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A selection of scientific results produced by NERSC users.

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Baby Brutes

Simulations Help Solve the Mysteries of Massive Young Star-Forming Galaxies

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Astronomers have in recent years been surprised to find hulking brutes among the baby galaxies of the early Universe. Studded with bright, giant clumps of rapidly forming stars, these big galaxies hail from a time when the cosmos was less than 4 billion years old, yet each contains about the mass of a modern Milky Way, which took 10 billion years to form.

Once considered oddities, these galaxies are now thought to be the engines that drove the Universe's most active period of star formation. It remains a mystery, however, how such massive galaxies came to be so quickly and what has happened to them in our modern Universe. Attempts to model the evolution of these so-called star-forming galaxies (SFGs) have failed. When modelers feed gas into a typical galaxy simulation at the high rates required for an SFG, the resulting galaxy can be misshapen or form too many stars too quickly, or both.

"There have been a lot of problems trying to understand galaxies. In fact, there are many aspects of galaxies that are still quite mysterious," said Joel Primack of the University of California, Santa Cruz, who is the principal investigator for the Galaxy Formation Simulation project that computes at NERSC. His group uses computer simulations and visualizations to explore questions about the structure, nature, and fate of the cosmos.

One of the team, Daniel Ceverino, may have cracked the SFG case. Zeroing in on single galaxies with high-resolution simulations and compensating for the effects of supernovae and runaway stars, Ceverino successfully simulated SFG-like galaxies using NERSC’s Bassi system.

"These are the best physics, highest resolution simulations anyone has run to date of forming galaxies," said Primack, who helped originate cosmology's standard model (Lambda Cold Dark Matter) under which simulations are run. "The Bassi machine at NERSC has been one of the best machines available for doing that kind of simulation," he added.

Ceverino of The Hebrew University, Jerusalem and collaborator Anatoly Klypin of New Mexico State University outlined their groundbreaking simulations in The Astrophysical Journal. In a second paper published in the same journal, Avishai Dekel, Re'em Sari and Ceverino, all of The Hebrew University, Jerusalem, used the simulations to explore a theory for how these unusual galaxies formed.
matter underpins the visible Universe. Galaxies form when the gravity of dense dark-matter knots snags streams of relatively cold gases (approximately 10,000 Kelvin). Compressed by gravity, the gases fuel star creation. Massive stars, in turn, slow the formation of additional stars by injecting energy, mass, and metals back into the galaxy-formation process through stellar winds and supernova explosions—a process called stellar feedback.

Because of the large scale and subsequent low resolution of many simulations, however, stellar feedback has been poorly accounted for in typical models, especially the feedback of runaway stars. Runaway stars are massive stars ejected from their natal molecular clouds by gravitational effects. A dramatic, though uncommon example would be when one of a binary pair goes supernova: losing the mass to hold its partner in co-orbit, it slings the other star out into space. Outside the damping effects of a giant molecular cloud, about 10 percent of runaway stars themselves explode as supernovae. The energy released from runaway supernovae ripples out for hundreds of light years, increasing their impact on galaxy formation.

Ceverino, a PhD candidate at New Mexico State University at the time, and Klypin, his advisor, adjusted their simulations to account for the feedback effects of both massive star clusters and runaway stars. Testing the changes on a galactic plane with a volume of 4,000 parsecs on a side (1 parsec = 3.26 light years), the researchers successfully reproduced the characteristics they expected of stellar feedback: chimneys of fast, hot outflows of gas, and smaller, hot gas bubbles (Figure 1) resulting in galactic winds.

**A More Realistic Model**

Using the adjusted simulation, Ceverino and Klypin then modeled three massive galaxies at "high redshift." Astronomers measure the distance (and thus the age) of galaxies based on how much their once-blue light has stretched, shifting it into the red spectrum. The redder the light, the higher the redshift value, the further away (and the longer ago) is an observed galaxy.

