# **ALCC Mission**

The mission of the ASCR Leadership Computing Challenge (ALCC) is to provide an allocation program for projects of interest to the Department of Energy (DOE) with an emphasis on high-risk, high-payoff simulations in areas directly related to the DOE mission and for broadening the community of researchers capable of using leadership computing resources.

The DOE mission is to ensure America's security and prosperity by addressing its energy, environmental and nuclear challenges through transformative science and technology solutions. See <u>https://www.energy.gov/mission</u> for more details on the Department's mission objectives

# How to Apply

The call for proposals for the 2019-2020 ALCC allocation process will open in January 2019. The call will close at 11:59 p.m. (Eastern Time) on Wednesday, Feb 13, 2019. ALCC Applicants submit proposals through an online system at <a href="https://apps.orau.gov/ALCC/Account/Login">https://apps.orau.gov/ALCC/Account/Login</a>. Application requirements are described below.

For any questions please contact the ALCC program manager, Betsy Riley, or the assistant program manager, Christopher Miller, via <u>alcc-ascr@science.doe.gov</u>.

### **Allocation Performance Period**

The 2019-2020 ALCC performance period is July 1, 2019 to June 30, 2020.

### **System Descriptions**

Allocations are provided in units of node-hours \*10^6. Since the node-hour is no longer a standard unit across architectures, we have provided descriptions below for what is considered to be a node for this allocation period. There is also a table below giving an indication of the relative processing power of the "nodes". The following high performance computing resources are available during the ALCC 2019-2020 performance period:

• OLCF Summit: OLCF will have 6.0M node-hours available on Summit, an IBM Power System AC922 system. Each of the 4,608 nodes contains two 22-core IBM POWER9 CPU processors and six NVIDIA Tesla V100 graphics processing unit accelerators (GPUs). The IBM POWER9 processor supports hardware threads. Each POWER9 processor is connected via dual NVLINK bricks, each capable of a 25 GB/s transfer rate in each direction. The memory per node is 512 GB of DDR4 combined with 96 GB of High Bandwidth Memory (HBM2) for use by the accelerators. The system uses a dual-rail Mellanox EDR 100 Gb/s Infiniband interconnect.

For applications requesting time on Summit, projects capable of using GPUs or developing GPU capabilities are strongly encouraged. For more details about Summit see: https://www.olcf.ornl.gov/for-users/system-user-guides/summit/ https://www.olcf.ornl.gov/for-users/system-user-guides/summit/system-overview/

• ALCF Theta: ALCF will have 5.9M node-hours available on Theta, a CrayXC40 system with Intel Xeon Phi CPU (a.k.a. Knights Landing or KNL) processors. Each of the 4,392 nodes has an Intel Xeon Phi Processor 7250 (KNL) with 64 cores. Each of the 64 cores supports four hardware threads for a total 256 threads per node. The memory per node is 192 GB of DDR4 combined with 16 GB of high-bandwidth multi-channel DRAM (MCDRAM). The system uses the Cray Aries high speed "dragonfly" topology interconnect.

For more details about Theta see: https://www.alcf.anl.gov/user-guides/computational-systems#theta-(xc40)

• NERSC Cori: NERSC will have 4.5M node-hours available on Cori's KNL partition, a CrayXC40 system with Intel Xeon Phi CPU (a.k.a. Knights Landing or KNL) processors. Each of the 9,668 nodes has an Intel Xeon Phi Processor 7250 (KNL) with 68 cores. Each of the 68 cores supports four hardware threads each for a total of 272 threads per node. The memory per node is 96 GB of DDR4 combined with 16 GB high-bandwidth MCDRAM. The system uses the Cray Aries high speed "dragonfly" topology interconnect.

