MPI usage at NERSC: Present and Future [*]

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1. ABSTRACT

In this poster, we describe how MPI is used at the National Energy Research Scientific Computing Center (NERSC). NERSC is the production high-performance computing center for the US Department of Energy, with more than 5000 users and 800 distinct projects. Through a variety of tools (e.g., User Survey, application team collaborations, etc.), we determine how MPI is used on our latest systems, with a particular focus on advanced features and how early applications intend to use MPI on NERSC's upcoming Intel Knights Landing (KNL) many-core system[1] - one of the first to be deployed. In the poster, we also compare the usage of MPI to exascale developmental programming models such as UPC++ and HPX, with an eye on what features and extensions to MPI are plausible and useful for NERSC users. We also discuss perceived shortcomings of MPI, and why certain groups use other parallel programming models on the systems. In addition to a broad survey of the NERSC HPC population, we follow the evolution of a few key application codes[2] that are being highly optimized for the KNL architecture using advanced OpenMP techniques. We study how these highly optimized on-node proxy apps

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[1]Cori Phase-2 system will be a Cray XC system based on the second generation of Intel Xeon Phi Product Family, called Knights Landing (KNL) Many Integrated Core (MIC) Architecture. The system will have a sustained performance that is at least ten times that of the NERSC-6 "Hopper" system, based on a set of characteristic benchmarks.

[2]http://www.nersc.gov/users/computational-systems/cori/application-porting-and-performance/application-case-studies/
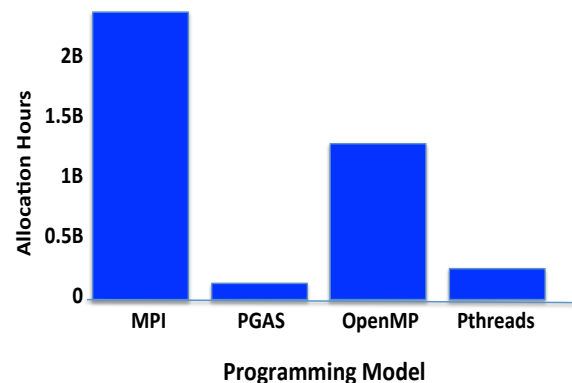
Figure 1: Approximate distribution of parallel programming models used at NERSC based on 2015 allocation requests to US Department of Energy. Total exceeds 100% because some codes use multiple models.

and full applications start to make the transition to using full hybrid MPI+OpenMP implementations on the self-hosted KNL system.

CCS Concepts

•Software and its engineering → General programming languages;

Keywords

MPI, programming models

2. ACKNOWLEDGMENTS