Rare open-access quantum computer now operational
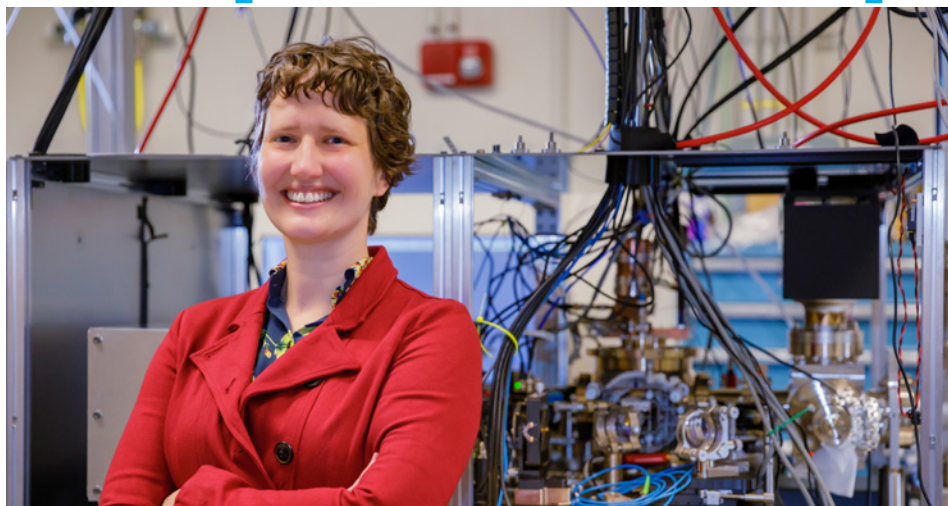
QUANTUM FOR ALL — Sandia physicist Susan Clark leads the team that built the Quantum Scientific Computing Open User Testbed. The ion-based quantum computer was made for outside researchers to use. **Photo by Bret Latter**

Scientists worldwide can use ion-based testbed

By Troy Rummler

A new DOE open-access quantum computing testbed is ready for the public. Scientists from Indiana University recently became the first team to begin using Sandia's **Quantum Scientific Computing Open User Testbed**, or QSCOUT.

Quantum computers are poised to become major technological drivers over the coming decades. But to get there, scientists need to experiment with quantum

Finding fire and ice: Modeling the probability of methane hydrate deposits on the seafloor

Sandia scientists use machine learning to find fuel source, climate-change driver

By Mollie Rappe

Methane hydrate, an icelike material made of compressed natural gas, burns when lit and can be found in some regions of the seafloor and in Arctic permafrost.

Thought to be the world's largest source of natural gas, methane hydrate is a potential fuel source. If it "melts" and releases methane gas into the atmosphere, it is a potent greenhouse gas. For these reasons, knowing where methane hydrate might be located, and how much is likely there, is important.

A team of researchers from Sandia and the **U.S. Naval Research Laboratory** have developed a new system to model the likelihood of finding methane hydrate and methane gas that was tested in a region of seafloor off the coast of North Carolina.

While methane hydrate deposits have been found in a variety of locations, there are significant unknowns in terms of how much methane hydrate exists on the seafloor and where. It is challenging to collect samples from the seafloor to find methane hydrate deposits. This

SANDIA & THE MARS MISSION

TABLE of CONTENTS

LABNEWS Notes

Spinning lights first step to computing future

By Michael Ellis Langley

Most of us rarely look up when we trek into a Costco, Home Depot or other large retailer. Usually, there's nothing of interest on the ceiling. But if one of Sandia's newest patents becomes an industry standard, those huge lights illuminating huge spaces may light the way to cooling computers and other electronics.

Engineer Jeff Koplow and his team have developed a way to use less energy to cool light fixtures. Their outside-the-box idea is to spin the LED emitters at 1,000 rpm to cool them. The 1,000 watts of electricity required to power the LEDs also powers the spinning emitters, Jeff said.

The rotating LED emitter array generates no perceptible flicker, and thus imposes no degradation of lighting quality. The cooling method also will extend the life of lighting fixtures, because keeping LED junction temperature low drastically improves LED service lifetime and requires less maintenance.

LAMPS IN ACTION — Two lights fitted with Sandia Cooler technology were put on display at the Light Fair International conference and trade show in Philadelphia, in May 2019.

Photo courtesy of Jeff Koplow

"We wanted to pursue an application with lighting first," Jeff explained. "It's a high-visibility application that demonstrates that the Sandia Cooler technology is now viable to businesses and consumers. That gets the conversation started that there is a new approach to cooling for electronics."

