energy barriers to forming those structures were too high for clusters to surmount in the cold environment of the neon jet.

The analysis therefore came down to distinguishing contact ion pairs from undissociated structures, and the Townes–Dailey nuclear-spin effect was crucial. The two classes of structures can be hard to differentiate from the arrangements of atoms alone, because shifting an H atom a fraction of an angstrom from an HCl molecule to an H_3O^+ ion might not have much of an effect on the cluster's rotational energy levels. But it makes all the difference to the hyperfine splitting.

From the splitting that they measured, the DESY researchers calculated the clusters' ionic character on a scale from 0 (for a nonpolar covalent bond, as in a Cl_2 molecule) to 1 (for a Cl^- ion). As figure 2 shows, a zero-water HCl cluster—that is, just an isolated HCl molecule—already has an ionic character of almost 0.4. That's because the H–Cl bond is polar, with more of its electron density on the Cl than on the H. For clusters with one to four water molecules, the ionic character doesn't change much. But for five- and seven-water clusters, there's a clear jump: The Cl is almost completely ionic.

What about clusters with six water molecules? The researchers have every reason to think that those will also form contact ion pairs, but they're still working on the spectral assignments. Perhaps counterintuitively, six-water clusters are harder to study than seven-water clusters, because they tend to have lower symmetry. With five or seven water molecules, the Cl^- and H_3O^+ ions can sit in the middle of the cluster, with the rest of the H_2O molecules arranged in pairs or trios symmetrically around the edges. With six water molecules, there's no such option, and the lower-symmetry clusters give rise to more complicated spectra.

The more pressing questions are the ones the researchers don't know the answers to. Can the clusters be made to form separated ion pairs, not just contact ion pairs, either by adding more water molecules or changing the experimental conditions? Do other acids behave the same way as HCl? Spectroscopic study of acid–water clusters is not going to get any easier, as the simplest remaining structures have their spectral lines assigned. But with the right combination of experimental and theoretical tricks—including the Townes–Dailey nuclear-spin effect—further progress may be possible. "Nuclear spin is really cool," says Xie. "It can reveal molecular properties that are difficult to assess in other ways."

Johanna Miller

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How to make a midsize black hole

Detailed simulations of star formation show that runaway collisions in a giant molecular cloud could produce very massive stars that are precursors to intermediate-mass black holes.

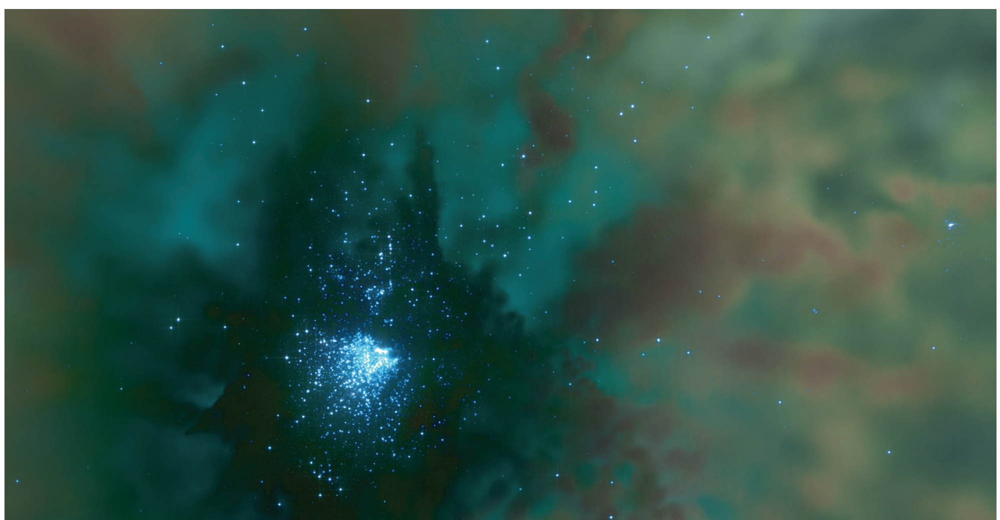

FIGURE 1. A CLUSTER OF STARS (blue dots) forming in a giant molecular cloud, as visualized in this artistic rendering. Simulations indicate that runaway collisions of stars in a gas cloud can create the very massive stars that can produce intermediate-mass black holes. Although astronomers have documented the existence of stellar-mass and supermassive black holes, the black holes' midsize counterparts have proved more elusive. (Courtesy of Michiko Fujii and Takaaki Takeda.)

Found at the center of galaxies, supermassive black holes have the mass of more than 100 000 suns. The largest ones tip the scales at billions of solar masses. Stellar-mass black holes, widely observed in binary systems with a partner star, are typically less than 50 solar masses. But observations of black holes with masses somewhere in between have been relatively sparse. That gap has long puzzled astronomers, who have wondered how supermassive black holes could get so enormous without any intermediate-mass black holes to grow from.

