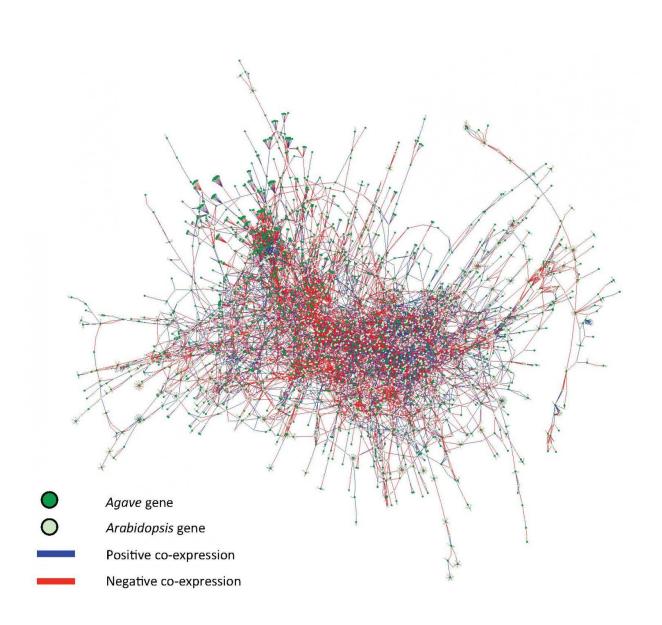


Research team uses supercomputing to understand processes leading to increased drought resistance in food and fuel crops

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This network shows the cross-species co-expression relationships between genes in Arabidopsis and Agave. Dark green nodes represent Agave genes, light green nodes represent Arabidopsis genes, blue edges represent positive co-expression relationships, and red edges represent negative co-expression relationships. The co-expression network was used in the paper to investigate the co-expression relationships of genes within the same gene family. Credit: ORNL

Photosynthesis, the method plants use to convert energy from the sun into food, is a ubiquitous process many people learn about in elementary school. Almost all plants use photosynthesis to gather energy and stay alive.

Not all photosynthetic processes are the same, though. In recent years, researchers have grown increasingly interested in desert <u>plants</u>' preferred method of photosynthesis—crassulacean acid metabolism (CAM), a process named after the *Crassulaceae* family of plants, which include succulents like <u>friendship plants</u>, <u>pig's ears</u>, and <u>hens and chicks</u>.

These plants caught researchers' attention because of their seemingly opposite photosynthetic schedule, and understanding this process may be the genetic key to helping plants of all kinds conserve water. With a more fundamental understanding of CAM, scientists aim to help the plants upon which society relies for food and fuel become more drought resistant, thereby expanding the area where crops can grow and thrive.

"One of the benefits of CAM photosynthesis is water efficiency," said Oak Ridge National Laboratory (ORNL) computational biologist Dan Jacobson, who is part of a multi-institutional team that recently published a CAM study in <u>Nature Plants</u>. "When you think of bioenergy and food crops, you want them to be able to tolerate drought stress or grow in areas that aren't currently arable land. That means they have to



be able to withstand some kind of environmental stress, most commonly drought stress. CAM species are very good at this."

To that end, Jacobson works with a large group of experimentalists and computational scientists to more fully understand the CAM process. This cross-omics team (combining expertise in metabolomics, proteomics, and genomics) uses computing resources at the Oak Ridge Leadership Computing Facility (OLCF)—a US Department of Energy Office of Science User Facility located at ORNL—to catalog how plants' CAM processes vary and ultimately uncover how CAM processes may be genetically engineered into feed stock, food crops, and crops for bioenergy applications.

Shining a light on photosynthesis

When most people think of photosynthesis, they are actually thinking of a specific form, called C3 photosynthesis. This process follows the Calvin Cycle, in which plants capture light energy during the day and convert it into energy-bearing adenosine triphosphate (ATP).

ATP helps plants split water atoms into their hydrogen and oxygen constituent particles. Meanwhile, a C3 photosynthetic plant opens up small pores—called stomata—to absorb carbon dioxide from the atmosphere. Then at night, the newly freed hydrogen particles combine with carbon dioxide absorbed during the day to create the carbohydrates plants use to live and grow.

CAM photosynthesis works the same way, but stomata open for respiration at night and stay tightly closed during the day, allowing plants to conserve more water. This helps plants like cactus and *Agave* survive in climates where water is scarce.

Less than 10 percent of known plant species use this specialized form of



photosynthesis, but researchers hope that by understanding how CAM works, they can apply this water-saving method to other plants. To do that, though, researchers need to understand how molecules interact during CAM photosynthesis and how metabolites and proteins change over time.

Data-intensive design

In addition to simulating processes too dangerous or complex for experiments, supercomputers also help scientists make connections in vast amounts of data. For this project, researchers from ORNL, the University of Tennessee, Newcastle University in the United Kingdom, and the University of Nevada, Reno gathered photosynthesis data from *Agave* (a CAM plant) and compared it with the *Arabidopsis* genus of plants (C3 plants). To conduct a study between *Agave* and a C3 plant, the team selected the *Arabidopsis* genus plant thale cress, one of the first plants to have its genome sequenced and a good candidate for plant studies.

The team then studied what gene expressions control stomata opening and closing in both CAM and C3 plants and how proteins regulated this process. Collecting this data in both a common CAM and a C3 species allowed the team to distinguish traits ubiquitous to CAM plants from species-specific traits. However, finding these connections required a machine capable of comparing large <u>data sets</u> against themselves.

Jacobson and his collaborators used the OLCF's Eos analysis cluster to run "all-versus-all" comparisons of the team's data sets. These comparisons scan large data sets and compare each individual plant's data with all others. This helps the team form relationships between the metabolic processes underpinning CAM in individual *Agave* specimens as well as the differences between *Agave*'s CAM properties from thale cress's C3 properties.



"These all-against-all vector comparisons for correlation networks allowed us to look for different types of patterns and different times of day where the [gene expression] transcripts are correlated with each other, where they were correlated to proteins or metabolites, or times of the day where they shift dramatically," Jacobson said.

The team members gained access to OLCF resources through the OLCF's Director's Discretionary program, and after familiarizing themselves with Titan's hybrid architecture, they plan to expand research into other CAM species, comparing larger data sets and more fully cataloging CAM processes. "As we gain more knowledge from these various approaches, we hope to tease apart the underlying mechanisms for CAM and how it is regulated," Jacobson said. "That starts to build toward having enough knowledge to deploy CAM in a new species."

Jacobson also indicated that without access to high-performance computing, the team would not have been able to find these meaningful connections in a timely manner. "This is the first study looking at a crossomics, time-course experiment to try and explore CAM at this molecular detail," he said. "I think the ability to use supercomputing infrastructure enabled things that wouldn't have been possible otherwise. We were able to have a pretty big impact on the analysis of this work because of those resources."

More information: Paul E. Abraham et al. Transcript, protein and metabolite temporal dynamics in the CAM plant Agave, *Nature Plants* (2016). DOI: 10.1038/nplants.2016.178

Provided by Oak Ridge National Laboratory

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