

# Unveiling User Behavior on Summit Login Nodes as a User

Sean R. Wilkinson<sup>[0000–0002–1443–7479]</sup>, Ketan Maheshwari<sup>[0000–0001–6852–5653]</sup>,  
and Rafael Ferreira da Silva<sup>[0000–0002–1720–0928]</sup>

Oak Ridge National Laboratory, Oak Ridge, TN, USA\*\*  
{wilkinsons, maheshwarikc, silvarf}@ornl.gov

**Abstract.** We observe and analyze usage of the login nodes of the leadership class Summit supercomputer from the perspective of an ordinary user—not a system administrator—by periodically sampling user activities (job queues, running processes, etc.) for two full years (2020–2021). Our findings unveil key usage patterns that evidence misuse of the system, including gaming the policies, impairing I/O performance, and using login nodes as a sole computing resource. Our analysis highlights observed patterns for the execution of complex computations (workflows), which are key for processing large-scale applications.

**Keywords:** High Performance Computing · Workload Characterization  
· User Behavior.

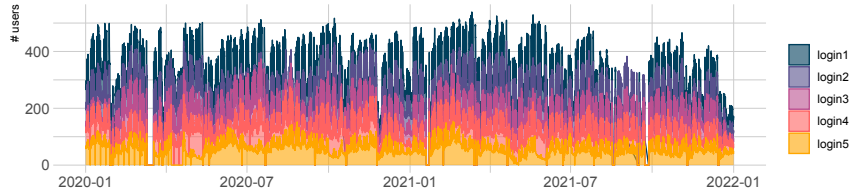
## 1 Introduction

HPC systems have been designed to address computing, storage, and networking needs for complex, high-profile applications. Specifically, leadership class supercomputers [16] meet the needs of applications that require high-speed interconnects, low latency, high I/O throughput, and fast processing capabilities (currently petascale, and soon exascale) [6]. Understanding the performance of these systems and applications is a cornerstone for the design and development of efficient, reliable, and scalable systems. To this end, several works have focused on the development of system- and application-level monitoring and profiling tools that can provide fine-grained characterizations of systems’ and applications’ performance.

The current landscape of HPC systems performance research is mostly focused on the system’s performance—which is utterly valuable for systems design [4, 9, 15]. However, the *user perception* of the system is often disregarded, and there is a common misconception that application execution performance is the only consideration for user satisfaction. Although application performance is one of the chief goals of HPC, there are several additional factors that impact

---

\*\* This manuscript has been authored by UT-Battelle, LLC, under contract DE-AC05-00OR22725 with the US Department of Energy (DOE). The publisher acknowledges the US government license to provide public access under the DOE Public Access Plan (<http://energy.gov/downloads/doe-public-access-plan>).



**Fig. 1.** Distribution of users over 5 Summit login nodes (Jan 2020–Dec 2021). Gaps in the time series indicate outages or system downtime.

user experience. More specifically, before experiencing the capabilities of the HPC nodes, users’ first interactions are with the *login nodes*, where users share resources like CPU, memory, storage, and network bandwidth while performing basic tasks like compiling code, designing experiments, and orchestrating services. The login nodes on an HPC system represent a gateway to the system which is often overlooked when considering the capabilities and performance of the overall system. We argue that the experience on the login nodes may impact a user’s perception of and behavior on the system, thus influencing whether and how the user continues to utilize that system in future work.

In this paper, we attempt to identify long-term usage patterns by collecting observational data on the login nodes from the Summit leadership class supercomputer hosted at the Oak Ridge Leadership Computing Facility (OLCF) at Oak Ridge National Laboratory (ORNL). Every hour for two years (2020–2021), we have collected data about the login nodes’ performance with respect to CPU, memory, and disk usage, and we also collected data about their activity with respect to logged-in users, the programs they were running on the login nodes, and the status of all user jobs. Figure 1 shows the number of users per login node within this time window. In addition to examining traditional metrics like system usage and distribution of jobs and users across the nodes, we also seek to (i) highlight atypical usage and user misconducts, (ii) relate these behaviors to potential performance issues, (iii) identify usage patterns of a complex class of applications such as scientific workflows, and (iv) establish relationships between users’ sessions length and system load.