Jeff believes the same technology can be adapted to cooling of computer central processing units and graphics processing units by transmitting the internal data stream across a narrow air gap.

Compact and easy to install

The cooler is extremely compact for such a large lighting fixture, essentially fitting inside the lamp. Traditional heat sink units for such lights are many, many times the size of the fixture and far more challenging to install.

"The idea here was you could get the best of all worlds," Jeff said. "Use the minimum number of LEDs, keep them really cool so they would last the whole life of

the light fixture and do that in a really lightweight and compact form factor without making any sacrifices to efficiency."

Most of the prototype was built by Sandians.

"Construction of the three product demo units was intensely collaborative," Jeff recalled. "There isn't a supplier making the Sandia Cooler. The parts would come in and we would put them together and test successive prototypes. There was also a learning curve from the standpoint of design for manufacturability, but we got there."

Jeff also complimented Sandia's involvement with DOE's Technology Commercialization Fund.

"I thought to myself throughout the process, 'This is exactly what the TCF was designed to do,'" he said. "Bring together a really productive collaboration with people whose incentives are fully aligned, work toward a product and overcome all the hurdles together. The whole process was really satisfying." 🏢

COOL INNOVATION! — The Sandia Cooler technology attached to the top of a traditional light fixture promises to save energy and the cost of replacing the bulbs.
Illustration courtesy of Jeff Koplow

Open-access quantum

machines that relatively few universities or companies have. Now, scientists can use Sandia's QSCOUT for research that might not be possible at their home institutions, without the cost or restrictions of using a commercial testbed.

"QSCOUT serves a need in the quantum community by giving users the controls to study the machine itself, which aren't yet available in commercial quantum computing systems. It also saves theorists and scientists from the trouble of building their own machines. We hope to gain new insights into quantum performance and architecture as well as solve problems that require quantum computation," said Sandia physicist and QSCOUT lead Susan Clark.

She said the new testbed is a rare machine in three ways: first, as a free, open-access testbed; second, as one made with trapped ion technology; and third, as a platform that gives users an uncommon amount of control over their research.

Last month, Sandia began running the testbed's first user experiment for scientists from Indiana University. Researchers from IBM, Oak Ridge National Laboratory, the University of New Mexico and the University of California, Berkeley, also have been selected to begin experiments soon. Their projects range from testing benchmarking techniques to developing algorithms that could someday solve problems in chemistry too complex for normal computers.

Make a proposal

Now, Sandia is calling for more research proposals. Anyone in the world can submit a proposal to use QSCOUT, and computing time is free thanks to funding from the DOE Office of Science, Advanced Scientific Computing Research program. The next group of projects is expected to be selected in the spring.

On top of providing an exceptional research opportunity, QSCOUT has a rare design for a testbed. Most commercial testbeds use technology called superconducting circuits. Such machines need to be kept at ultralow temperatures, making them expensive to build and operate. But Sandia's

testbed uses what is called an ion trap instead. This means Sandia's testbed can run at warmer temperatures. Trapped ions also yield clearer signals than circuits and hold on to information longer, enabling scientists to perform different types of experiments and compare the two platforms.

Trapped ions are held inside QSCOUT in a so-called "trap on a chip," a flat, bow tie-shaped device, about 2 cm (0.8 inches) long, overlaid on a semiconductor chip. Three electrically charged atoms of the element ytterbium are suspended in place by radio waves and an electric field above a hairline channel that runs down the center of the device. Lasers encode information in each ion as a qubit, comparable to a bit in a conventional computer, to perform calculations.

Sandia plans to expand the system from three to 32 qubits over the next three years so scientists can perform more sophisticated tests.

QSCOUT resides at Sandia's Microsystems Engineering, Science, and Applications complex, which also produces microelectronics for the nation's nuclear stockpile. 🏢

Sandia contributes to the Mars 2020 mission

RED PLANET PANORAMA — On the third day of the mission, a zoomable pair of cameras aboard NASA's Perseverance Mars rover captured this 360-degree panoramic photo of the red planet, which was stitched together on Earth from 142 individual images.   **Photo courtesy of NASA/JPL-Caltech/ASU/MSSS**

By **Mollie Rappe**

A team of Sandia scientists and engineers, led by Daniel Clayton, worked tirelessly since 2016 to assess the launch risks and ensure the safe launch of the **Mars 2020 rover Perseverance** last July.

Using Sandia's state-of-the-art supercomputers, they assessed the various risks posed by the rover's **radioisotope thermoelectric generator** in the unlikely event of a catastrophic accident during the launch of the rocket carrying Perseverance. The radioisotope thermoelectric generator powers Perseverance's vital scientific instruments throughout the frigid Mars nights and is built with a rugged, multilayer containment system to minimize the risk of releasing radioactive material.

