# Interactive Supercomputing on 40,000 Cores for Machine Learning and Data Analysis

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Abstract—Interactive massively parallel computations are critical for machine learning and data analysis. These computations are a staple of the MIT Lincoln Laboratory Supercomputing Center (LLSC) and has required the LLSC to develop unique interactive supercomputing capabilities. Scaling interactive machine learning frameworks, such as TensorFlow, and data analysis environments, such as MATLAB/Octave, to tens of thousands of cores presents many technical challenges - in particular, rapidly dispatching many tasks through a scheduler, such as Slurm, and starting many instances of applications with thousands of dependencies. Careful tuning of launches and prepositioning of applications overcome these challenges and allow the launching of thousands of tasks in seconds on a 40,000-core supercomputer. Specifically, this work demonstrates launching 32,000 TensorFlow processes in 4 seconds and launching 262,000 Octave processes in 40 seconds. These capabilities allow researchers to rapidly explore novel machine learning architecture and data analysis algorithms.

#### Keywords-Scheduler, interactive, machine learning, manycore, high performance computing, data analytics.

#### I. INTRODUCTION

Interactive supercomputing has been an ongoing focal point of high performance computing (HPC) at Lincoln Laboratory [Reuther 2004]. Since its inception, users have connected their desktops and laptops to Lincoln's interactive supercomputer and been able to launch parallel pMatlab jobs from their desktop/laptop integrated developer environment (IDE) [Reuther 2005].

This system architecture has evolved into the MIT SuperCloud, a fusion of the four large computing ecosystems – supercomputing, enterprise computing, big data and, traditional databases – into a coherent, unified platform that enables rapid prototyping capabilities across all four computing ecosystems. The MIT SuperCloud has spurred the development of a number of cross-ecosystem innovations in high performance databases [Byun 2012], [Kepner 2014a], database management [Prout 2015], data protection [Kepner 2014b], database federation [Kepner 2013], [Gadepally 2015], data analytics [Kepner 2012] and system monitoring [Hubbell 2015].

This capability has grown in many dimensions. The MIT Lincoln Laboratory Supercomputing Center (LLSC) provides interactive supercomputing to thousands of users at MIT Lincoln Laboratory and at the MIT Beaver Works Center for Engaging Supercomputing. LLSC not only continues to support parallel MATLAB and Octave jobs, but also jobs in Python [Van Rossum 2007], Julia [Bezanson 2017], R [Ihaka 1996], Tensorflow [Abadi 2016], PyTorch [Paszke 2017], and Caffe [Jia 2014] along with parallel C, C++, Fortran, and Java applications with various flavors of message passing interface (MPI). Furthermore, the TX-Green flagship system now has nearly 60,000 cores available for users' parallel jobs. The most significant jump in core count was the addition of 648 Intel Xeon Phi 64-core nodes [Byun 2017, Cichon 2016], each of which has 64 compute cores in a single processor socket laid out in a mesh configuration [Jeffers 2016]. This equals 41,472 total cores across the 648 compute nodes, all connected by a non-blocking 10-Gigabit Ethernet network and a non-blocking Intel OmniPath low-latency network.

Scaling immediate interactive launches to such a large number of cores was a significant challenge; this paper discusses the technical experimentation and engineering involved in scaling the interactive parallel launching capability of TX-Green to the scale of 40,000 core jobs. In the Section II, we review the background of interactive supercomputing, discuss the components of a supercomputing scheduler, review the results of a previous study comparing state-of-the-art HPC schedulers and resource managers. Section III details the experimentation and steps taken to enable interactive supercomputing launches to the scale of 40,000 core jobs, while

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Section IV discusses the scaling launch time results on the 64-core Xeon Phi compute nodes. Finally, the paper is summarized in Section V.

## II. INTERACTIVE SUPERCOMPUTING LAUNCH

Whether on a laptop or smartphone, interactivity is inherent in our daily interactions with computers since that computer is dedicated exclusively to ourselves when we are interacting with the device. However, supercomputers are almost always a shared set of resources. Traditionally, supercomputer jobs were submitted to a job queue, from which the scheduler chose the optimal job to execute next when resources became available. This scheduling technique is called batch scheduling, and it introduces latency between job submission and job execution as depicted in Figure 1 [Reuther 2007]. However, one component of interactive supercomputing is enabling very fast parallel on-demand (immediate) job launches, while the other main component is supporting parallel high productivity software packages including MATLAB/Octave, Python, Julia, and R along with domain specific packages like Tensorflow, Caffe, and PyTorch. In this paper, we focus on the job launches to enable the efficient use of such high productivity software packages. Such terastive lancebes are abordepicted in Figure 1, and in this work flow does not have time spent in the pending state.