Unlike previous models, the galaxies in the adjusted simulation looked very much like the star-forming galaxies astronomers observe (Figure 2). Instead of smooth, large central bulges, their visualizations formed thickened disks with clumpy arms, much like SFGs (Figure 3). The simulations also supported the theories of astronomer Avishai Dekel, who had proposed in a January 2009 Nature article an explanation of how SFGs form. If incoming gas streams could remain "cold" (about 10,000 Kelvin) and stream continuously into the galaxy core, Dekel proposed, SFGs could form. Ceverino's models showed streams of cold, often clumpy gas streams feeding early-stage galaxies.

The models also suggest that these wild, violent galaxies may have settled down considerably in the space of a few billion years. In the simulations, star-forming clusters make a few galactic rotations before being drawn into a central bulge, which slows star formation and "quenches" galaxy growth. Cranking up the resolution was key. Lower-resolution simulations didn't properly account for stellar feedback. At resolutions poorer than 50 parsecs, the models lost resemblance to observed galaxies. Ceverino ran simulations at resolutions high as 35 parsecs, ten times that of typical simulations.

On both cosmological and computational scales, that's unusually fine. Our own Milky Way galaxy measures 30,000 parsecs across. At the
finest resolutions, these galactic models were imaging only portions of a single galaxy. "If you're doing simulations that fine, then you can resolve the regions where stars form, though not the individual stars themselves," Primack said.

The models may also help scientists finally identify some of the oldest and most mysterious cosmic structures ever observed: Lyman-alpha blobs. Primack and colleagues are exploring whether these glowing globs of gases may actually be evidence of the cosmic streams that fed SFGs. Ceverino's close-up, high-resolution models will also help increase the accuracy of larger-scale simulations aimed at understanding how dark matter and visible, or baryonic, matter interact.

"Nobody has the computer power or the understanding of underlying physics to try to do everything in one go," said Primack. "We learn what we can from the small-scale simulations and extend that up to larger-scale models."

The Next Challenge: Black Holes

Meanwhile, Ceverino's simulations have reached 6.2 billion years, almost half the age of the Universe, and continue to run at NERSC. The Bassi system is set for early 2010 decommissioning, but his work will continue on the Franklin (Cray XT4) and Hopper (Cray XT5) systems. Primack's group may also test this and other codes on NERSC's Magellan, a scientific cloud computing testbed.

Primack's next challenge is to incorporate the effects of black holes found at the center of massive galaxies into models. "Black holes are 1,000 times more effective than stars at releasing energy from matter, so there's no doubt these black holes play a huge part in galaxy formation," said Primack.
A typical event in the STAR detector that includes the production and decay of an antihypertriton candidate (H3 with a bar indicates an antithydrogen 3 nucleus; the lambda with a bar indicates that it contains an antilambda). The dashed black line is the trajectory of the candidate, which cannot be directly measured. The heavy red and blue lines are the trajectories of an antihelium nucleus and a pion, decay daughters which are directly measured.

Translated, the newly detected "antihypertriton" means a nucleus of antihydrogen containing one antiproton and one antineutron—plus one heavy relative of the antineutron, an antilambda hyperon.

Most of the objects in the cosmos today consists of matter, comprised of "normal" particles like positively charged protons and negatively charged electrons. Each of these fundamental particles has a corresponding "antiparticle." Antiparticles have primarily the same properties as their normal counterparts, with a few reversals. For example, antiprotons have the same mass as protons but a negative charge, and positrons have the same properties as electrons but with a positive charge. Just as most "normal" hydrogen is comprised of a proton and electron, antihydrogen is comprised of an antiproton and positron.
"STAR is the only experiment that could have found an antimatter hypernucleus," says Nu Xu of the Lawrence Berkeley National Laboratory's Nuclear Science Division, the spokesperson for the STAR experiment. "We've been looking for them ever since RHIC began operations. The discovery opens the door on new dimensions of antimatter, which will help astrophysicists trace back the story of matter to the very first millionths of a second after the Big Bang."

