2019 INCITE Call for Proposals: New Proposal Preparation Instructions for Authors

Fifty percent of the allocable time on the IBM/NVIDIA "Summit" machine and the Cray XK7 "Titan" at the OLCF and the Intel/Cray "Theta" machine and the IBM Blue Gene/Q "Mira" at the ALCF will be allocated for calendar year (CY) 2019 through the INCITE program. For each resource, allocations are anticipated to be between 300k and 800k Summit node-hours, 2M and 5M Titan node-hours, 13M and 25M Mira node-hours, and 1M and 2M Theta node-hours. Individual awards may be higher.

INCITE seeks research enterprises for capability computing: production simulations and data science applications - including ensembles - that use a large fraction of the machine. Please note that requests smaller than 20% of the average award on any particularly resource may be considered too small for the INCITE program, unless the proposal is (i) for algorithm development or other computer science activities requiring a large fraction of the machine but not a large amount of time or (ii) clearly articulates the need for other aspects of the architecture and/or infrastructure associated with leadership computing resources. Please contact the INCITE program manager (incite@doeleadershipcomputing.org) if you have questions regarding the allocation request for your proposed project allocation size.

INCITE provides several resources to help you prepare your proposal.

- The INCITE Overview and Policies includes a description of the basis for award decisions, etc.

- The questions used by reviewers to assess proposals are available, as are a sample proposal and templates for the narrative sections of the proposal.

- See "Presentations" at www.doeleadershipcomputing.org/faqs/ for the slides from the most recent INCITE proposal writing webinar.

- Early access on LCF Resources can be requested through the Director's Discretionary program if you wish to generate benchmarking data on these systems.
    - https://www.olcf.ornl.gov/support/getting-started/
    - https://www.alcf.anl.gov/dd-program

Experts will carry out scientific and technical reviews of the potential impact of the proposal and the ability of the applicant's team to effectively use the Titan, Mira, Summit, and Theta systems. Potential scientific impact is the predominant determinant for awards. INCITE awards are large-often one hundred times greater than more generally available allocation programs-and a limited number of projects are selected each year. Campaigns chosen by the INCITE program typically cannot be performed anywhere else and require extremely large high-performance computing systems, large awards of time, or the unique Leadership Computing Facility (LCF) architectural infrastructure to succeed.

General Information

Revisions for 2019 INCITE Call for Proposals:

- Allocation requests shall be made in the unit of "node-hour" for the CY2019 INCITE submission. Conversion factors from core-hours are available in the FAQs (#31).

It is strongly recommended that authors comply with the guidelines established below, which will be used to assist in the review of proposals. Templates for all sections are available.

The proposal must be clear, readily legible, and conform to the following requirements:

1. Each section of the proposal must be paginated. Footers should be used for paginating all files. Also, headers should be used to indicate the title of the proposal and the lead principal investigator (PI).

2. Proposal titles may not be longer than 80 characters.

3. One of the two typefaces must be used: Arial or Times New Roman (font size 11). A font size of less than 11 points may be used for mathematical formulas or equations, figure, table, or diagram captions, or when using a symbol font to insert Greek letters or special characters. PIs are cautioned, however, that the text must still be readable.

4. Margins must be at least 1 inch in all directions. These requirements apply to all sections of the proposal, including supplementary documentation.

5. Proposals should be prepared using single line spacing. The proposal elements should not exceed the specified page count limits.

6. References should be gathered at the end of the narrative. References are **not** included in the total page count.

7. The total file size should be limited to 5 MB.

8. No letters of collaboration or letters of support will be accepted with the application. Current and pending support documentation is not required.

Adherence to type size and spacing requirements is necessary to ensure readability and that no proposer will have an unfair advantage by using smaller type or spacing to accommodate more text.

Submission Instructions

All proposals must be submitted electronically via the INCITE website (https://proposals.doeleadershipcomputing.org). Electronic applications will be accepted starting Monday April 16, 2018, thru 8:00 pm EDT on Friday, June 22, 2018. All proposals must follow these instructions. **INCITE reserves the right to decline consideration of proposals not compliant with these instructions and guidelines.** Hardcopies will not be accepted for review. The final file size must not exceed 5 MB.