The safety assessment team ran mechanistic-based computer models of various potential launch accidents, validated with experimental data from smaller-scale tests and previous launch accidents. These smaller-scale tests included burning solid rocket fuel at Sandia's **Thermal Test Complex** and impact tests conducted at Sandia's **Rocket Sled Track** and Los Alamos National Laboratory.

THREE, TWO, ONE, LIFTOFF — Years before the rocket took off from Kennedy Space Center, a team of Sandia scientists assessed the launch risks to ensure the safe launch of the Mars 2020 Perseverance rover.   **Photo courtesy of NASA/Joel Kowsky**

Identifying risk sources

"The results of the assessment are used to identify the main sources of risk, allowing us to reduce the overall risk of the mission before launch," said Daniel. "Right after the launch, I felt a great sense of relief and excitement that everything went the way it was supposed to. Even though our job was to look at what would happen if things went wrong, we really wanted everything to go right. Then when Perseverance landed, the team and I felt a great sense of accomplishment that our analysis helped make this mission possible."

The Sandia-led safety assessment team collaborated with experts from Los Alamos, Idaho and Oak Ridge national laboratories; NASA's **Jet Propulsion Laboratory** and **Kennedy Space Center**; and the **University of Dayton Research Institute**.

Their work, in the form of a Final Safety Analysis Report, was reviewed by DOE, NASA, Environmental Protection Agency, Department of Defense and others, before being eventually briefed to the **Office of the President** in early 2020. This paved the way for Perseverance's launch on July 30, and ultimately its Feb. 18 landing on the red planet.

SAFE LANDING – As shown in this illustration, NASA's Perseverance rover landed safely on Mars after a seven-month journey through space. The event could only take place following a safe launch that had been vetted by Sandia scientists.　　**Courtesy of NASA/JPL-Caltech**

FIRST LOOK — NASA's Perseverance Mars rover captured this first high-resolution, color image after its landing on Feb. 18. The Perseverance rover is part of NASA's Mars Exploration Program, a long-term effort of robotic exploration of the red planet.　　**Photo courtesy of NASA/JPL-Caltech**

Finding fire and ice

is where Sandia's computer modeling expertise comes in.

"This is the first time someone has been able to approach methane hydrate distribution in the same way we approach weather forecasting," said Jennifer Frederick, a computational geoscientist and lead researcher on the project.

"When you hear a weather forecast for a 60% chance of two inches of rain, you don't necessarily expect exactly two inches. You understand that there is uncertainty in that forecast, but it is still quite useful," she said. "In most places on the seafloor we don't have enough information to produce an exact answer, but we still need to know something about methane and its distribution. By using a probabilistic approach, similar to modern weather forecasting, we can provide useful answers."

The new system combines Sandia's longstanding expertise in probabilistic modeling with machine learning algorithms from the Navy. The system was tested and refined by modeling the area around Blake Ridge, a hill on the seafloor 90 to 230 miles southeast of North Carolina's Outer Banks with known deposits of methane hydrate and methane gas.

The team shared its model for Blake Ridge and compared it with previous empirical data in a paper soon to be published in Geochemistry, Geophysics, Geosystems.

'Forecasting' methane with machine learning

The Naval Research Laboratory's **Global Predictive Seafloor Model** provides site-specific details on seafloor properties, such as temperature, overall carbon concentration and pressure. If data is missing for a certain region, the Naval Research Laboratory's model uses advanced machine-learning algorithms to estimate the missing value based on information about another area that may be geographically distant but similar geologically.

The research team imported the data from the Naval Research Laboratory's model into Sandia software that specializes in statistical sampling and analysis, called **Dakota**. Using Dakota, they determined the most likely value

for influential seafloor properties, as well as the natural variation for the values.

Then, in a statistical manner, they inserted a value from this expected range for each property into PFLOTRAN. **PFLOTRAN** is another software maintained and developed at Sandia, which models how chemicals react and materials move underground or under the seafloor. The team conducted thousands of methane production simulations of the Blake Ridge region. All the software involved in the system is open source and will be available for other oceanographic researchers to use.

"One of the biggest things we found is that there is almost no formation of methane hydrates shallower than 500 meters, which is to be expected given the temperature and pressure needed to form methane hydrate," said William Eymold, a postdoctoral fellow at Sandia and primary author of the paper. Solid methane hydrate is known to form in low-temperature, high-pressure environments where molecules of methane are trapped within well-organized water molecules.