Cosmologists believe that equal quantities of matter and antimatter were created in the Big Bang, yet most of the cosmic objects observed today are made of matter. So why is there more matter than antimatter in the universe? This is one of the greatest mysteries in science, and solving it could tell us why human beings, indeed why anything at all, exists today.

**Computers and Colliders Collaborate to Find Antimatter**

So far, scientists have only been able to study antimatter by colliding particles in accelerators. By colliding gold ions at high energies in RHIC, the STAR collaboration is attempting to recreate what is believed to be the conditions in the universe just microseconds after the Big Bang. The enormous energy density that existed at that time would have separated the constituents of protons and neutrons, called quarks.

This very hot cosmic stew of free floating fundamental particles, including quarks, antiquarks and gluons is known as the quark-gluon plasma. As the universe expanded and cooled, the quarks recombined in a variety of ways to make

The diagram above is known as the 3-D chart of the nuclides. The familiar Periodic Table arranges the elements according to their atomic number, Z, which determines the chemical properties of each element. Physicists are also concerned with the N axis, which gives the number of neutrons in the nucleus. The third axis represents strangeness, S, which is zero for all naturally occurring matter, but could be non-zero in the core of collapsed stars. Antinuclei lie at negative Z and N in the above chart, and the newly discovered antinucleus (magenta) now extends the 3-D chart into the new region of strange antimatter.
protons and neutrons (consisting solely of up and down quarks), hyperons (which contain strange quarks) and all of the associated antiparticles. Because quarks and antiquarks exist in equal numbers in the quark-gluon plasma, the cooling gas produces both matter and antimatter. Eventually, a small fraction of these particles combined to form light nuclei and their antiparticles like the antihypertritons detected by the STAR collaboration. To identify this hypernucleus, physicists used supercomputers at NERSC and other research centers to painstakingly sift through the debris of some 100 million collisions.

The team also used NERSC's PDSF system to simulate detector response. These results allowed them to see that all of the charged particles within the collision debris left their mark by ionizing the gas inside RHIC's time projection chamber, while the antihypertritons revealed themselves through a unique decay signature—the two tracks left by a charged pion and an antihelium-3 nucleus, the latter being heavy and so losing energy rapidly with distance in the gas.

"These simulations were vital to helping us optimize search conditions such as topology of the decay configuration," says Zhangbu Xu, a physicist at Brookhaven who is part of the STAR collaboration. "By embedding imaginary antimatters in a real collision and optimizing the simulations for the best selection conditions, we were able to find a majority of those embedded particles."

Physicists agree that the discovery also extends human knowledge of the nuclear terrain. Physicists represent this terrain graphically by placing each kind of nucleus on a three-dimensional graph with the three axes being Z, the number of protons in a nucleus; N, the number of neutrons; and S, the degree of strangeness. Each of these three axes has positive and negative sections, allowing for the representation of both particles and antiparticles. This latest result extends the nuclear terrain below the N–Z plane for the first time.

Jinhui Chen, a postdoctoral researcher at Kent State University and currently a staff scientist at the Shanghai Institute of Applied Physics, and Zhangbu Xu were among the lead authors of the paper that was published in the March issue of Science Express. Their work utilized more than 100,000 processor hours on NERSC's PDSF and was partially supported by the Offices of Nuclear Physics and High Energy Physics in the Department of Energy's Office of Science. Data generated by RHIC's STAR experiment, located at the Brookhaven National Laboratory in New York, travels to NERSC, managed by Lawrence Berkeley National Laboratory in Berkeley, Calif., via DOE's
high-bandwidth Energy Sciences Network (ESnet).

This story was adapted from an article published on physicsworld.com and the Berkeley Lab feature "STAR Discovers the Stranges Antimatter Yet."