Any questions should be directed to the INCITE program manager at INCITE@doeleadershipcomputing.org.

Proposal Contents

1. **Project Executive Summary (1-page limit):** The executive summary should accurately describe the proposed research and the high-impact scientific or technical advances you will realize with the proposed INCITE allocation. Industry organizations should also summarize the potential economic or strategic business impact of the proposed research.

2. **Project Narrative: The narrative should not exceed 15 pages.** Visual materials, such as charts, graphs, pictures, etc., are included in the 15-page limit. References do not count toward the 15-page limit and should be included at the end of the Project Narrative. URLs that provide information related to the proposal should not be included. **The 15-page limit will be strictly enforced.** The Project Narrative should address the following points:

   1. **Significance of Research:** List any previous INCITE award(s) received and discuss the relationship to the work proposed. Explain what advances you expect to be enabled by an INCITE award that justifies an allocation of petascale resources (e.g., anticipated impact on community paradigms, valuable insights into or solving a long-standing challenge, etc.). Place the proposed research in the context of competing work in your discipline or business. The information should be sufficient for peer review in your area of research and also appropriate for general scientific review comparing your proposal with proposals in other disciplines. Potential scientific or business impact is the predominant determinant for awards. This factor will be assessed by a peer-review panel. **This section is typically about 4 pages.**

   2. **Research Objectives and Milestones:** Describe the proposed research, including its goals and milestones and the theoretical and computational methods it employs. Goals and milestones should articulate simulation and developmental objectives and be sufficiently detailed to assess the progress of the project for each year of any allocation granted. Milestones should correlate with those in Section 4, "Milestone Table." It is especially important that you provide clear connections between the project's overarching milestones, the planned production simulations, and the compute time expected to be required for these simulations (e.g., should correlate with Section 2.3.i, "Use of Resources Requested") in the research proposal. You should also make clear any dependencies of milestones on other milestones. **This section is typically about 6 pages.**

   3. **Computational Readiness:** Proposals will be assessed on the need for, readiness to use, and reasonableness of the request for resources. Proposals should summarize the requirement(s) that best exemplifies the proposed computational work. Leadership targets in the INCITE program typically include one or both of the following categories:

      - Use of 20 percent or more of the system for production calculations. Simulation, data science and/or learning projects should all use a significant fraction of the LCF resources; compute, memory, network or disk, for example. Parameter sweeps, ensembles, design of experiments, and other statistical methods that require large numbers of discrete or loosely coupled simulations may be considered capability-class campaigns. See the FAQs for details and qualifiers.
      - Specific architectural needs that can only be met by the LCF.

This section, including the following subsections, is typically about 5 pages.

i. **Use of Resources Requested:** Describe your proposed production simulations and state how the runs are tied to each of your project's goals and milestones (Section 4, "Milestone Table"). Also describe the data requirements of your production simulations. If at any point during your project the sum of your data storage needs in the scratch filesystems exceed 1 petabyte, specific justification is required. **See the Project Narrative Template for a detailed listing of information required in this section.**

NOTE: The LCF data management plans can be found at

ALCF: http://www.alcf.anl.gov/user-guides/data-policy

OLCF: https://www.olcf.ornl.gov/for-users/system-user-guides/

ii. **Computational Approach:** Provide a detailed description of your computational approach, including a discussion of the state of the art in the field. The description should also mention:

1. Particular libraries required by the production and analysis software, algorithms and numerical techniques employed (e.g., finite element, iterative solver), programming languages, and other software used.

2. Parallel programming model(s) used (e.g., MPI, OpenMP/Pthreads and vector intrinsics (QPX/AVX-512) for BG/Q or Xeon Phi; MPI, OpenMP/Pthreads, CUDA, OpenACC or AVX intrinsics for XK7).

3. Project workflow including the role of analysis and visualization; identify where the analysis will be done and any potential bottlenecks in the analysis process. Describe any analysis and/or data reduction tools used.

