ALCF Newsbytes

Argonne Leadership Computing Facility

Argonne National Laboratory

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Call for Proposals for Mira Access Opens April 11

Mira, the ALCF's IBM Blue Gene/Q, is expected to begin arriving in May. Once fully operational, Mira will be one of the world's fastest and most energy-efficient supercomputers, thanks to innovations in chip design and water cooling. Lauded as a stepping-stone to exascale-class computers, scientists around the globe will have their first opportunity to compete for 2013 system time on Mira with the opening of the 2013 INCITE Program call for proposals (April 11– June 27, 2012).

Moving breakthrough science to action through INCITE

To enable research for game-changing advances in science, the DOE Office of Science sponsors high-performance computing facilities equipped with some of the world's most advanced supercomputers. Sixty percent of these supercomputing resources are awarded through INCITE—the Innovative and Novel Computational Impact on Theory and Experiment Program.

The INCITE award selection process is aimed at ensuring these leadership-class supercomputing resources are used to their fullest potential by researchers who can leverage the massive compute power to accelerate their science. Awards of system time to scientists in academia, industry, and research institutions are allocated on a competitive basis. Teams vying for the coveted resources must successfully demonstrate to a committee of peers that their work addresses "grand challenges" in science and engineering, and that their project is computationally ready to run on machines that are among the world's most powerful.

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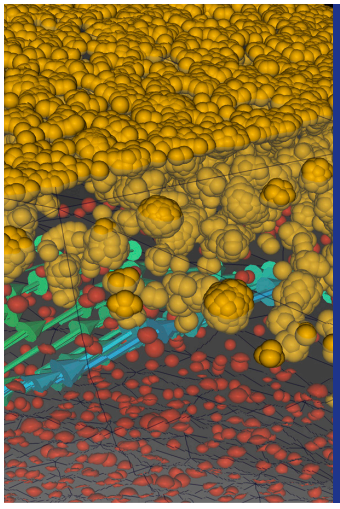

Join the "Preparing for INCITE 2013" informational webinar, April 24th

Both prospective and returning users are invited to join in this opportunity to gain tips and to have their specific questions answered about the INCITE submission and review processes. Representatives from INCITE, Argonne, and Oak Ridge will be present. To register, visit *https://www.alcf.anl.gov/incite2013.*

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Events of Interest

ALCF Hosts Leap to Petascale Workshop
May 22-25, 2012
Argonne National Laboratory

Take your code to the next level! Work hands-on with ALCF experts in performance and computational science to fine-tune your code. And developers of performance tools and debuggers will share ways to improve your code's performance.

Register today:
http://www.alcf.anl.gov/workshops/l2p-workshop

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Call for Proposals for Mira Access Opens April 11 (continued)

A time machine for your science

Says ALCF Director of Science, Paul Messina, "Access to resources like Mira could mean a huge leap forward in their work, so we tell scientists applying for INCITE to think well beyond today, and to imagine propelling their research forward several years. We essentially offer a time machine for their science."

Through INCITE, ALCF resources have been instrumental in major advances in "grand challenge" problems, including research efforts to design technologies to reduce carbon emissions, enhance the efficiency and reliability of nuclear energy, assess the impacts of climate change, and gain insight into deadly human blood diseases.

In addition to an assessment of scientific relevance, INCITE reviewers also gauge each project's ability to utilize the enormous scale of a leadership-class system. "The reality is, it does take work to scale code to a system the size of ours, and you need to have already done some of that work to be an INCITE contender," Messina notes. Reviewers look for previous success on a large-scale machine, including work done at the ALCF through start-up allocations available through the facility's Director's Discretionary program.

"Think of the computer as an experimentalist would think of an apparatus: By understanding the apparatus, an experimentalist can fully utilize the tool for scientific discovery. The same is true of researchers who understand their code and the resources at the ALCF. They don't just consider it to be a black box—by really understanding the apparatus, they derive the most from it."
–Paul Messina, ALCF Director of Science

Membership has its perks

To maximize scientific impact, the massive number of compute hours available through INCITE are divvied up amongst a selected number of recipients. This year, a total of 732 million compute hours were awarded to 31 prestigious research teams, yielding average allocation awards exceeding 20 million hours. Average allocations in 2013 will be around 100 million hours.