The team also found methane gas formed closer to shore. They were able to compare their model to methane hydrate values calculated by past studies and samples collected a few decades ago by the **National Science Foundation's Ocean Drilling Program**, he said. For example, methane hydrate was detected in a seafloor sample collected from a hole drilled on Blake Ridge called Site 997.

"The fact that we predicted methane hydrate formation in similar amounts to past studies and observations really showed that the system appears to be working pretty well and we will be able to apply it to other geographic locations that may have less data," William said.

Importance of methane to the Navy

The location of methane hydrate deposits and methane gas near the seafloor is important to the Navy.

"Understanding how sound interacts with the seafloor is really important for any kind of naval operation," said Jennifer. "Methane gas affects the acoustics dramatically.

"Even if only 1% or 2% of the pore space in the seafloor sediment is filled with a gas bubble, the speed of sound decreases a hundredfold, or more," she

FIRE AND ICE — Sandia researchers used advanced computer models to predict the likelihood of finding methane hydrate, an ice-like material made of compressed natural gas that burns when lit.

Photo courtesy of U.S. Geological Survey
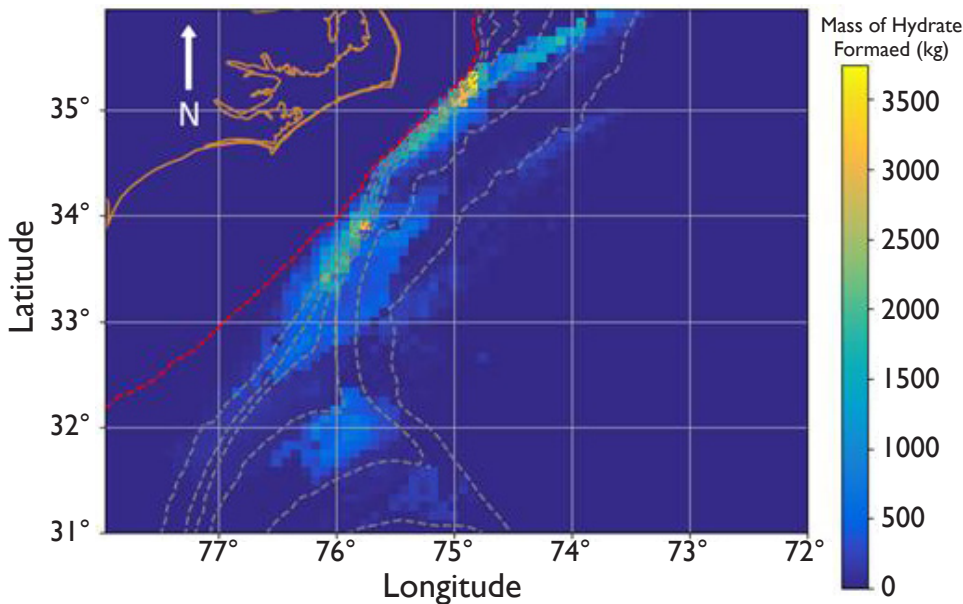
CLOUDY WITH A CHANCE OF METHANE — Using Sandia's longstanding expertise in probabilistic modeling and machine learning algorithms from the Navy, the researchers determined the probability of finding methane hydrate off the coast of North Carolina's Outer Banks where methane hydrate has been found.   **Image courtesy of William Eymold**

said. "This is a very large effect and if you don't account for it properly, then you're not going to get precise acoustics."

Jennifer compared a submarine using sonar to the early arcade game Breakout, where a player moves a paddle horizontally in order to keep a ball bouncing to destroy a wall of bricks. In this analogy, the seafloor serves as the "paddle" to reflect or refract sound waves, or the "ball," in order to get a complete view of obstacles in the ocean. If the paddle started to bounce the ball differently — or held on to the ball for varying lengths of times — depending on where the paddle was located, the game would become far more challenging.

Future modeling projects

So far, the team has used their system to create models of a region of the Norwegian Sea between Greenland and Norway and the shallow waters of the Arctic Ocean offshore of the North Slope of Alaska, two areas of interest to the Navy.

Jennifer has also worked with a large team of international experts to assess the amount of methane and carbon dioxide stored in the shallow Arctic seafloor, and how sensitive those deposits would be to rising temperatures.

The team has also created a much coarser model of the whole globe and has started looking at the mid-Atlantic, where methane gas was spotted bubbling out of the seafloor a few years ago.