depicted in Figure 2. At one extreme, all jobs are scheduled as batch jobs which can incur high latency before execution, while at the other extreme all jobs are scheduled immediately, which can cause scheduler flooding. Most supercomputing centers use batch queuing with reservations, which allow users to reserve a set of resources sometime in the future for a window of interactive computing. For the LLSC, we have chosen the route of interactive, immediate launches with user resource limits. This enables immediate interactive jobs, while avoiding scheduler flooding:<sup>COMPUTING CENTER</sup>



To better understand how we have implemented MIT LINCOLN LABORATORY SUPERCOMPUTING CENTER s of the job scheduler. At its simplest level, job schedulers are resperent and the sources. The users and utern users on computational resources. The users and utern jobs will have different resource requirements and priorities. Similarly, the computational resources have different resource availabilities and capabilities, and they must be managed in such a way that they are



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A cluster job scheduler has four key operational lifecvcle management. tasks: iob resource management, scheduling, and job execution, as shown in Figure 3. The job lifecycle management task receives jobs from users through the user interface and places them in one of the job queues to wait for execution (regardless of whether jobs are scheduled and executed on demand or batch queued). Various resources for the job including memory, licenses, and accelerators (such as GPUs) are requested through the user interface by the user. The job lifecycle management task is also responsible for prioritizing and sorting candidate jobs for execution by using the queue management policies. The scheduling task periodically requests a prioritized list of candidate queued jobs and determines whether resources are available to execute one or more of the jobs. The scheduler receives the state of all the resources from the resource management task, which in turn is receiving resource state and availability information from the compute nodes. The scheduling task allocates resources (usually one or more job slots on compute nodes) and assigns the job to the resource(s) if adequate resources are available to execute each job. The job execution task is responsible for dispatching/launching the job on the resources. Upon the completion of each job, the job execution task manages the closing down of the job and reporting the statistics for the job to the job lifecycle management task, which records it in logs.

In recent studies [Reuther 2016, Reuther 2018], we conducted a detailed comparison of traditional supercomputing schedulers and Big Data schedulers. Two of the most important takeaways from this comparison were:

- 1. The traditional supercomputing schedulers including Slurm [Yoo 2003], LSF [Zhou 1993], and GridEngine [Slapnicar 2001] were capable of launching synchronously parallel (MPI-style) jobs as well as loosely parallel job arrays. Big Data schedulers including Mesos, Apache YARN [Vavilapalli 2013], and the open-source Kubernetes project [Hindman 2011] supported only parallel job arrays.
- 2. Several schedulers including Slurm, Mesos, and Kubernetes were designed to handle 100,000+ jobs, both in its queues and executing on compute nodes.

Since Slurm supports both synchronously parallel jobs and job arrays and scaled to managing 100,000+

jobs, it substantiated the continued use of Slurm as the job scheduler for LLSC systems.

# III. LAUNCHING 40,000 CORE JOBS

Recently, LLSC upgraded its flagship system with 648 Intel Xeon Phi compute nodes. Each node has a 64-core Intel Xeon Phi 7210 processor, for a total of 41,472 cores, along with 192 GB RAM, 16 GB of onpackage MCDRAM configured in 'flat' mode, local storage, 10-GigE network interface, and an OmniPath application network interface each. The Lustre [Braam 2003] central storage system uses a 10 petabyte Seagate ClusterStor CS9000 storage array that is directly connected to the core switch. As with all of the LLSC systems, enabling interactive jobs was a top priority. However, the first attempts at launching interactive MATLAB/Octave jobs through slurm onto 40,000 processors resulted in 30- to 60minute launch times; these launch times were a hindrance to any interactivity with the jobs.

To enable truly interactive launches, a number of experiments and engineering trade-offs were explored. First, we investigated how fast launches could be enabled. We started by allocating a block of nodes through Slurm with the salloc command, feeding the node list into pMatlab [Kepner 2009], and using a hierarchical secure shell (ssh) process spawning mechanism to launch a large set of interactive processes. This gave us a baseline for how fast we could expect to launch 10,000+ core jobs launches of less than a minute should be possible. We went on to explore the use of job arrays and synchronously parallel launches, which each had their trade-offs. Synchronously parallel jobs using srun enabled the fastest launches, but the resources for a job remained allocated until all of the computational processes completed. Conversely, each job array process relinquishes its resources as soon as it finishes its work. Launch times were similar. We also experimented with various queue evaluation periodicities and job queue evaluation depth values to find the most effective combination.

