**• Please fill out the following to the best of your ability.   
• If you have multiple projects and/or codes represented by this case study, note this in the text and then fill out the table at the end using aggregate numbers where appropriate (e.g., total hours used) and maximum values elsewhere (e.g., number of compute cores used per job).   
• If needed, include a different table for each major code.   
• For reference, review the graph of historical usage at   
http://www.nersc.gov/science/requirements-workshops/case-study-faq/**

**• If a question is not applicable to your project, please enter "N/A."**

# Case Study Title: (enter a title here)

**Principal Investigator:**

**Worksheet Author(s) (if not PI):**

**NERSC Repositories**:

# Project Description

## Overview and Context

**Please give a brief, high-level description of your research and its relationship to High Performance Computing (HPC) and storage. (1-3 short paragraphs)**

## Objectives for 2017

**What are your project’s goals for 2017? (1-3 paragraphs)**

# Computational Strategies (now and in 2017)

## Approach

**Give a short, high-level description of your computational problem and your strategies for solving it.**

## Codes and Algorithms

**Please briefly describe the codes you use and algorithms that characterize them (1-2 sentences per). In what science areas are these codes and/or algorithms used? If there are specific science teams that you are working with, please list them here.**

# HPC Resources Used Today

## Computational Hours

**How many hours on conventional cores (not GPUs) will your project(s) use at NERSC in 2013?****How many hours on conventional cores (not GPUs) will your project(s) use at other facilities in 2013?**

## Parallelism

**How many (conventional) compute cores are typically used for production runs at NERSC today using the codes you described above? (You can give a range.)**

**What is the maximum number of cores that these codes could use today?**

**If the typical number is less than the maximum, briefly explain why fewer than the maximum are used.**

**Which is more important for your software or project, strong scaling or weak scaling? Why? (Strong: you have a problem of a given size and you'd like to use parallel computing to solve it faster. Weak: you have a problem of a given size and you'd like to use parallel computing to solve a bigger problem in the same time.)**

## Scratch Data

**What is the maximum amount of temporary disk space (space that can be purged) you need?**

## Shared Data

**NERSC provides “project directories,” which are permanent, global, shared storage areas for collaboration. Does your project have a NERSC project directory? If so, what is its name? What is the primary reason you have this space?**

## Archival Data Storage

**How much data do you have stored on the NERSC HPSS data archive in 2013?**

# HPC Requirements in 2017

## Computational Hours Needed

**How many compute hours will your project require in CY 2017? Please state this requirement normalized to a Hopper-equivalent core hour if possible.** **Include all hours your project will need to reach the goals you listed in 2.2 above.**

**If you expect to receive significant allocations from sources other than NERSC, please list them here.**   
  
  
  
**If you expect to need more compute hours in 2017 than you used at NERSC in 2013, what is the primary factor driving the need for more hours?**

## Parallelism

**How many MPI tasks (or equivalent) do you expect your code use in 2017? How much additional fine-grained parallelism will be associated with each task? (Please describe the target architecture if applicable).**

**What do you expect is the maximum that could be used in 2017?**

## I/O

**Does your application have built-in checkpoint/restart?**

**How much data will you need to read and write per run in 2017 (including checkpoint/restart data)?**   
  
**Please estimate your I/O bandwidth requirement (bandwidth = data read or written / time to read or write).**

**What percentage of your total runtime are you willing to devote to I/O?**

## Future Data Needs (Please replace "X" or fill in the blank)

**In 2017, we expect to need \_\_X\_\_ TB of temporary scratch disk space, \_\_X\_\_ TB of NERSC project space (globally accessible shared data), and \_\_X\_\_ TB of storage on NERSC HPSS. The growth in these requirements relative to 2013 is due primarily to \_\_\_\_\_\_\_\_\_\_\_\_\_\_.**

**Of the data that you store at NERSC in the project space or on HPSS, how long does your data need to be retained after the project is done? (N years, would like permanent repository, etc.)**

## Memory Required

**For NERSC to plan for future systems, we need to know your memory requirements. How much memory will your codes require per node (in a discrete memory space)? How much aggregate memory will be required?**

## Emerging Technologies and Programming Models

**Please discuss the status of efforts to transition your software to emerging architectures. Please answer the questions below and provide any additional information that will help us understand what needs to done to successfully transition codes to run efficiently on next-generation architectures.**

**Does your software have CUDA/OpenCL extensions? If so, are they used, and if not, are there plans to add them?**

**Does your software run in production now on Titan or elsewhere using GPU hardware?**

**Does your software have OpenMP directives now? If so, are they used, and if not, are there plans to add them?**

**Does your software run in production now on Mira or Sequoia (BG/Q) using threading?**

**Is porting to, and optimizing for, the Intel MIC architecture underway or planned?**

**Have there been, or are there now, other funded groups or researchers engaged to help with these activities?**

**If you answered "no" for the questions above, please explain your strategy for exploiting these technologies.**   
  
**What role should NERSC play in the transition to these architectures?**

**What role should DOE and ASCR play in the transition to these architectures?**

**Other needs or considerations:**

## Software Applications and Tools

**What HPC software (applications / libraries / tools / compilers / languages / etc) will you need to be installed at NERSC in 2017? Be sure to include analytics applications and I/O software**.

## HPC Services

**What NERSC services will you require in 2017? Possibilities include consulting and account support, data analytics and visualization, training, support servers, collaboration tools, web interfaces, federated authentication services, gateways, etc**.

**Do you need web resources from NERSC to publish your data or results?**

## Additional Data Intensive Needs

**Will you have additional needs we have not considered regarding data? These could be related to workflow, management, transfer, analysis, sharing or access, or visualization**.

**Do you already have a data management plan for your project and does it include archival storage?**

**Do you need help from NERSC in defining or implementing a data management plan for your project?**

## Additional Data Intensive Needs: Burst Buffer

**Please look at the primary scenario and seven secondary scenarios for possible Burst Buffer use on http://www.nersc.gov/assets/Trinity--NERSC-8-RFP/Documents/trinity-NERSC8-use-case-v1.2a.pdf and comment which of these would be most useful for your work.**

## What Else?

**Are there any other services or facilities you would like NERSC to provide?**

**Do you have present or future concerns you’d like to discuss?**

# Requirements Summary Worksheet

Please try to fill out this worksheet, based on your answers above, to be best of your ability prior to the review.

|  |  |  |
| --- | --- | --- |
|  | **Used at NERSC in 2013** | **Needed at NERSC in 2017** |
| Computational Hours\* |  |  |
| Typical number of cores\*\* used for production runs |  |  |
| Maximum number of cores\*\* that can be used for production runs |  |  |
| Data read and written per run | TB | TB |
| Maximum I/O bandwidth | GB/sec | GB/sec |
| Percent of runtime for I/O |  |  |
| Scratch File System space | TB | TB |
| Shared filesystem space | TB | TB |
| Archival data | TB | TB |
| Memory per node | GB | GB |
| Aggregate memory | TB | TB |

\*Normalized to Hopper-equivalent (NERSC MPP) hours

\*\* “Conventional cores.” For GPUs and accelerators, please fill out section 4.7.

# Additional Storage and I/O Questions

These questions are optional but your answers will provide additional useful data for NERSC. If you don't know the answer to any of these leave them blank.

**For Scratch data (like Question 5.4)**:

• **Is your I/O more serial or parallel?**

• **Is your I/O more single-node or multiple-node?**

• **Is your I/O more shared (N-to-1) or distributed (N-to-N)?**

•  **Is your I/O more small-file or large-file?**