi_{\rm eff}^2}{\tilde{a}^2} + \frac{1}{2} & \text{if } \chi_{\rm eff} > 0. \end{cases} \tag{3}$$

Since θ_1 and θ_2 are independent, the distribution of $\chi_{\rm p}$ is obtained by the product of the distributions for each of the two angles:

$$N_{22}(\leq \chi_{\rm p}) = \left(1 - \sqrt{1 - \frac{\chi_{\rm p}^2}{\tilde{a}^2}}\right)^2. \tag{4}$$

We note that similar distributions for $\chi_{\rm eff}$ and the $\chi_{\rm eff}$ *vs* $\chi_{\rm p}$ correlation were obtained by Refs. [59,60].

We now asses the accuracy of the analytical model by comparing its predictions to the results of globular cluster models evolved using the fast cluster code cBHBd [61]. Unless specified otherwise, our initial conditions and numerical modeling are the same as in [22]. In all models considered here we adopt an initial cluster half-mass density $\rho_{\rm h} = 10^5 M_\odot {\rm pc}^{-3}$ and the delayed supernova mechanism from [62].

We report the results from four population models that differ by the choice of the initial BH spin distributions and the maximum mass of 1G BHs, $m_{\rm cut}$. In one model, the initial BH spins are all set to zero and $m_{\rm cut} \simeq 70 M_\odot$. In the other three models, we assume that $m_{\rm cut} \simeq 50 M_\odot$ and that the BH spin distribution follows a beta distribution with shape parameters $(\alpha, \beta) = (2, 18)$, (2,5), and (2,2); these distributions peak at ≃0.06, 0.2, 0.5 and their corresponding median values are ≃0.1, 0.26, and 0.5, respectively. All but the last model (with the highest spins) give differential merger rates at primary masses above $m_{\rm cut}$ consistent with those measured from LIGO/Virgo data [6]. Above this mass, the merger rate is dominated by 1G + 2G mergers in all models [see Supplementary Material (SM) [63]].

In Fig. 1 we show the CDFs of $\chi_{\rm eff}$ and $\chi_{\rm p}$ for 1G + 2G and 2G + 2G mergers, as well as the analytical predictions based on equations (1)–(4), and the spin parameter distributions from the cluster Monte Carlo models of [19]. These distributions almost perfectly align with each other across the entire range of parameter values. We note that while the differences near the tails of the distributions increase with initial BH spins, higher spins tend to reduce the merger rate above $m_{\rm cut}$ due to increased BH ejection from their host clusters, so these models are statistically disfavored; on the other hand, the small deviations seen in

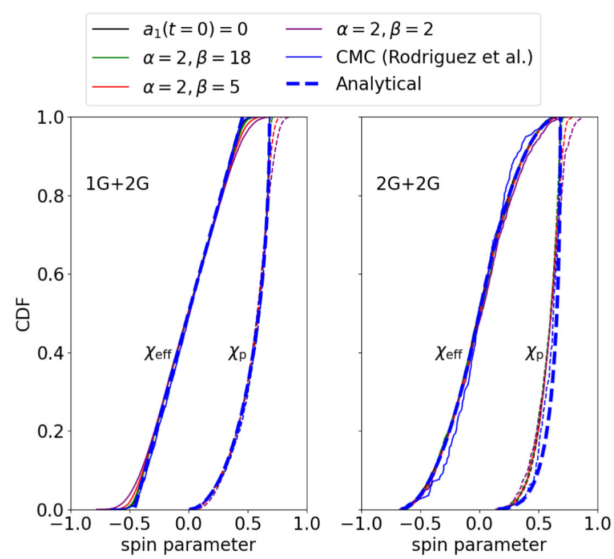

FIG. 1. CDF of $\chi_{\rm eff}$ and $\chi_{\rm p}$ obtained from our cluster models and the expected CDFs based on our analytical approximations. The lines are hard to distinguish because they lie on top of each other, showing the independence of these distributions on model assumptions and initial conditions.

the lower-spin models are unlikely to be discernible from the data. Thus, if hierarchical mergers are the most common class of merger above some threshold mass, our models predict a near-universal spin distribution, simply represented by equations (1) and (2). In the following, we test this prediction against GW data.

Bayesian inference—Since the value of χ_p is less well measured in GW observations than $\chi_{\rm eff}$ [4,7], we predominantly consider hierarchical inference of the effective spin distribution. For this study, we use the subset of BHs from GWTC-3 with false alarm rates below 1 yr^{-1}, consistent with Ref. [6]. This results in a total of 69 binary BHs in our sample. In parallel with $\chi_{\rm eff}$, we hierarchically fit the distribution of q, m_1, and redshift z. We incorporate selection effects using the set of successfully recovered binary BH injections provided by the LIGO-Virgo-KAGRA Collaboration and spanning their first three observing runs [6,7].