## 2 Characteristics of the Summit Login Node Data

Table 1 summarizes the main characteristics of the collected data. The dataset represents activity from 1,967 unique users, who connected using 9,841 unique IPs and submitted 1,783,867 jobs, of which 1,073,754 completed successfully while 705,103 had a non-zero exit code. Figure 2 shows the distribution of users’ geolocations, which were resolved through an IP geolocation tool [1]. For the sake of privacy, any user-specific data had been previously anonymized and not retained.

**Table 1.** Characteristics of Summit login node data for a period of two years (Jan 2020–Dec 2021). Totals for “Unique Users” and “Unique IPs” do not sum additively due to Summit users whose use spanned both years. Additionally, the total number of jobs may not coincide with the sum of individual years because jobs may be carried over from one year to the next.

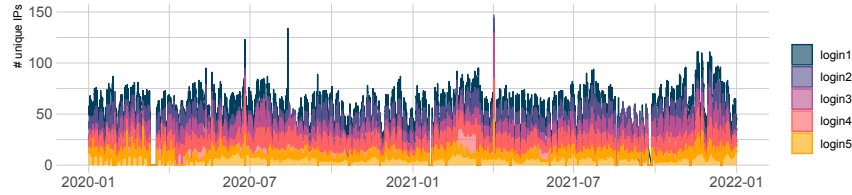
Year	# Unique Users	# Unique IPs	# Jobs			total
			completed	suspended	exited	
2020	1,509	5,094	480,550	1,869	313,257	795,676
2021	1,514	5,467	668,580	3,264	410,493	1,082,337
Total	1,967	9,841	1,073,754	5,010	705,103	1,783,867



**Fig. 2.** Users’ geolocation distribution obtained with IP lookup (~93% of total users).

**System Characteristics and Data Collection** – Summit is equipped with 5 login nodes [18]. Each login node runs Red Hat Enterprise Linux v8.2 and comes equipped with two 3.8 GHz 16-core IBM POWER9 CPUs (4 threads per core), 512 GiB of DDR4-2667, 4 NVidia V100 GPUs each with 16 GiB of HBM2, and connection to a 250 PB GPFS scratch filesystem. Data were collected hourly, starting January 1, 2020, on all five login nodes. A shell script ran in the user space as a `while` loop within a Linux `tmux` session because user cronjobs are not allowed, and it collected traditional system usage performance metrics as well as user behavior (e.g., running processes and jobs). One caveat is that the hourly sampling frequency may have failed to capture fine grained behavior, as many things can happen between samples. Nevertheless, we believe that the large volume of samples sufficiently captures most of the representative system and user activity. More precisely, at each iteration of the script we collect the following data:

- List of currently logged-in users using the `w` command;
- CPU and memory usage using the `top` and `ps` commands (which also provides the list of running processes), and statistics from `meminfo` and `vmstat` in the `/proc` filesystem;



**Fig. 3.** Distribution of unique IPs across Summit login nodes (Jan 2020–Dec 2021).

- Status of users’ batch jobs via the `bjobs` command;
- Disk usage statistics using the `df -h` command and disk throughput by measuring the timespan for writing a 1GB data file to GPFS.

**Data Preparation** – Real-world data may be incomplete, noisy, and inconsistent, which can obscure useful patterns [20]. Data preparation techniques cannot be fully automated; it is necessary to apply them with knowledge of their effect on the data being prepared. We used our prior knowledge about the execution of scientific applications on HPC to extract and combine relevant information from each source of data. We have then pre-processed the dataset by removing redundancies and missing data (e.g., due to outages and system downtimes), sanitizing lists of programs and users for long-running processes and jobs, and resolving IP addresses for filtering and identifying individual users and their locations, among other things.

### 3 System Metrics

In this section, we examine overall characteristics and performance metrics from Summit. The assessed set of metrics are restricted to an ordinary user’s perspective of the system, as viewed from a login node. Although these metrics are often reported and analyzed in-depth from the system’s perspective by using system-wide monitoring and profiling tools, here we have used a subset of these metrics to support our claims regarding user experience and behavior.