To further speed up launches, we decided to allocate whole compute nodes and launch a single scheduler-issued launcher process per compute node. This launcher process subsequently spawns and backgrounds each of the application processes that are to be launched on its compute node.

We made several improvements in tuning the launching of applications themselves. First, we

copied the entire installations of five MATLAB versions, two Octave versions, and five versions of Anaconda Python including TensorFlow, Caffe, and PyTorch onto the local hard drive of every compute node. This reduced the latency of loading thousands of instances from sthe central file system and across the 10Gig-E network. We also used the thing flag<sup>T E R</sup>interactive machine learning experience. with MATLAB to record what segments of MATLAB startups used the most time and reduced its launch time further. This prompted us to also create a MATLAB-lite version which loaded only the base MATLAB toolboxes and did not include the internal Java invocation. With all of these improvements, we met the interactive launching goals that we had set out to achieve.

## **IV. PERFORMANCE RESULTS**

Training machine learning models requires high level programming environments for building the models and rapid interaction with the analyst to converge on the best training parameters. Standard approaches take minutes to hours to launch models on thousands of cores. However, with the improvements we discussed in the previous section, we are able to launch hundreds of machine learning models in a matter of seconds.



Figure 4: Tensorflow launch scaling results Supercomputing Center

TensorFlow is one of the leading deep neural network model frameworks available today. TensorFlow is supported by Geogles, and the provides a productive Python API for generating and training deep neural networks [Abadi 2016], Figure 4 is a log-log plot scaling up the number of processor cores on the x-axis versus the launch time on the y-axis. We

have achieved launch times of less than 5 seconds for 32,000+ cores (512 64-core Xeon nodes). In other words, we are able to launch 512 TensorFlow models simultaneously. This enables very rapid trade-off analyses of neural network batch size, convergence rates, input set randomization, etc. for a truly



Figure 5: MATLAB/Octave launch scaling

Many researchers at MIT frequently use MATLAB and Octave for rapid prototyping, algorithm development, and data analysis. These activities require rapid interaction and fast turnarounds to make significant progress and convergence to a solution. We achieved similar launching results with pMatlab and parallel Octave jobs. Figure 5 is a log-log plot scaling up the number of processor cores on the xaxis versus the launch time on the y-axis. We have achieved launch times of less than 10 seconds for launching 32,000+ MATLAB/Octave jobs (512 64core Xeon nodes) launching one MATLAB/Octave process per core. Furthermore, we have achieved parallel launches of 260,000+ MATLAB/Octave process launches in under 40 seconds. Each of the cores on a Xeon Phi processor has four hyperthreads, and this parallel launch involves launching 512 MATLAB/Octave processes per Xeon Phi processor, two for each hyperthread.

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Figure 6: Launch times in seconds of parallel MATLAB/Octave jobs over Nnode nodes and Nproc MATLAB/Octave processes per node.



Figure 7: Launch rates of parallel MATLAB/Octave jobs over Nnode nodes and Nproc MATLAB/Octave processes per node.

We have further measured the launch time and launch rate for the parallel MATLAB/Octave jobs, varying the number of nodes from 1 to 512 in powers of 2, and varying the number of processes per node from 1 to 512 in powers of 2. The launch time results are show in Figure 6; launch times remain under 10 seconds for all but the largest number of nodes onto which the processes were launched. Further, launch times are under 20 seconds but for the very largest node numbers and processes per node. Figure 7 displays the launch rates in process launches per second. This plot shows that the scheduler and the local launchers can sustain launch rates of 6,000 processes per second. We have found that Slurm handles the many parallel launches onto each of the nodes quite well. Our two-tiered launching mechanism is very effective on manycore processors such as the Intel Xeon Phi. We have determined that the rise in launch time for high node counts and processes per node arises from backpressure from our low-latency, high-bandwidth Lustre central file

system, which serves a few files to each of the launching processes. However, serving a few files to each process when there are many processes does add up.

## V. SUMMARY

High performance launch at scale is a generally enabling capability of interactive supercomputing. It allows the processing of larger sets of sensor data, the creation of higher-fidelity simulations, and the development new algorithms for space observation, robotic vehicles, communications, cyber security, machine learning, sensor processing, electronic devices, bioinformatics, and air traffic control. In this we have discussed the technical paper. experimentation and engineering involved in scaling the interactive parallel launching capability of TX-Green to the scale of 40,000 core jobs. The applications for which we shared results are the TensorFlow machine learning framework and the MATLAB/Octave rapid prototyping language and environment. These launching capabilities enable very large Monte Carlo and parameter trade-off analyses using these very familiar frameworks and programming environments.

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