4. Software workflow solution (e.g., pre- and postprocessing scripts that automate run management and analysis) to facilitate this volume of work.

5. I/O requirements (e.g., amount, size, bandwidth, etc.) for restart, analysis, and workflow. Highlight any exceptional I/O needs.

iii. **Parallel Performance:** Provide direct evidence, **including supporting quantitative data,** for your production application's parallel performance for the intended research simulations. Ideally, the proposing team will have generated the data and this data will be representative of the entire workflow of the project proposed. If you cite work by others, explain why it is applicable here. You should use the application code you intend for the production work, not a related code. Data for sample systems not related to the intended research is undesirable. Performance benchmarking should reflect all I/O and workflow requirements. Parallel performance data in either strong or weak scaling mode *must* be provided. Explain how the strong or weak scaling applies to the proposed work. See the examples at the end of this document.

NOTE: You may apply for a startup account at one of the centers to conduct performance studies. Applications are available at

ALCF: http://www.alcf.anl.gov/getting-started/apply-for-dd

OLCF: https://www.olcf.ornl.gov/for-users/documents-forms/olcf-directors-discretion-project-application/

    iv. **Developmental Work:** For the computational approach above, describe what, if any, development work has been carried out to date, especially on the architecture of the requested resource. Describe what development work will be executed, and when, during the proposed INCITE campaign, and an estimate of the computational resources required for this work. If applicable, identify the milestones and production simulations in Section 2.3.i that are dependent on the developmental work and provide a plan for validating this developmental work.

3. **Personnel Justification and Management Plan:** A personnel justification and management plan must be included in the proposal. (Does not count toward the 15-page Project Narrative limit).

    1. **Personnel Justification:** What personnel are already in place and what are their roles on the project? If applicable, describe (i) personnel that will be hired for the project in the future and their responsibilities and (ii) potential personnel turnover that may occur during the project and a strategy for replacing them. The INCITE program welcomes proposals from individual PIs or teams of collaborators.

    2. **Management:** Describe the project's leadership team and how decisions are made to allocate time to individuals or, for proposals with multiple collaborating teams, subgroups within the project. Describe the focus of each individual or subgroup. Successful proposals will include a management plan that conveys to reviewers the interrelationship between subgroups and how the sum of the parts will lead to scientific discovery or engineering solutions that are the overarching goal of the project. Also identify points of contact who will provide updates on the status of the work including publications, awards, and highlights of accomplishments.

4. **Milestone Table**: Proposals must be accompanied by a summary table of planned milestones for each year of the proposed work. Milestones should be clearly articulated and appropriate for the size and length of the requested award (e.g., large requests should have sufficient milestones to allow reviewers to assess the planned project workflow). Future modification to the project scope and milestones will be tracked in part through the milestone table. Use the template provided. Below is a description of what should be provided for each column in the table. (Does not count toward the 15-page Project Narrative limit).

    Milestones: Clearly state the scientific and technical (e.g., development) milestones for each year of the proposed work

    Details: Include the following details as appropriate for each milestone.
- Resource: List the primary computing resource.
- Node hours: List the number of node-hours associated with this milestone.
- Filesystem storage: Provide an estimate in terabytes of the required temporary storage needed on the filesystem while the data is analyzed and reduced or before it is moved to archival storage. Also provide the estimated time period when this storage is needed.

- Archival storage: Provide an estimate in terabytes of the required archival storage associated with this milestone for the duration of the project. Also provide the estimated time period when this storage is needed.
- Application: Software application or code needed for this milestone.
- Tasks: Briefly summarize the work that will be done by listing the subtasks, computational runs, and data analysis and reduction tasks associated with each milestone.
- Dependencies: Note dependencies between the scientific milestones and on proposed development work.

Date: List the projected start and completion date for each milestone.

Status: For renewal proposals only.

5. **Publications Resulting from INCITE Awards**: Provide a list of publications resulting from previous INCITE awards to this project team for work related to the proposal under consideration. Only those publications that include an acknowledgement to INCITE and/or the LCF may be included. This list may **not** be used in lieu of references in Section 2, "Project Narrative." If applicable, list the citations in both Sections 2 and 5. (Does not count toward the 15-page Project Narrative limit).