Each INCITE team is assigned a "Catalyst" from the ALCF staff of computational scientists who serves as project advocate and intermediary, helping to coordinate full lifecycle support for the project, including performance analysis, debugging, I/O, and visualization assistance. In addition to sizeable allocations and one-on-one Catalyst support, INCITE projects receive priority access to the ALCF systems.

For more information, or to apply for a start-up account at the ALCF, visit
http://www.alcf.anl.gov/getting-started/getting-time

Are you ready for INCITE?

How do you know if INCITE is right for your research? Your answers to these five questions may help you decide.

1. Is your research groundbreaking?
   INCITE research is game-changing: During the INCITE review, panelists assess the likelihood that your proposed work will contribute significantly to its respective field. INCITE research is also far reaching: Successful candidates are those who think years ahead, or who seek answers to fundamental questions that have eluded explanation for years, or even centuries.

2. Does your code scale to large systems?
   Successful INCITE candidates have production runs that scale to thousands of cores. Intrepid users should have production runs that typically use at least 8192 cores. On Mira, the number of cores will be significantly higher. In your proposal, you'll need to show that your production runs will make effective use of a significant portion, in most cases 20% or more, of the ALCF system(s) you request. Include previous large runs or plans for full-machine runs to help illustrate your "computational readiness" for INCITE. Also share your plans for addressing potential bottlenecks.

Are you ready for INCITE? (continued)

3. Can you use an INCITE-sized allocation?
   The average 2012 INCITE allocation at the ALCF was 27 million compute hours, and the largest award was 63 million.

   In addition to time on the ALCF's Blue Gene/P, Intrepid, in 2013, Mira, the ALCF's new Blue Gene/Q, will also have production hours for INCITE. You may request time on Intrepid, on Mira, or on both systems. Because the exact number of Mira hours available in 2013 won't be known until after the INCITE open call ends, researchers who request time on Mira must provide project plans for each of three possible resource scenarios:

   - Scenario 1: ALCF resources of 3 billion Mira core hours
   - Scenario 2: ALCF resources of 2 billion Mira core hours
   - Scenario 3: ALCF resources of 768 million Mira core hours

   The number of hours you request should be based on your best estimate of the time required for each phase of your research plan.

4. Do you have a long-range plan for your science?
   In the interest of encouraging far-reaching advances, INCITE encourages multi-year proposals. All proposals must include specific, intermediate milestones to allow for tracking of the project's progression throughout the duration of the award period.

5. Do you have a path forward for your code and the skill sets on your team to evolve your code?
   Successful INCITE teams are engaged with their software and have a coordinated plan for its evolution. Be prepared to explain how you will utilize your code to propel your science forward. You will also need to demonstrate that your project has sufficient personnel resources with the right skill sets to get the job done.

5 Tips for INCITE Proposal Writers

1. **Follow proposal instructions carefully**
   For full consideration, review and follow the ***proposal instructions*** thoroughly.

2. **Write a detailed proposal**
   INCITE is extremely competitive. Each proposal is reviewed by a panel of leaders in their respective fields (more than half are society or laboratory fellows, department chairs or heads, or center directors). In 2012, 33% of new proposals received allocations. ALCF's Director of Science, Paul Messina, recommends, "Write your INCITE proposal with the level of detail you would use in a proposal for science in which you were requesting millions of dollars."

3. **Include data about your specific problem, not benchmark runs**
   Your proposal must include performance data from runs of the actual science problem you are seeking to solve, or as close to that problem as possible on your code. A common mistake made by INCITE applicants is to submit results of benchmark runs that represent science problems other than those specified in the proposal.