Although astronomers generally agree that stellar-mass black holes form from the collapse of individual stars, the formation mechanisms for intermediate-mass and supermassive black holes are not as well understood. Ideas include the formation and collapse of very massive stars, the merging of smaller black holes, and the accumulation of mass once a black hole has formed. Findings show that some of the largest observed supermassive black holes formed when the universe was less than a billion years old,[1] but it's unclear how they grew so quickly.

New star-by-star simulations by the University of Tokyo's Michiko Fujii and colleagues lend support to one possibility: Stars that grow in dense molecular clouds can merge with the speed and efficiency needed to grow into very massive stars that will eventually collapse to form intermediate-mass black holes.[2] The results suggest that astronomers looking for the elusive midsize black holes should continue to target dense groups of stars known as globular clusters, which are found in the galactic halo of the Milky Way.

Merging codes

Fujii and her team had set out not to simulate the formation of intermediate-mass black holes but rather to investigate the growth of globular clusters from a molecular gas cloud. To do that, the researchers brought together two disparate codes. One simulates the process of star formation from molecular gas clouds, and the other, known as an *N*-body code, models the gravitational interactions of individual stars.

By making improvements to the algorithms in the *N*-body code, Fujii's team could run simulations that contain millions of individually resolved stars. Previous *N*-body codes couldn't include so many individual stars because of computational limitations, so researchers have relied on simplifying assumptions to model star clusters: grouping many stars together as individual particles or using Monte Carlo simulations that contain other simplified parameters.

Fujii and colleagues integrated the more sophisticated *N*-body code with a model of star formation in gas clouds, as illustrated in figure 1. The new code enabled the researchers to simulate the birth of the Orion Nebula and, with the latest study, dense star clusters from their inception. "That they include both gas and stars and have a realistic number of stars is really impressive," says Nathan Leigh of the University of Concepción in Chile. "This brings simulations into a more realistic regime."

Accumulating mass fast

Fujii and colleagues' simulations begin with a gas cloud that contains 10^5–10^6 solar masses worth of matter. The high-density gases form filaments and clumps that eventually collapse to form stars that proceed to grow, interact, and merge amid the cloud.

Generally, as stars grow larger, they generate stronger stellar winds that cause them to lose mass. The competition between mass loss and mass accumulation can thus limit their growth. But the simulations show that the gravitational potential from the dense gas cloud around the stars keeps the star cluster compact. So as more stars merge, mass accumulates faster than it is lost. Eventually, stars can form that are more than 1000 solar masses, much more massive than any stars ever observed. As shown in figure 2, those very massive stars, as they're known, gain most of their mass in under 100 000 years. "We expected some collisions of stars to proceed inside globular clusters, but it was surprising to us that we formed such a big star," says Fujii.

Though such massive stars have never been observed, their existence has been predicted by theorists. There are many reasons such enormous stars may not have been sighted—they could have a cool surface that makes them hard to spot in the sky, or they could be short-lived before they collapse into black holes. Other theoretical work has estimated that such a star would collapse into an intermediate-mass black hole after about 2 million years. Fujii and colleagues used stellar-evolution calculations to estimate mass loss from a very massive star over that duration, as shown in figure 2. But because very massive stars remain only theoretical, the calculations of how they would evolve are a best guess.

"Nobody knows how a 1000 solar mass star evolves, what is the nuclear burning process in these extraordinary massive objects," says Simon Portegies Zwart of Leiden University.

To assess whether the growth of very massive stars would be limited to the early universe or could be ongoing, Fujii and colleagues explored different values of metallicity, the proportion of elements heavier than helium. Stars that formed earlier in the universe's history have lower metallicity. Generally, stars with higher metallicity generate stronger stellar winds that reduce their mass, so lower metallicity is considered favorable for the formation of very massive stars.

The simulations contained varied metallicities, from levels similar to those observed in Milky Way globular clusters to a value five times as high. Models with lower metallicity produced the largest stars in the simulations, but runaway collisions still produced very massive stars in the high-metallicity scenarios. That finding suggests that very massive stars could still be forming today.

Seeing in the dark

What Fujii and colleagues found in their simulations supports results from simpler models published decades ago that identified globular clusters as potential sites for the growth of intermediate-mass black holes.[3] The new result encourages ongoing exploration of those clusters, but obstacles to finding midsize black holes remain. Observational challenges that are unique to the intermediate-mass range may partially explain their seeming absence. "It's strange to have a gap of four orders of magnitude," says Jillian Bellovary of Queensborough Community College in New York. "It doesn't mean they aren't there. We haven't discovered the stuff in the middle because it's hard."