For more details on the Cori KNL nodes see:

http://www.nersc.gov/users/computational-systems/cori/configuration/cori-intel-xeon-phinodes/

Please note that due to fundamental differences between the system architectures, the FLOPs achievable per node-hour are NOT equivalent across the three systems. The following table, which is based on the Top500 ranking of the systems, provides a rough comparison of the computational power per node:

	Node Architecture	Nodes	TFLOPs *	Node-hours
Machine			per Node	available
Summit	IBM Power System AC922	4,068	49.35	6.0M
	(IBM POWER9 CPU,			
	NVIDIA Tesla V100 GPU)			
Cori	Cray XC40 (Intel KNL CPU)	9,688	2.87	4.9M
Theta	Cray XC40 (Intel KNL CPU)	4,392	2.65	5.9M

Proposers should also use the respective webpages to familiarize themselves with the descriptions of the data management resources available to users of the ASCR Facilities. Oak Ridge Leadership Computing Facility (OLCF)

https://www.olcf.ornl.gov/for-users/system-user-guides/summit/file-systems/

Argonne Leadership Computing Facility (ALCF)

https://www.alcf.anl.gov/user-guides/xc40-file-systems

https://ww.lcf.anl.gv/user-guides/data-storage-file-systems

National Energy Research Scientific Computing Center (NERSC) http://www.nersc.gov/users/computational-systems/cori/file-storage-and-i-o/

## Eligibility

- The proposed research should be in areas related to the DOE mission
- The proposed research results must be open and cannot contain proprietary information unless the project meets the criteria for the Industrial Partnership User Agreement. (Interested parties from industry should contact the "Contacts for Industry" <u>here</u> for more information).

# **Review Process**

ALCC proposals undergo scientific merit reviews through a peer review process. The proposals are evaluated against the following criteria, which are listed in descending order of importance as codified in the<u>Code of Federal Regulations</u> (10 CFR 605.10)

- Scientific and/or technical merit of the project (for ALCC, this includes an evaluation of the project's relevance and importance to the DOE mission)
- Appropriateness of the proposed method or approach
- Competency of applicant's personnel and adequacy of proposed resources
- Reasonableness and appropriateness of the proposed allocation request

# **Application Requirements**

### 2019-2020 ALCC Year: July 1, 2019 to June 30, 2020

[1] A complete online application must be received by 11:59 PM Eastern Time on Wednesday, February 13, 2019. Late applications will automatically be deemed ineligible. The online application is divided into 12 sections. Requirements for each section are described below. Note, the application includes three PDFs prepared separately by the applicant: Abstract (Section 7), Proposal Narrative (Section 8), and CV of application team (Section 9). If you are unable or have difficulty submitting a PDF, please contact the ALCC program manager at alccascr@science.doe.gov.

[2] Applicants are asked to identify whether their project is a Consortium/End-Station project (see Section 2). A consortium proposal, also called an end-station proposal, is a single allocation request for resources that will respond to the allocation needs of a group of Principal Investigators, research teams, or institutions. This group may be built around shared use of codes, shared scientific interests, or some other common use criteria. Most proposals are not consortium proposals. Consortium projects must include a management plan as part of the proposal narrative. Peer reviewers are notified if your project is a consortium project and are asked to adjust their comments accordingly. Additionally, peer reviewers will be asked to evaluate the management plan.

[3] The Proposal Narrative has five required elements as indicated below (see Section 8); there is a sixth required element for Consortium/End-Station projects. If your proposal does not include

these elements, it may be rejected without peer review.[4] Each proposal must have a completed Application Content Agreement (see Section 11).

# **Online Application**

To complete the online application, you will need to include the following information for each section (each item is required unless indicated otherwise);

### Section 1 – Team and Contacts

- Contact information for primary PI
- Name and affiliation of collaborators (if applicable)
- Institutional Contact Information this is the agent who has the authority to sign the user agreement on behalf of your institution. The person may be someone in a contracts or procurement department, department head, or grants department.