We fit the $\chi_{\rm eff}$ distribution to a mixture model comprising a Gaussian distribution, representing the bulk of the population at $m_1 \lesssim \tilde{m}$, and a uniform distribution, representing 1G + 2G hierarchical mergers at $m_1 \gtrsim \tilde{m}$, where $\tilde{m}$ is the value of m_1 at which the transition between the Gaussian and uniform descriptions of $\chi_{\rm eff}$ occurs:

$$\pi_{\mathcal{N}+\mathcal{U}}(\chi_{\rm eff}|m_1) = \begin{cases} \mathcal{N}(\chi_{\rm eff};\mu,\sigma) & (m_1 < \tilde{m}) \\ \mathcal{U}(\chi_{\rm eff}; w = 0.47) & (m_1 \geq \tilde{m}). \end{cases} \quad (5)$$

Here, $\mathcal{N}(\chi_{\rm eff};\mu,\sigma)$ denotes a normalized Gaussian distribution with mean μ and standard deviation σ truncated within $[-1, 1]$, and $\mathcal{U}(\chi_{\rm eff}; w)$ is a uniform distribution defined over the range $|\chi_{\rm eff}| < w$. We set $w = 0.47$, as predicted for hierarchical mergers. We use broad uninformative priors; the prior on $\tilde{m}$ is uniform between 20 and $100 M_\odot$. For more details on the implementation of the models and prior assumptions see SM [63].

We consider additional models with increased complexity. Our second model, $\pi_{\mathcal{N}+\mathcal{U}_w}(\chi_{\rm eff}|m_1)$, is similar to $\pi_{\mathcal{N}+\mathcal{U}}$, but with w now being a parameter that we infer from the data. The third model is

$$\pi_{\mathcal{N}+\mathcal{N}\mathcal{U}_w}(\chi_{\rm eff}|m_1) = \begin{cases} \mathcal{N}(\chi_{\rm eff};\mu,\sigma) & (m_1 < \tilde{m}) \\ (1-\zeta)\mathcal{U}(\chi_{\rm eff}; w) + \zeta\mathcal{N}_{\rm u}(\chi_{\rm eff};\mu_{\rm u},\sigma_{\rm u}) & (m_1 \geq \tilde{m}), \end{cases} \quad (6)$$

where the mixing fraction $0 \leq \zeta \leq 1$. In this latter model, the potentially asymmetric distribution of $\chi_{\rm eff}$ above $\tilde{m}$ (if $\mu_{\rm u}$ is nonzero) allows us to assess how well the data support the theoretical expectation of the symmetry of $\chi_{\rm eff}$ around zero for $m_1 > \tilde{m}$ without this being enforced by the model.

If $\tilde{m}$ cannot be constrained or its posterior distribution rails against the limits of the prior, this would imply that a model with a separate spin distribution population above $\tilde{m}$ cannot be statistically distinguished from a Gaussian model applied across the entire mass range. A well-measured $\tilde{m}$, in turn, implies that there is a distinct mass threshold above which the population of binary BH mergers has a measurably distinct distribution of $\chi_{\rm eff}$. We measure $\tilde{m} = 44^{+6}_{-4} M_\odot$ for the $\pi_{\mathcal{N}+\mathcal{U}}$ model (hereafter, reported measurements are median and 90% credible interval). The posterior distributions of $\tilde{m}$ and w are shown in Fig. 2. We infer $w = 0.5^{+0.3}_{-0.2}$ and $0.5^{+0.3}_{-0.3}$ under the $\pi_{\mathcal{N}+\mathcal{U}_w}$ and the $\pi_{\mathcal{N}+\mathcal{N}\mathcal{U}_w}$ models, respectively. While the recovered posteriors on w are quite broad, they peak close to the expected value $w \simeq 0.47$ for hierarchical mergers. We show in Fig. 2 the distribution of $\chi_{\rm eff}$ as inferred under $\pi_{\mathcal{N}+\mathcal{N}\mathcal{U}_w}$. Below $\tilde{m}$, the distribution is a narrow Gaussian with mean $\mu = 0.05^{+0.03}_{-0.04}$; above $\tilde{m}$ the distribution is consistent with being symmetric around zero and favors a large width as expected from a