#### 3.1 Users Access

Figure 1 shows the distribution of user sessions per login node. The average percentage of user distribution is 21.9% ( $\pm 9.2\%$ ), 20.7% ( $\pm 9.2\%$ ), 17.9% ( $\pm 7.8\%$ ), 20.2% ( $\pm 8.8\%$ ), and 19.3% ( $\pm 8.1\%$ ) for login nodes 1–5, respectively. Although this distribution is relatively balanced among login nodes, by inspecting the distribution of unique IPs per login session (Figure 3) we observe that there is an imbalance on the disposition of individual users among the nodes. Specifically, the average percentage of unique IPs distribution is 20.5% ( $\pm 8.8\%$ ), 20.8% ( $\pm 9.2\%$ ), 16.7% ( $\pm 8.6\%$ ), 23.5% ( $\pm 10.1\%$ ), and 18.5% ( $\pm 8.1\%$ ) for login nodes 1–5, respectively. This indicates that a subset of users may be (involuntarily) benefitting from an increased number of concurrent login sessions; thus, their





**Fig. 4.** CPU utilization on Summit login nodes (Jan 2020–Dec 2021).



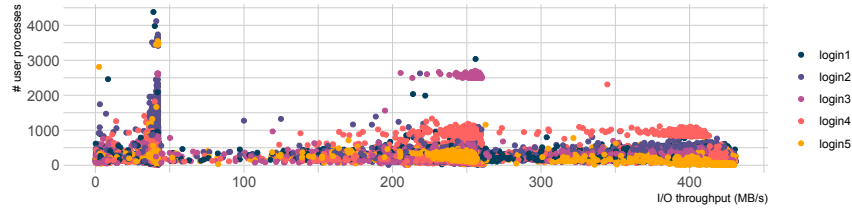
**Fig. 5.** User processes on Summit login nodes (Jan 2020–Dec 2021).

perceived experience of the system may be more favorable when compared with users who share resources with a larger number of individual users.

To support (or contrast) the above claim, we examined CPU utilization and the number of user processes per login node (Figures 4 and 5). Overall, CPU utilization is relatively balanced among nodes (around 15% in average across nodes) with some spikes on login nodes 2, 3, and 5. Unsurprisingly, the number of user processes follows similar trends as for the distribution of unique IPs. Both of these results corroborate the claim that a small subset of users have been benefited from lower concurrency. More precisely, the balanced distribution of CPU utilization on login nodes 3 and 5 indicates that this small set of users consumes as many resources on these nodes as the larger set of users on the other nodes.

### 3.2 I/O Throughput

Every hour, we have measured the I/O throughput of Summit’s GPFS for writing a 1 GB randomly generated binary data file to a shared folder. Notice that we do not aim to assess peak write speeds; instead our goal is to identify potential low performance caused by user-related I/O operations within the login nodes. Figure 6 shows the distribution of the number of user processes running per login node in relation to the I/O throughput for writing a 1 GB file. Note that the performance of the GPFS filesystem may also be affected by I/O operations occurring on the compute nodes; thus a weak correlation is expected with processes running on the login nodes. That said, we can observe that a low performance is highly correlated with an increased number of user processes running on the login nodes. Specifically, throughput values as low as 42MB/s are reported when more than 3,000 user processes are running for more than



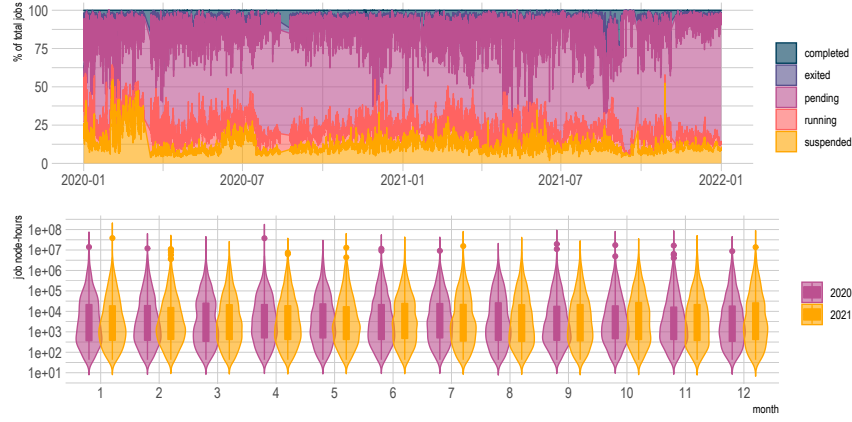
**Fig. 6.** I/O throughput of Summit’s GPFS for writing a 1 GB file in relation to the number of user processes.