Read more about Berkeley Lab’s Computing Sciences: http://www.lbl.gov/cs
It's raining helium on Jupiter—and as these droplets fall towards the planet's deeper interior, they are bringing neon down with them.

This new result, published in the March 26 issue of *Physical Review Letters*, solves a 15-year-old mystery that was initiated on December 7, 1995, when NASA's Galileo probe plunged into Jupiter's atmosphere and found only one-ninth the amount of neon that should have been there based on measurements of the Sun's composition. The authors, Burkhard Militzer and Hugh Wilson of the University of California, Berkeley, were able to answer this decade-old question with some supercomputing help from the Department of Energy's National Energy Research Scientific Computing Center (NERSC).

Since 1995, astronomers have suspected that neon in Jupiter's interior was dissolving into droplets of condensed helium. However, Wilson notes that the UC Berkeley team was the first to actually test the hypothesis.

"Because the pressures on Jupiter currently cannot be reproduced in a laboratory, we had to rely on computer simulations to determine whether neon would prefer to be dissolved in hydrogen or helium, since these two elements make up the majority of
A slice through the interior of Jupiter shows the top layers that are depleted of helium and neon, the thin layer where helium drops condense and fall, and the deep interior where helium and neon
Sun and the gas on Jupiter should have very similar composition. As asteroids and comets collided with the planet over time, concentrations of elements other than hydrogen and helium became enhanced. The fact that Galileo detected most of these enhanced chemical concentrations in Jupiter’s atmosphere, except for neon, reaffirmed widely accepted theories about Jupiter’s formation. But until helium rain, scientists didn't have an explanation for the missing neon.

"We are very grateful to NERSC for providing us with CPU hours in the beginning stages of our research. This time allowed us to run a large number of relatively short runs at a critical stage of our research," says Wilson.

"We only used about 10,000 to 20,000 computing hours at NERSC for this project, but it was very useful. These simulations showed us that science puzzles can also be solved with relatively small allocations," says Militzer.

Militzer is a NERSC user and assistant professor of earth and planetary science at UC Berkeley. Wilson is a postdoctoral fellow at UC Berkeley. The team used both density functional theory and molecular dynamic supercomputer simulations to achieve their result.

About NERSC and Berkeley Lab
The National Energy Research Scientific Computing Center (NERSC) is the primary high-performance computing facility for scientific research sponsored by the U.S. Department of Energy’s Office of Science. Berkeley Lab is a U.S. Department of Energy national laboratory located in Berkeley, California. It conducts unclassified scientific research and is managed by the University of California for the DOE Office of Science.

For more information about computing sciences at Berkeley Lab, please visit: www.lbl.gov/cs
Simulations Reveal That Earth’s Silica Is Predominantly Superficial

Simulations Reveal That Earth's Silica Is Predominantly Superficial

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Silica is one of the most common minerals on Earth. Not only does it make up two-thirds of our planet's crust, it is also used to create a variety of materials from glass to ceramics, computer chips and fiber optic cables. Yet new quantum mechanics results generated by a team of physicists from Ohio State University (OSU) show that this mineral only populates our planet superficially—in other words, silica is relatively uncommon deep within the Earth.

Using several of the largest supercomputers in the nation, including the National Energy Research Scientific Computing Center's (NERSC) Cray XT4 "Franklin" system, the team simulated the behavior of silica in high-temperature, high-pressure environments that are particularly difficult to study in a lab. These details may one day help scientists predict complex geological processes like earthquakes and volcanic eruptions. Their results were published in the May 10 online early edition of the Proceedings of the National Academy of Sciences (PNAS).