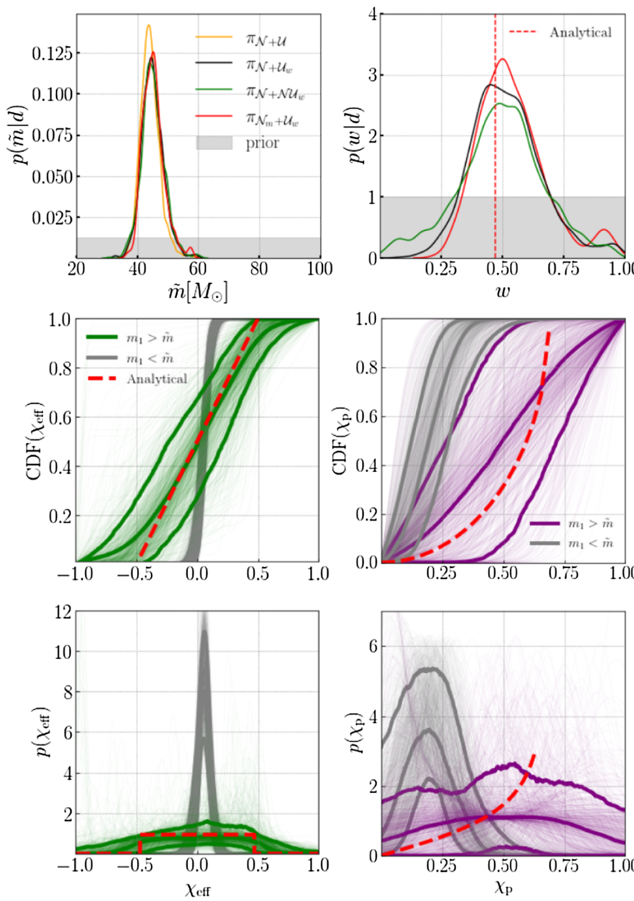

FIG. 2. Posteriors of $\tilde{m}$ (upper-left panel) and w (upper-right panel) obtained under our models. In the middle-left and bottom-left panels we show the distribution of $\chi_{\rm eff}$ for the $\pi_{\mathcal{N}+\mathcal{N}\mathcal{U}_w}$ model, for both the Gaussian component at $m_1 \lesssim \tilde{m}$ and the Uniform + Gaussian component at $m_1 \gtrsim \tilde{m}$. We also show the distribution of χ_p obtained by using equation (8) in the middle-right and bottom-right panels. Thick lines are median, 10th and 90th quantiles, while light lines are individual draws from the posterior. Analytical lines are from Eqs. (1) and (2).

hierarchically formed population of mergers. In SM [63] we show that our inference is unlikely to be affected by Monte Carlo uncertainty in the population likelihood estimator.

The precise measurement of $\tilde{m}$ implies that these models are strongly favored over models in which black holes of all masses share the same spin distribution. More quantitatively, we compute the Bayes factors of models $\pi_{\mathcal{N}+\mathcal{U}}$, $\pi_{\mathcal{N}+\mathcal{U}_w}$, and $\pi_{\mathcal{N}+\mathcal{N}\mathcal{U}_w}$ relative to a model where the entire population is represented by a single Gaussian in $\chi_{\rm eff}$ (e.g., [6]). We find $\log_{10}\mathcal{B} = 4.7, 4.5$ and 4.2, respectively. These results indicate strong evidence in favor of the hierarchical merger model over the Gaussian model above $\simeq 45M\odot$.

Ref. [50] identified a broadening in the distribution of $\chi_{\rm eff}$ with increasing mass and/or redshift. Consistent results were obtained by Ref. [49] using flexible models that allow for a nonmonotonic dependence of the mean and variance of the $\chi_{\rm eff}$ distribution on primary mass. The behavior we identify in this work—the transition to a broad $\chi_{\rm eff}$ distribution above $\approx 45M_\odot$—is likely responsible for this conclusion. To verify this, we consider a fourth model, in which the fixed Gaussian spin distribution below $\tilde{m}$ is replaced with one whose mean and variance evolve linearly with primary mass, as in [50]:

$$\pi_{\mathcal{N}_m+\mathcal{U}_w}(\chi_{\rm eff}|m_1) = \begin{cases} \mathcal{N}(\chi_{\rm eff};\mu_\chi(m_1),\sigma_\chi(m_1)) & (m_1 < \tilde{m}) \\ \mathcal{U}(\chi_{\rm eff};w) & (m_1 \geq \tilde{m}), \end{cases} \quad (7)$$

where $\mu_\chi(m_1) = \mu + \delta\mu(m_1/10M_\odot - 1)$ and $\log\sigma_\chi(m_1) = \log\sigma + \delta\log\sigma(m_1/10M_\odot - 1)$. Under the $\pi_{\mathcal{N}_m+\mathcal{U}_w}$ model we infer that mean and variance of effective spins below $\tilde{m}$ are now consistent with no or mild change with mass ($\delta\mu = 0.00^{+0.02}_{-0.02},\ \delta\log\sigma = -0.24^{+0.22}_{-0.07}$). In fact, the data prefer a reversal of the trend inferred in previous work [50], with the $\chi_{\rm eff}$ distribution slightly narrowing with mass below $\tilde{m}$. Our interpretation is that the population above $\tilde{m}$ may drive the mass- and redshift-dependent broadening reported in [50].