"It will be interesting to see if our model is able to predict these regions of methane seeps on the seafloor," Jennifer said. "We'd like to see if we can predict the distribution of these methane seeps and whether they are consistent with the thermodynamic properties of methane-hydrate stability. When you see a seep, that means that there is a lot of gas beneath the seafloor. That will significantly impact how sound travels through the seafloor, and thus sonar. Also, these deposits could be a source of natural gas for energy production, will impact the ocean ecology and nutrient cycles, and if that gas reaches the atmosphere, it will have climate change implications."

This research was funded by Sandia's Laboratory Directed Research and Development program. Jennifer is seeking funding to continue the project with her collaborators at the Naval Research Laboratory.

Recent Patents

September–December 2020

- **Andrea Ambrosini and Eric Nicholas Coker:** Redox-active oxide materials for thermal energy storage. Patent #10800665

- **Hongyou Fan:** Method to synthesize metal halide perovskite particles with high luminescence and stability. Patent #10800798

- **Cy Fujimoto:** Block copolymers including poly(phenylene) and methods thereof. Patent #10800889

- **Mark D. Allendorf, Michael S. Kent and Vitalie Stavila:** Conversion of lignin into a water-soluble polyacid using a MOF catalyst. Patent #10800891

- **Charles J. Mueller:** Ducted fuel injection. Patent #10801395

- **Mark Daniel Rintoul, Christopher G. Valicka and Andrew T. Wilson:** Trajectory prediction via a feature vector approach. Patent #10801841

- **Kevin Youngman:** Power supply including a nonlinear transmission line that receives a single input pulse and outputs a plurality of pulses. Patent #10804804

- **Brad Boyce, Zachary Casias, Nathan Heckman, Todd Huber, Bryan James Kaehr, Nicholas Leathe, Brian T. Lester and William Mook:** Topological damping materials and methods thereof. Patent #10808794

- **Edward Steven Jimenez Jr and Kyle R. Thompson:** Material identification system. Patent #10816485

- **Christopher D. Jenkins:** Systems and methods for monitoring traffic on industrial control and building automation system networks. Patent #10819721

- **Giorgio Bacelli and David G. Wilson:** Nonlinear controller for nonlinear wave energy converters. Patent #10823134

- **Adam Cook, Bryan James Kaehr and William Reinholtz:** Methods of preparing a safety battery. Patent #10826050

- **Timothy J. Draelos and Matthew Gregor Peterson:** Systems, methods and computer program products for self-tuning sensor data processing. Patent #10837811

- **Patrick D Burton and Keith Eugene Frakes:** Blast mitigation foam concentrates and foams made therefrom. Patent #10843154

- **Steve Xunhu Dai:** Interfacial bonding oxides for glass-ceramic-to-metal seals. Patent #10843964

- **Matthew Gregor Peterson, David John Stracuzzi and Charles Vollmer:** Method for enhancing a computer to estimate an uncertainty of an onset of a signal of interest in time-series noisy data. Patent #10859721

- **Travis Mark Anderson, Kyle R. Fenton, Kevin Leung, Harry Pratt, Susan Rempe and Chad Staiger:** Organosilicon-based electrolytes for long-life lithium primary batteries. Patent #10862163

- **John P. Korbin, Carianne Martinez, David Peterson, Kevin Matthew Potter, Matthew David Smith and Charles Snider:** Device and method for constructing and displaying high-quality images from imaging data by transforming a data structure utilizing machine learning techniques. Patent #10867415

- **Timothy J. Boyle:** Molecular tracers and modified proppants for monitoring underground fluid flows. Patent #10871066

- **Harumichi Arthur Kariya and Jeffrey P. Koplow:** Heating and cooling devices, systems and related method. Patent #10876773

- **Eric Christopher Forrest and Joshua Stanford:** Passive millimeter wave radiometer system for calibration of infrared cameras. Patent #10876898

- **Karla Rosa Reyes, Peter Anand Sharma and Josh A. Whaley:** Apparatus, methods and system for temperature gradient aging with in-situ electrical monitoring. Patent #10876987

- **Thomas Edwin Beechem III, Paul Davids, Michael Goldflam, David W. Peters and Isaac Ruiz:** Tunable graphene-based infrared reflectance filter having patterned nanoantenna layer and unpatterned graphene layer. Patent #10877194

Note: Patents listed here include the names of active Sandians only; former Sandians and non-Sandia inventors are not included.

Following the listing for each patent is a patent number, searchable at the U.S. Patent and Trademark Office website (uspto.gov).

Mileposts

Tom Lutz   45

Lawrence Sanchez   20

Recent Retirees

Veronica Argo   28

Kevin Harrison   27

Ken Hatfield   20