Appendix

**Examples of Performance Required Materials**

Quantitative data for production application performance should be provided in either tabular or graphical form or both. This data should reflect the performance of the application for the production simulations proposed and should include all I/O requirements of the production simulations.

Where appropriate, characterize the production application's single-node performance (e.g., percent of peak). For example, describe the most computationally expensive portion of your algorithm and describe the on-node parallelization scheme employed. Any optimization strategy to improve single-node performance, including code restructuring, GPU strategy, and exploiting OpenMP/Pthreads and vectorized instructions, should be described. For Titan and Summit, provide any evidence of speedup using GPUs compared to using all CPU cores. For Mira and Theta, demonstrate the efficient use of many CPU cores per node, and if not all cores can be used effectively, explain why. For all architectures indicate the degree of utilization of any architecture-specific features.

Weak scaling behaviors are probed by holding per-node computational work constant (e.g., the size of the mesh on a processor is held constant) as the total problem size grows with processor count. Strong scaling behaviors are probed by holding the total problem size constant as the processor count grows, thereby decreasing the per-processor computational work. Note that in the examples provided, a logarithmic scale is preferred.

In addition, where appropriate the proposal should describe the entire computational workflow of the proposed project. In particular, the project should demonstrate that the entire workflow is tenable on the proposed architecture or supporting analysis resources at the LCFs, or discuss where any pre- and post-processing or data analysis will be conducted and how relevant files will be transferred.

Weak Scaling Example

Weak Scaling Example
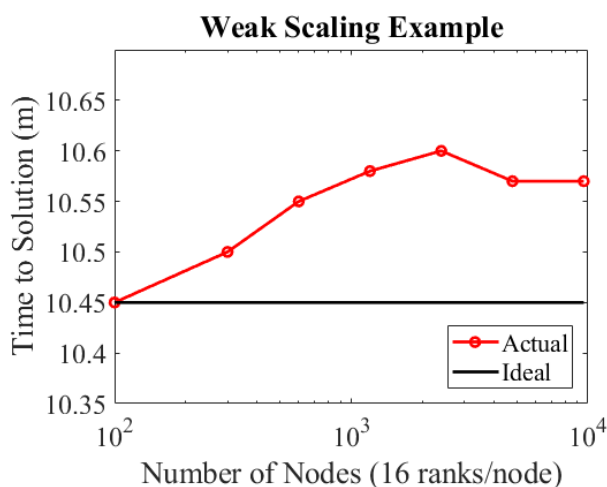
nNodes (16 procs/node)	Time to Solution (m)	Ideal Time to Solution (m)
100	10.45	10.45
300	10.50	10.45
600	10.55	10.45
1200	10.58	10.45
2400	10.60	10.45
4800	10.57	10.45
9600	10.57	10.45

Strong Scaling Example
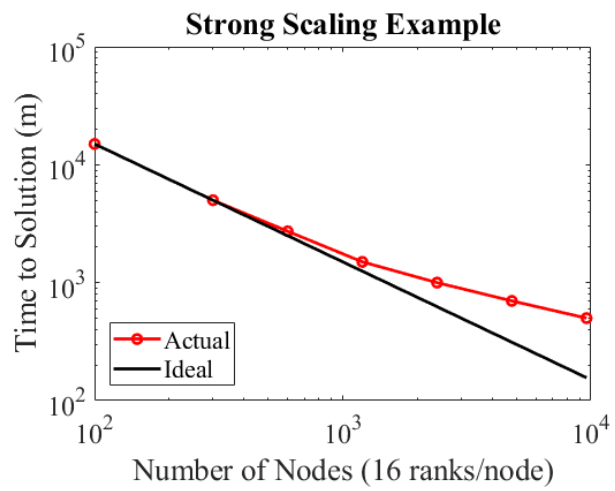
nNodes (16 procs/node)	Time to Solution (m)	Ideal Time to Solution (m)
100	15000	15000
300	5000	5000
600	2725	2725
1200	1500	1250
2400	1000	625
4800	700	313
9600	600	156