Finally, we consider a model where we also fit for the distribution of $\chi_{\rm p}$, which is represented by a mixture of two Gaussian distributions truncated within [0, 1], one below and one above $\tilde{m}$:

$$\pi_{\chi_{\rm p}}(\chi_{\rm eff},\chi_{\rm p}|m_1) = \begin{cases} \mathcal{N}(\chi_{\rm eff};\mu,\sigma)\mathcal{N}(\chi_{\rm p};\mu_{\rm p,l},\sigma_{\rm p,l}) & (m_1 < \tilde{m}) \\ \mathcal{U}(\chi_{\rm eff};w)\mathcal{N}(\chi_{\rm p};\mu_{\rm p,u},\sigma_{\rm p,u}) & (m_1 \geq \tilde{m}). \end{cases} \quad (8)$$

Under this model, we infer $\tilde{m} = 46^{+6}_{-4}M_\odot$ (see SM [63] for more details). We show the derived distribution of $\chi_{\rm p}$ in Fig. 2. The two distributions above and below $\tilde{m}$ can be nearly separated and the latter is broadly consistent with the theoretical expectation.

Implications—We compare the predicted distribution of the effective spin parameters $\chi_{\rm eff}$ and $\chi_{\rm p}$ for hierarchical mergers to that of the population of observed BH binaries, finding evidence that the spin properties of observed binary BHs change at $\simeq 44M_\odot$. Above this mass, the $\chi_{\rm eff}$ distribution is consistent with the hypothesis of a (P)PISN gap in BH birth masses, which is repopulated by hierarchical mergers in dense clusters. We infer that a fraction $p(m_1 > \tilde{m}) = 0.009^{+0.01}_{-0.007}$ of binary BHs lie in the high-mass and isotropically spinning subpopulation, with no appreciable variation across the different models. This can be interpreted as $\gtrsim 1\%$ of binary BH mergers being of hierarchical origin—as these can also occur below $\tilde{m}$, albeit at a subdominant level—under our models.

Sequential mergers in triples or quadruples [88,89] are also possible, though the expected low merger rate makes this less likely [90]. BHs in the (P)PISN mass gap can also arise from gas accretion and/or hierarchical mergers in AGN disks [91,92] and stellar mergers in star clusters [93,94]. These latter scenarios are unlikely to give rise to the same $\chi_{\rm eff}$ distributions as hierarchical BH mergers in clusters [24,95,96] and are therefore disfavored, although not excluded, by our analysis as a primary formation mechanism.

Our findings align with previous work showing that the BH properties change above a certain mass, suggesting formation in clusters for some fraction of the population [34,37,42,43,45,51,97]. Refs. [43] and [45] found evidence for a high-mass population consistent with hierarchical formation by studying the correlation between the component spin distributions and mass. However, the component spin is not a parameter that is easily inferred from the GW data, and its distribution lacks robust constraints. Other parameters, e.g., mass, mass ratio, and merger rate, cannot be robustly predicted from astrophysical models. We have used $\chi_{\rm eff}$ instead, which is both well constrained from the data and has a distribution that can be predicted from basic principles. This strengthens our conclusions and enables very stringent constraints on a hierarchical formation scenario with future data. Ref. [34] also considered the $\chi_{\rm eff}$ distribution and found that the data allow for the presence of a high-mass population consistent with hierarchical mergers but do not require it. Here, we showed that the data do require the presence of such a population.

The hierarchical formation hypothesis for high-mass BHs makes other predictions that will enable tighter constraints from future GW observations with a growing population of BHs. From the cluster population models, we find that a 1% fraction of hierarchical mergers in the (P)PISN mass gap implies that $\simeq 20\%$ of the BH binaries in the overall astrophysical population are formed in clusters. Therefore, a significant fraction of the detected binaries should present a residual eccentric signature [98–100], of which traces are already claimed to exist in the data [64,101]. If mass-gap BHs form only through hierarchical mergers in clusters, we should expect ~5% of mass-gap mergers to be measurably eccentric. Additionally, because BHs with mass above $\sim 90 M_\odot$ can only be formed from at least two previous mergers and these are rare, we might expect a drop or discontinuity in the merger rate (and binary properties) near this mass.

Software used in this work: astropy [65]; `bilby` [66]; `cBHBd` [61]; `jax` [67]; `numpy` [68]; `numpyro` [69,70]; `scipy` [71].

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Data and code availability—The cluster and hierarchical inference codes used to produce the results in this Letter and the resulting data products are available under reasonable request.

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