Being black objects against a black background, black holes can be difficult to observe. Orbital dynamics are one reliable way to spot them. Supermassive black holes at the center of galaxies are more easily identified because of their enormous size and also because lots of stars orbit them. Stellar-mass black holes frequently form in binary systems, where their partner stars' mutual orbits can be observed. In both of those systems, frictional heating from the siphoning of matter into the black hole also generates observable x rays and radio waves.

Intermediate-mass black holes are less likely to have easily discerned orbiting stars that would make their presence known. The high density of stars in globular clusters makes it hard to decipher individual orbits, although a recent study may have broken through that barrier: An analysis of two decades of data from the *Hubble Space Telescope* reveals seven stars at the center of Omega Centauri, a Milky Way globular cluster, that are moving so fast that they should escape the cluster unless they are orbiting a black hole of at least 8200 solar masses.[4]

One of the clearest to-date observations of an intermediate-mass black hole took place in 2019, when the merger of two stellar-mass black holes produced a black hole of about 142 solar masses. Nine solar masses' worth of energy radiated from that merger as gravitational waves, which were detected by the twin detectors of the Laser Interferometer Gravitational-Wave Observatory (LIGO) in the US and the Virgo observatory in Italy.

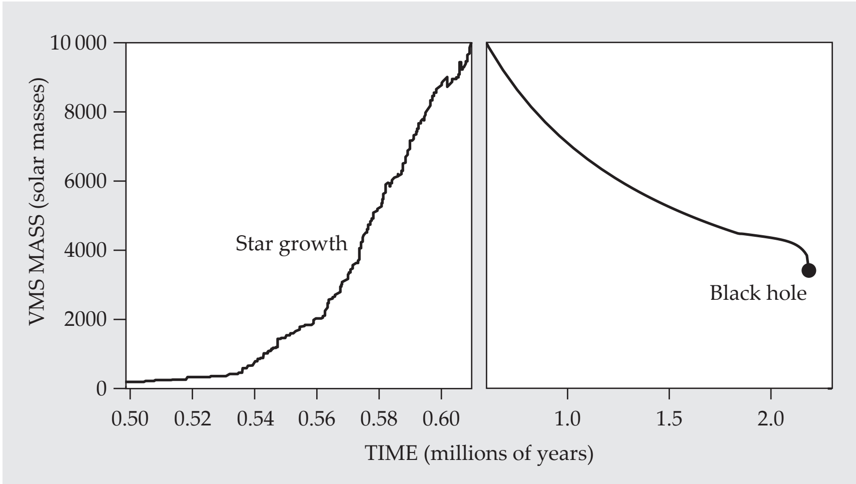

FIGURE 2. VERY MASSIVE STARS (VMSs) can be produced by runaway collisions of smaller stars in a globular cluster. This detailed simulation indicates that a very massive star accumulates most of its mass in less than 100 000 years. After formation stops, such a large star could evolve and collapse into an intermediate-mass black hole over a few million years. (Adapted from ref. 2.)

The LIGO–Virgo observation shows that the collisions of stellar-mass black holes represent one viable method for producing black holes at the smaller end of the intermediate-mass range. Such collisions of stellar-mass black holes, not to mention collisions of stars, are most likely to occur in dense star clusters. But a merger of black holes of different sizes produces asymmetrical gravitational waves that can kick the resulting black hole out of the star cluster, where it is less likely to merge with other objects.

Tidal dissipation allows stars to absorb more of the energy from mergers, so stellar collisions don't produce the same kind of kick that merging black holes do. Thus a very massive star that collapses into an intermediate-mass black hole has been favored as a formation mechanism over the merging of smaller black holes. But there's no reason both can't happen. Once a black hole is massive enough, a merger with a small black hole no longer produces a kick large enough to displace the merged black hole.

The size scale of LIGO and Virgo limits the frequencies of gravitational waves that they can pick up, so they can't detect mergers of black holes at the larger end of the intermediate-mass range. The Laser Interferometer Space Antenna (LISA) mission—led by the European Space Agency in collaboration with NASA and the LISA Consortium—aims to fill that gap (see PHYSICS TODAY, July 2010, page 14). Scheduled to launch in the mid 2030s, LISA is made of three spacecrafts that will be separated by millions of kilometers and will trail Earth in its orbit like a cartwheeling triangle. By sending lasers between its three crafts, LISA will use the same interferometry technique that LIGO and Virgo do, but it will be able to detect gravitational waves at the low frequencies needed to find larger collisions.

As the hunt for more intermediate-mass black holes continues, Fujii and colleagues' simulations confirm that globular clusters are good targets. Fujii plans to continue expanding the size of the star-by-star simulations. Her next goal is to simulate the first star clusters that formed in the universe with almost no metallicity because they may have the potential to form even more massive stars.

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