

## 2023 INCITE Proposal: Computational Review Questionnaire

Computational experts conduct reviews to gauge the state of readiness of INCITE submittals to effectively utilize the requested Leadership Computing Facility (LCF) resources. Reviewers focus on the benchmarking data and other information provided in the proposal to assess the need for leading-class systems, readiness to effectively use INCITE resources, and the reasonableness of the computational campaign the authors defined for the proposed production simulations.

### 1. Machine Requested (choose one or more):

- a) Summit
- b) Frontier
- c) Theta
- d) Polaris
- e) Aurora

### 2. Need for and Effective Use of INCITE's Leadership-class Systems

State one or more of the following that best exemplifies the proposed computational work. Is the work:

- a) capability computing (use of 20% or more of the system for production runs: individual simulations or ensembles)
- b) data-intensive computing or other nontraditional use models
- c) specific architectural requirements (e.g., large memory, GPU's, file system)
- d) other

Describe the reason for your selection in your assessment.

Assess the need for LCF resources and how effectively the project team can use the requested systems. For example, could the work be performed elsewhere? How well is the application optimized for the resources requested (in terms of efficiency, scalability, convergence of the solution, throughput, data input/output, workflow tools for ensemble runs, etc.)? The most valuable performance data is that which is most related to the proposed work, and ratings should appropriately reflect this.

*For multiple-resource requests, please comment on the merit of allocations at both centers.*

### 3. Computational Plan

Assess the computational plan (e.g. system and software requirements, milestones, data management, post processing and analysis), project staffing and technical expertise, and the timeliness of the project to begin computing next year.

- a) Is the request for resources clearly explained and the amount of time and storage requirements reasonably estimated and associated with relevant project milestones?
- b) Does the Personnel Justification and Management Plan clearly articulate who is responsible for application performance? Is the level of effort sufficient?
- c) How much time would it take for the project to begin production runs?

#### **4. Summary Rating:**

The ratings below summarize the scale on which computational readiness of the submittal is assessed. The appropriateness of LCF resources can be either capability computing, defined as using approximately 20% of the LCF resources available, or specific architectural requirements that only can be met by the INCITE program. To receive an assessment of appropriate for LCF resources, the project must utilize key components of the compute resources (e.g. many-core architecture of the KNL on Theta or GPUs on Summit) or the project must have specific memory needs, data storage requirements, or time to solution expectations, etc. that cannot be obtained elsewhere.

##### **Ready**

The project is highly appropriate for the requested resource: the planned work could not be accomplished without INCITE resources; the project codes and workflow are already optimized and demonstrated to operate at scale on the requested resource; a clear plan and justification for the requested resources is provided; and the project is ready to begin efficiently computing immediately.

##### **Mostly Ready**

The project is very appropriate for the requested resource: the planned work could not be accomplished without INCITE resources; a very high degree of confidence exists that the project code and workflow can transition to efficient operation at scale on the requested resource; a reasonably clear plan and justification for the requested resources has been provided and the project can be computing efficiently within 1 calendar month.

##### **Approaching Ready**

The project is appropriate for the requested resource: the planned work may not be possible without INCITE resources; the project code has several minor technical issues but can be brought to efficient operation at scale on the requested INCITE resource. The project provides a sufficiently clear plan and justification for the requested resources and can be computing efficiently in less than 3 calendar months using project-provided resources plus normal site user support.

##### **Less Than Ready or Aspects Not Appropriate**

Aspects of the project may not be appropriate for the requested resource: the planned work may not require INCITE resources; the project code has significant technical issues that could negatively impact the ability to effectively use INCITE resources. Minor aspects of the project plan or justification for requested resource may be unclear. The project can only be brought to efficient operation at scale on the requested INCITE resource in no less than 6 calendar months using project resources or project resources plus additional implementation support beyond normal site user support.

##### **Not Ready or Not Appropriate**

The project is not appropriate for the requested resource: INCITE resources are not needed to accomplish the goals; the code cannot run efficiently at scale and there are no plans to scale up; or the project has not provided a clear plan or provided insufficient data to gauge computational readiness.