"Silica is one of the simplest and most common minerals, but we still don't understand everything about it. A better understanding of silica on a quantum-mechanical level would be useful to earth science, and potentially to industry as well," says Kevin Driver, an OSU graduate student who was a lead author on the paper. "Silica adopts many different structural forms at different temperatures and pressures, not all of which are easy to study in the lab."
Over the past century, seismology and high-pressure laboratory experiments have revealed a great deal about the general structure and composition of the Earth. For example, such work has shown that the planet's interior structure exists in three layers called the crust, mantle, and core. The outer two layers—the mantle and the crust—are largely made up of silicates, minerals containing silicon and oxygen. Still, the detailed structure and composition of the deepest parts of the mantle remain unclear. These details are important for complex geodynamical modeling that may one day predict large-scale events, such as earthquakes and volcanic eruptions.

Driver notes that even the role that the simplest silicate—silica—plays in the Earth's mantle is not well understood. "Say you're standing on a beach, looking out over the ocean. The sand under your feet is made of quartz, a form of silica containing one silicon atom surrounded by four oxygen atoms. But in millions of years, as the oceanic plate below becomes subducted and sinks beneath the Earth's crust, the structure of the silica changes dramatically," he said.

As pressure increases with depth, the silica molecules crowd closer together, and the silicon atoms start coming into contact with more oxygen atoms from neighboring molecules. Several structural transitions occur, with low-pressure forms surrounded by four oxygen atoms and higher-pressure forms surrounded by six. With even more pressure, the structure collapses into a very dense form of the mineral, which scientists call alpha-lead dioxide.

Driver notes that it is this form of silica that likely resides deep within the earth, in the lower part of the mantle, just above the planet's core. When scientists try to interpret seismic signals from that depth, they have no direct way of knowing what form of silica they are dealing with. They must rely on high-pressure experiments and computer simulations to constrain the possibilities. Driver and colleagues use a particularly high-accuracy, quantum mechanical simulation method to study the behavior of different silica forms, and then compare the results to the seismic data.

In *PNAS*, Driver, his advisor John Wilkins, and their coauthors describe how they used a quantum mechanical method to design computer algorithms that would simulate the silica structures. When they did, they found that the behavior of the dense, alpha-lead dioxide form of silica did not match up with any global seismic signal detected in the lower mantle. This result indicates that the lower mantle is relatively devoid of silica, except perhaps in localized areas where oceanic plates have
The structure of a six-fold coordinated silica phase called stishovite, a prototype for many more complex mantle minerals. Stishovite is commonly created in diamond anvil cells and often found naturally where meteorites have slammed into earth. Driver and co-authors computed the shear elastic constant softening of stishovite under pressure with quantum Monte Carlo using over 3 million CPU hours on Franklin.

"As you might imagine, experiments performed at pressures near those of Earth's core can be very challenging. By using highly accurate quantum mechanical simulations, we can offer reliable insight that goes beyond the scope of the laboratory," said Driver.

**Supercomputers Dissect Silica with Quantum Monte Carlo Calculations**

The team's work was one of the first to show that quantum Monte Carlo (QMC) methods could be used to study complex minerals deep in the planet's interior. Although the algorithms have been around for over half a century, Driver notes that applying them to silica was simply too labor- and computer-intensive, until recently.

"In total, we used the equivalent of six million CPU hours to model four different states of silica. Three million of those CPU hours involved using NERSC's Franklin system to calculate a shear elastic constant for silica with the QMC method. This is the first time it had ever been done," said Driver.

He notes that the QMC calculations on Franklin were completed during the system's pre-production phase, before the system was formally accepted by NERSC. During this phase, the center's 3,000 science users were encouraged to try out the Cray XT4 system to see if it could withstand the gamut of scientific demands from different disciplines. Driver notes that the Franklin results allow him to measure how silica deforms at different temperatures and pressures.

"From computing hardware to the consulting staff, the resources at NERSC are really subducted.
excellent. The size and speed of the center’s machines is something that I don’t normally have access to at other places," says Driver.

"This work demonstrates both the superb contributions a single graduate student can make, and that the quantum Monte Carlo method can compute nearly every property of a mineral over a wide range of pressures and temperatures," said Wilkins. "The study will stimulate a broader use of quantum Monte Carlo worldwide to address vital problems."