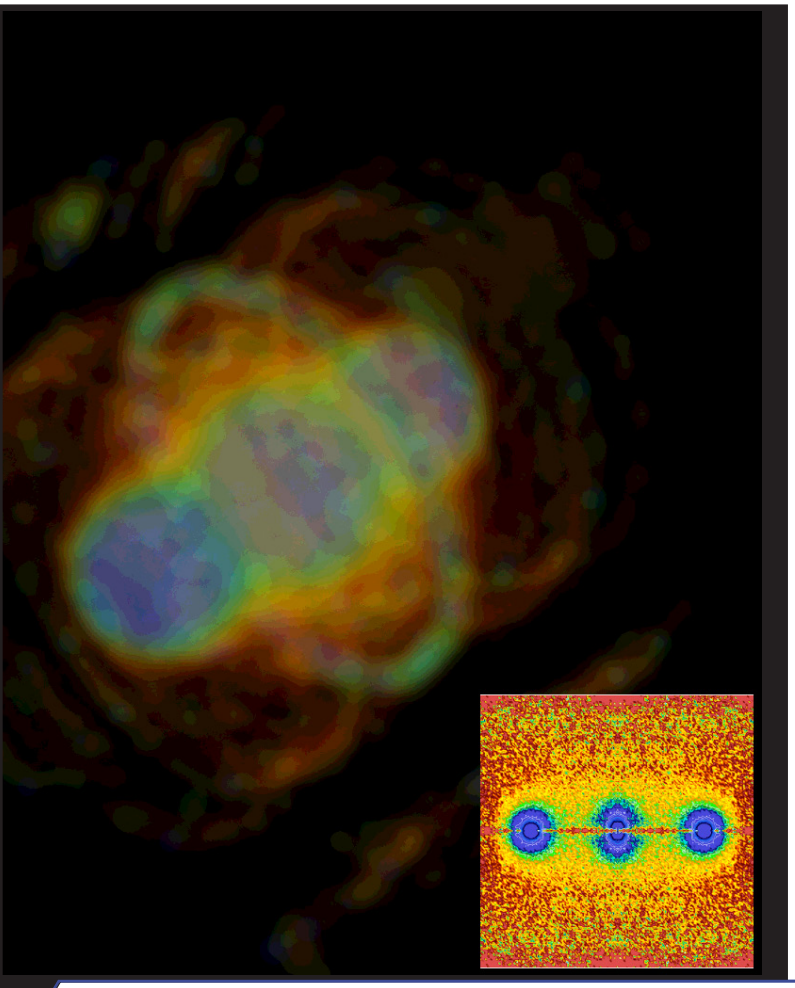
4. **Join the "Preparing for INCITE 2013" informational webinar, April 24th, 2012**
   Both prospective and returning users are invited to join in this opportunity to gain tips and to have their specific questions answered about the INCITE submission and review processes. Representatives from INCITE, ALCF, and OLCF will be present. Click ***here*** to register.

5. **Be prepared to sell your story**
   Your INCITE proposal will include your project narrative. This is your opportunity to describe the significance and impact of your work in terms of the type of "game-changing" science that defines INCITE. Think "big picture" and include how the scientific community, the nation, or the world will benefit from your efforts.

Staving Off Global Climate Change with CO_2 Capture

INCITE researcher, William Lester, Jr., UC Berkeley, will use his award to study carbon sequestration techniques that may further the development of clean energy systems.

Our amazing planet has the power to heal itself. Through the intricate flow of the carbon cycle, it maintains a delicate balance that is fundamental to life on Earth. These regulating mechanisms, however, are not without limits. Today, the amount of manmade carbon dioxide (CO_2) and other greenhouse gases released into the atmosphere far outpaces the planet's normal ability to mitigate them. The United Nations Environment Program reports that energy-related CO_2 emissions have skyrocketed globally from 200 million tons a year in 1850, to 29 billion tons a year today, with projections for a rise of another 54 percent by 2030. The resulting imbalance in the carbon cycle carries grave global climate repercussion, including the potentially catastrophic effects of global warming.



The situation gets heated

Gases in the Earth's atmosphere trap heat and cause the planet's temperatures to rise. Given the amount and speed at which carbon dioxide and other gases are being released today, some studies suggest that the Earth's average temperature could rise between 2.5 and 10 degrees Fahrenheit by 2100, putting global temperatures at their highest levels in thousands of years. Left unchecked, global climate models predict this global warming will have devastating affects on the planet, including:

- Floods caused by a rise in sea level (as much as three feet across the globe) in areas populated by millions,
- Devastating droughts in our farmlands,
- Storms (including hurricanes) of increasing intensity and frequency,
- Extinction of animal and plant species unable to adjust to habitat changes brought about by global warming.

The imperative to reduce and remove CO_2 is clear. In response, the Energy Department is arming top scientists with the resources of leadership-class supercomputing facilities, like those found at the Argonne Leadership Computing Facility (ALCF). Here, scientists from around the globe have access to the compute power of Intrepid, a 557-teraflops IBM Blue Gene/P supercomputer to aid in their search for transformative science and technology solutions to today's pressing global issues.