## Section 2 – Project Topic

- Project Title
- Consortium Proposal Identification you must identify if your project is a consortium proposal. A consortium proposal, also called an end-station proposal, is a single allocation request for resources that will respond to the allocation needs of a group of Principal Investigators, research teams, or institutions. This group may be built around shared use of codes, shared scientific interests, or some other common use criteria. Most proposals are not consortium proposals.
- Non-technical summary (250 word maximum). This summary should be understandable to a non-specialist; the target audience is an educated layperson, not scientific colleagues.
- Project Website (optional, will not be sent to peer reviewers)
- Keywords (10 max)

### **Section 3 – Project Support**

- Identify primary source(s) of funding; ALCC allocates computing time and not financial support. For citations of DOE support only, it is requested you include the DOE program office and program manager name if known. For all sources of funding, only the name of the funding source is required (e.g. no grant numbers are requested).
- Current high performance resources supporting project (if applicable)

# Section 4 – HPC Resources Request

- Provide a table that lists the requested allocation by system; clearly explain whether your allocation request has concurrent and/or phased work linked to the project milestones articulated in your project narrative (e.g., "Construction of device X is dependent on modeling results from milestone A").
- Allocation requests should be stated in units of Machine Node-Hours x 10<sup>6</sup>. Please note that due to fundamental differences between the system architectures, the FLOPs

achievable per node-hour are NOT equivalent across the three systems. See the "System Descriptions" section above for more information.

• State the magnitude and duration of any related storage request. Summit has a 250PB IBM Spectrum Scale file system, called Alpine. Theta has a 10PB Lustre file system. Cori is connected to a 30PB Lustre scratch file space. More details about storage is available from links listed above under "System Descriptions".

### Section 5 – Previous ALCC Publications (if applicable)

#### Section 6 – Suggested Reviewers (optional)

- Name, Organization
- Phone and/or Email (optional)

### Section 7 – Abstract/Executive Summary (1 page maximum, PDF upload)

• The abstract/executive summary of your project. The target audience is peer reviewers and the allocation panel. The abstract is uploaded as a single PDF file independent of proposal narrative.

#### Section 8 – Proposal Upload (PDF upload)

Your main proposal is a single PDF upload. The main proposal is broken into three sections. (i) Narrative, (ii) Team Description, and (iii) Bibliography.

(*i*) Narrative (15 page maximum)

Proposal Narrative describing the proposed research. The narrative *must* contain:

- 1. A description of the project's relevance and importance to the DOE mission;
- 2. A plan to disseminate the results (e.g. conference submission, paper publication, data repository);
- 3. A breakdown of your project into intermediate goals/ milestones and computational resources requested for each milestone. If there is only one goal with no intermediate goals/milestones, state that explicitly. Please ensure that this narrative description of milestones is consistent with the allocation request table provided in section 4
- 4. A thorough description of the computational approach and the performance of the codes that will be used. Include whether the application software already contains the models necessary to simulate the problem to be studied and if not, an estimate of the person months needed to add those capabilities, (e.g. "adding new force fields may delay start of computing by 3 months"). For applications to Summit, projects capable of using GPUs or developing GPU capabilities are strongly encouraged.
- 5. Anticipated results of the research
- 6. For Consortium/End-Station proposals, the narrative must also contain a management plan that clearly explains how the consortium will function as a cohesive project.
- (ii) Team Description (1 page maximum)

• The proposal must contain a brief description of the expertise of the members of the project, their role, and their experience in comparable computational projects.

(*iii*) *Bibliography* (*no maximum*) **Section 9 – CV** (single PDF upload)

- CVs for the PI and project collaborators
- The CV of the primary PI must include a section that lists collaborators for the past four years with current affiliations.

#### Section 10 – Security

The security section asks a series of yes or no questions related to the content of your project/proposal. These questions are primarily to facilitate access to the center once an award is made and ensure proper handling of a proposal during the review process. The security questions are in three sections: Proprietary Information, Export Control, and Privacy Information. PDF of Security Questions

#### Section 11 – Application Content Agreement

The application content agreement is your assurance that your proposal submission does not contain any prohibited information (e.g. classified information, export control information). If your submission includes proprietary information, the agreement also grants your permission for peer-reviewers to read your proposal.

PDF of Application Content Agreement

Section 12 – Review and Submit