He and his colleagues expect that quantum Monte Carlo will be used more often in materials science in the future, as the next generation of computers goes online. Coauthors on the paper included Ronald Cohen of the Carnegie Institution of Washington; Zhigang Wu of the Colorado School of Mines; Burkhard Militzer of the University of California, Berkeley; and Pablo López Ríos, Michael Towler, and Richard Needs of the University of Cambridge.

This research was funded by the National Science Foundation and the Department of Energy. In addition to NERSC, computing resources were also provided by the National Center for Atmospheric Research, the National Center for Supercomputing Applications, the Computational Center for Nanotechnology Innovations, the TeraGrid and the Ohio Supercomputer Center. Click here to read the PNAS abstract.

Portions of this story were adapted from an OSU press release written by Pam Frost Gorder.

About NERSC and Berkeley Lab: The National Energy Research Scientific Computing Center (NERSC) is the primary high-performance computing facility for scientific research sponsored by the U.S. Department of Energy’s Office of Science. Berkeley Lab is a U.S. Department of Energy national laboratory located in Berkeley, California. It conducts unclassified scientific research and is managed by the University of California for the DOE Office of Science.

For more information about computing sciences at Berkeley Lab, please visit: www.lbl.gov/cs
Berkeley Lab Team Receives NASA Public Service Group Achievement Award

June 11, 2010

Three scientists from the Lawrence Berkeley National Laboratory’s (Berkeley Lab) Computational Cosmology Center (C3) are being honored with a NASA Public Service Group Award for developing the supercomputing infrastructure for the U.S. Planck Team’s data and analysis operations at the Department of Energy’s National Energy Research Scientific Computing Center (NERSC).

The award will be presented to current C3 members Julian Borrill, Christopher Cantalupo and Theodore Kisner, as well as former members Sara Ricciardi, Federico Stivoli and Radek Stomporon on June 15, 2010 at the Jet Propulsion Laboratory in Pasadena, Calif. All three researchers are also members of the U.S. Planck Team. The NASA Public Service Group Achievement Award honors a group’s outstanding accomplishment that has contributed substantially to a NASA mission.

The European Space Agency’s Planck satellite— in which NASA is a major partner— is currently gathering the most detailed observations ever made of the Cosmic Microwave Background (CMB), which is essentially the leftover light from the Big Bang that permeates our universe. Transforming these observations into maps of the CMB is a very significant computational challenge in which NERSC’s supercomputers play a leading role. Computing is so critical to the U.S. contribution to the mission that NASA and DOE

From top to bottom: Julian Borrill, Christopher Cantalupo, Theodore Kisner
have entered into a unique Interagency Implementation Agreement guaranteeing Planck long-term access to NERSC resources.

"The CMB is our most valuable resource for understanding fundamental physics and the origins of the universe. We have spent much of the last decade getting the Planck data analysis infrastructure set up at NERSC, and getting this award is really a great honor to our work," says Borrill.

In addition to developing and maintaining the massively parallel software for processing and analyzing data collected by the Planck's high- and low-frequency instruments, the C3 scientists also work closely with NERSC staff to ensure that both the data and the mission-specific and general CMB analysis tools are available on all of the facility's platforms and accessible to all members of the U.S. Planck Team.

The Berkeley Lab team is also named on a second award to the US Planck Data Analysis team for outstanding participation as a partner with European colleagues in conceiving and implementing the overall data analysis strategy for the Planck mission.

For more information about NERSC's legacy of computational cosmology, please read:

- NERSC Continues Tradition of Cosmic Microwave Background Data Analysis with the Planck Cluster
- Mapping the Universe to the Beginning of Time
- A Rising Tide of Cosmic Data

C3 is a joint center of the Berkeley Lab's Computational Research and Physics Divisions. For more information about Berkeley Lab Computing Sciences, please visit: www.lbl.gov/cs