One such team of researchers, led by William Lester, Jr., UC Berkeley, is focusing on new ways to capture (or "sequester") CO_2 to prevent or defer the climate changes it causes. Central to their work is a special class of solvent—called ionic liquids (ILs)—that shows promising abilities to sequester CO_2.

The main image shows a projection of the energetic landscape of a CO_2 molecule (oriented along the X-axis) from a high-dimensional space of QMC random walks into the real space. Inset: a matching two-dimensional slice containing the linear CO_2 molecule; blue colors correspond to the nuclear regions where electrons experience strong attractive potential.

Credit: Dmitry Yu. Zubarev, UC Berkeley (Lester Group) and Prabhat, Lawrence Berkeley National Laboratory

Staving Off Global Climate Change with CO_2 Capture (continued)

While scientists have known about ILs for the last hundred years, their use as novel solvent systems has only been investigated since the 1980s. Ionic liquids offer many promising advantages over other solvents: ILs are effective solvents for a broad array of materials, are stable and inert, can exhibit acidic or basic properties, and can act as catalysts in certain systems. Ionic liquids are also relatively inexpensive, easy to prepare, and offer a large working temperature range. Dubbed "designer solvents," the versatility of ionic liquids makes them useful for a range of conditions and functionality in ionic liquid-based processes, like CO_2 sequestration.

As research into ILs is relatively new, scientists must first understand exactly how CO_2 interacts with these solvents. Lester and his team will use complex and highly accurate Quantum Monte Carlo (QMC) computer algorithms to simulate IL/CO_2 interaction at the molecular level. Scientists believe that, together, the unique characteristics of the Blue Gene/P supercomputer coupled with the QMC algorithms will provide them with a comprehensive picture of these interactions that is chemically accurate. "We are excited about the potential to answer a fundamental question involving a major greenhouse gas through research made possible by the significant computational resources that we have been awarded," said Professor Lester. This research could spur the development of a comprehensive model of CO_2 absorption. Through their efforts, Lester's team is building a solid framework of computational results for use by researchers around the world with the common goal of clean energy systems to combat global climate change.

INCITE Researchers Explore How Aircraft Contrails Can Impact Climate

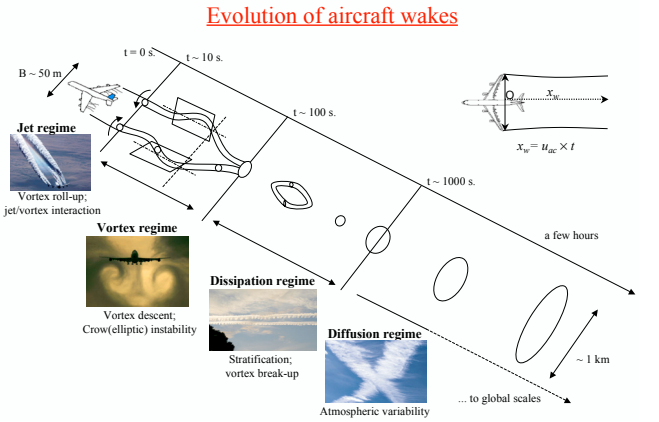
When aircraft in the United States were grounded for three days after the Sept. 11, 2001 terrorist attacks, scientists had a singular opportunity to study the effects of contrails—ice clouds generated by water exhaust gases from aircraft engines—on climate. The scientists measured day and night temperatures to find out if contrails contributed to regional warming and/or global climate change. Some studies indicated that the absence of contrails during this grounding period increased the daily temperature range at the Earth's surface, but this result is still a subject of scientific debate.

Nonetheless, there's no question that the environmental impact of aviation represents a source of increasing concern among scientists and policy makers as the demand for air travel continues to grow. Aviation is one of the fastest growing sectors, with a projected twofold increase by 2020.

Contrails are ice clouds that form by condensation of water vapor exhaust from aircraft engines and develop further in the aircraft wake as they are entrained by the airplane trailing vortices (see Fig. 1). When contrails spread to form cirrus clouds (see Fig. 2), they can persist for hours and extend over areas of several square kilometers. These "contrail cirrus," which artificially increase Earth's cloudiness and become almost indistinguishable from natural cirrus, are among the most uncertain contributors to the Earth's radiative forcing. (Radiative forcing is defined as the change of the net radiating flux resulting from changes in the atmospheric composition. A measure of the perturbation of Earth-atmosphere energy budgets, it is widely used as a climate metric.)

INCITE Researchers Explore How Aircraft Contrails Can Impact Climate (continued)

Researchers at CERFACS and Laboratoire d'Aérologie recently received an INCITE award of 20 million hours at the Argonne Leadership Computing Facility (ALCF) to study the contrail-to-cirrus transition. "This project aims at understanding the physics of the formation of contrail cirrus, which occurs when the effects of the atmospheric perturbations become predominant, compared to the dynamics of the aircraft wake where ice particles are initially trapped," notes INCITE PI Roberto Paoli, CERFACS. "The unique aspect of the research is that the key mechanisms that control this process will be analyzed separately using high-resolution large-eddy simulations over large computational domains to accommodate the spreading of the contrail and its transition into cirrus."



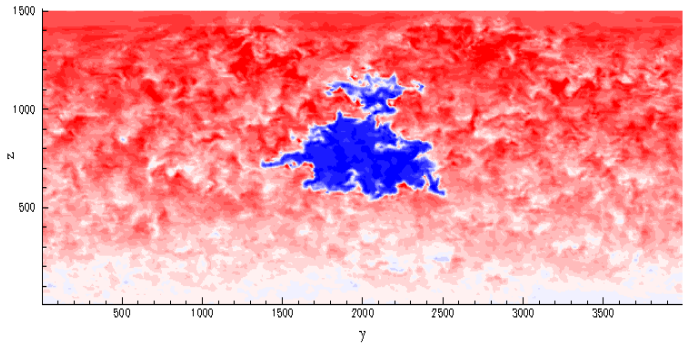


Figure 1 (Top). Representation of the evolution of aircraft wakes, from nozzle exit to dispersion in the atmosphere. Figure 2 (Bottom). Snapshot of ice supersaturation illustrating the initial spreading of a contrail.

Credit: Top image courtesy of Paoli, Cariolle, and Sausen, published in Geoscientific Model Development, 2011. Bottom image courtesy of Paugam, Paoli, and Cariolle, published in Atmospheric Chemistry and Physics, 2010.

The research team is examining the transition using the numerical code, Méso-NH, the mesoscale atmospheric model of the French research community to 1) characterize the 3-D structure of the cloud, as well as the spatial and size distribution of ice particles contained in the cloud; and 2) identify the relative importance of the mechanisms that control this process as a function of the age of the contrail. To that end, they are carrying out a parametric study through a set of dedicated simulations, where the effect of atmospheric turbulence, microphysics, and radiative transfer are being analyzed separately. First, various turbulent fields corresponding to different levels of turbulence will be generated using a stochastic forcing technique that reproduces the atmospheric conditions normally encountered in the upper troposphere. Then, the contrail resulting from the wake of a typical aircraft will be inserted on the top of each of these fields to analyze the transition into contrail cirrus —activating ice microphysics. Finally, radiative transfer will be activated to find out if and on which spatial and temporal scales the induced vertical motion prevails over the essentially horizontal motion of atmospheric turbulent diffusion in driving contrail-to-cirrus transition.

By understanding and characterizing the physical mechanisms that control the formation of contrail cirrus, this INCITE research will lead to more complete and effective representation of aviation impact into next-generation climate models.

Spotlight on ALCF Staff: Katherine Riley

This month, the Newsbytes spotlight shines on Catalyst Manager, Katherine Riley.

NEWSBYTES You're the manager for the Catalyst team. What is the role of the Catalyst at the ALCF?

KATHERINE RILEY The Catalysts are a team of computational scientists from a variety of scientific domains. Each Catalyst is assigned to a very small number of INCITE projects. Our goal is that the Catalyst is seen as a member of the research team who is skilled in using Intrepid and soon Mira for the team's particular science. As computational scientists and experts in their fields (or near it), Catalysts can be strong collaborators by organizing large computational campaigns, to guiding the code to new algorithms and approaches for even larger scaling. The Catalysts ensure that each INCITE project has full lifecycle support, including performance analysis, debugging, I/O, and visualization assistance by leveraging the resources available through the ALCF.

NEWSBYTES The ALCF provides some of the most advanced supercomputing resources in the world to science. With these types of resources, what does access to a Catalyst add?

RILEY As computational scientists, the Catalysts are experts in algorithms and applications and how those work on the ALCF resources. They can significantly accelerate the process of moving codes to scale for computation and can provide key insight as researchers plan for new computational resources. Through the Catalyst program, we lend research teams our expertise in computational science.

NEWSBYTES Working for a DOE leadership computing facility is exacting and demanding. What makes it worth it for you?

RILEY There are very few places in the world where you can work with the most cutting-edge and largest-scale computing resources, and the ALCF is one of them. The way you use these systems is different than using your desktop, and the resulting challenges are incredibly exciting. The resources allow us to tackle science that is unique and potentially world-changing. That's very exciting for me, too.

NEWSBYTES What does "success" look like for you and your team of Catalysts?

RILEY The past couple years we've really had a lot of fantastic successes. We've been able to work with projects that come to us with codes that were nowhere near ready to meet INCITE scalability requirements, and now they are running on Intrepid as successful INCITE projects. Also, we encourage PIs to share their codes with us. Having access to these codes gives our team the opportunity to view them through expert eyes that are skilled in using Intrepid. It's a big success for us when we can call PIs and tell them we've made significant performance improvements for them.

NEWSBYTES In your role, you're very involved with the annual selection of INCITE projects. What wisdom do you have to pass along to those applying for INCITE 2013 awards?

RILEY Well, I think it is very important for applicants to understand that INCITE is a science competition first. The entire review process is focused on ensuring that the best science is selected. We do have strong computational readiness demands, but they are not the primary criterion for the award. The science review panels are composed of worldwide experts in their respective fields. They look at each INCITE proposal for its potential global relevance and impact within the domain.

NEWSBYTES What's an aspect that makes the ALCF unique among HPC user facilities?

RILEY Our Catalyst team. We have experts in areas that include materials, chemistry, fluid dynamics, molecular dynamics, astrophysics, and plasma physics. Their unique expertise is in how to solve problems in these fields on the largest computation resources available. This often includes understanding a breadth of methods for different scales of computing. So, besides the significant effort Catalysts put into working with projects, they are also an incredible resource for understanding the computational challenges within their science domains, both now and in the future. They are an amazing resource for the ALCF and the scientific community. I am incredibly grateful for them.

For more information about the Catalyst Team, contact Katherine Riley: riley@alcf.anl.gov

Researchers Get Time on Mira Test and Development Prototypes at ESP Workshop

The first of two technical, hands-on workshops was held April 19-21 for representatives of the ALCF's Early Science Program (ESP) projects. ESP provides a small group of researchers with preproduction hours on Mira, the ALCF's next-generation, 10-petaflops Blue Gene/Q system. These hours give ESP projects an early opportunity to adapt to the new system while helping to bring system instabilities to light for resolution.

The April workshop was geared towards ESP team members responsible for code development, porting, validation, and optimization. It provided users with a jump start on Mira and an opportunity to set in motion the code development, testing, and benchmarking that will continue throughout the coming year.

Representatives from 13 of the 16 ESP projects attended, and with the help of ALCF Catalysts and Performance Engineers, most were able to compile and run on the ALCF's Very Early Access System (VEAS) Blue Gene/Q rack. Several tools and libraries were installed on VEAS prior to the workshop, including PETSc, PAPI, TAU, HPCToolkit, and Jumpshot. Developers were on hand at the workshop to assist attendees.

Working closely with ALCF Catalysts and Performance Engineers in extended hands-on sessions, ESP projects made significant progress, including, in some cases, substantial performance improvements. Said ESP PI Steve Pieper, "With help from Vitali Morozov [ALCF Performance Engineer], we were very pleased to achieve an 80 percent speedup of one kernel of GFMC on VEAS by modifying it to get access to the QPX capability of the Blue Gene/Q chip."

Other accomplishments made during the ESP workshop include:

- GTC code Poisson was ported.
- Nek5000 was profiled with HPCToolkit.
- Calls were added to Kernel_GetMemorySize in FLASH to show various memory usage statistics.
- GAMESS was compiled and ran up to 8 ranks per node successfully. Benchmarking was started.
- PHASTA code was ported and compiled with cmake, and a case successfully run in parallel. The team also adapted submit scripts to run in script mode.

A second workshop is planned for ESP project teams in late April. Visit our website for more information about ESP at the ALCF.

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Visit us online at www.alcf.anl.gov Contact the editor at info@alcf.anl.gov