3 consecutive hours. For the same set of datapoints, user processes running on login5 run for more than 5 consecutive hours, which coincides with the timespan in which the filesystem yields low performance (recall that login5 has, on average, a reduced number of concurrent unique users). Analogously, impaired performance (around 250 MB/s) is observed for a very small group of users who run more than 2,500 processes on login3 for more than 7 hours.

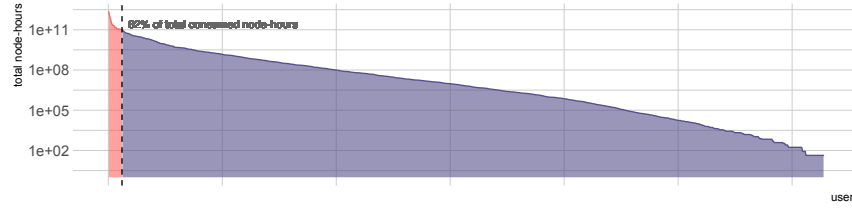
### 3.3 Computational Jobs

The fundamental purpose of leadership-class supercomputers is to improve science by running the largest-scale computational jobs. It is expected that user satisfaction is mostly dictated by the ability to execute batch jobs successfully with good performance and without long waits in the queue. Figure 7-*top* shows the percentage distribution of jobs based on their status. The workload average jobs submitted, running, and completed, as shown by the LSF scheduler, are 529 ( $\pm 271$ ), 81 ( $\pm 24$ ), and 90 ( $\pm 69$ ), respectively. Given that the number of individual users (see Table 1) is orders of magnitude higher than the average number of running jobs, the variation in the number of running jobs seems relatively low.

Figure 7-*bottom* shows the distribution of node-hours consumed per job. Intriguingly, the shape of the distributions are alike across years and months. More precisely, the average root mean square error (RMSE) is below 6 for every month comparison between the two years, with most jobs consuming between 1,000 and 10,000 node-hours. This result suggests that jobs are mostly submitted by a small set of users running similar, yet large, workloads. Indeed, by examining the number of jobs submitted per user, we observe that *only 29 users* ( $\sim 1.4\%$  of total number of users in the dataset), submitted more than 50% of all Summit jobs over the measured period of time. These jobs represent more than 82% of the total consumed node-hours in the dataset (Figure 8). As expected, most individual jobs consume between 1,000 and 10,000 node-hours, which corroborates the findings asserted from Figure 7-*bottom*. Most users submitted a very small number of jobs, though they span a wide range of node-hours consumption, with a few jobs consuming nearly all available compute resources. We can also observe that specific users submitted sets of individual jobs with a wide range of node-hours (e.g., from 96 up to 193,537), but also submitted more than 1,100 jobs with the same size (e.g.,  $\sim 4,300$  node-hours).



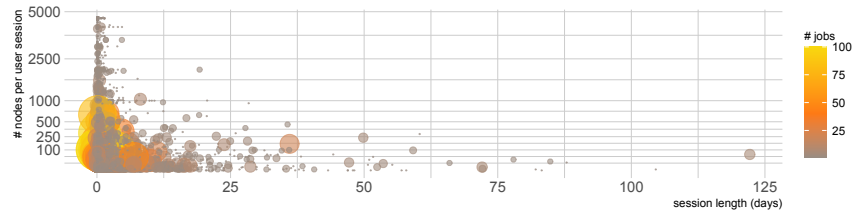
**Fig. 7.** Distribution of jobs’ statuses (*top*) and jobs’ sizes (*bottom*). Each “violin” represents the distribution of jobs’ sizes in a given month in terms of node-hours as a rotated kernel density plot on top of a box-plot that shows the first and third quartiles of the distribution; the width of the violin corresponds to the number of jobs, and the dots indicate outliers in the tails.



**Fig. 8.** Distribution of total node-hours consumed per user. (The dashed vertical line delineates the total node-hours consumed by 29 users, which represents more than 82% of the entire dataset.)

## 4 User Behavior

HPC performance metrics are traditionally associated with success metrics such as high system utilization and large number of users and jobs, which correlate to wide system adoption by the community and fulfillment of scientific goals. Understanding and modeling user behavior in HPC environments is key to exhibiting usage patterns that may help improve the design of the system, relate performance bottlenecks to specific behaviors, and ascertain violations of policies and best practices, among other things. Previous studies have mainly focused on job characteristics (performance metrics as presented in Section 3.3) and scheduling (queuing time, wall time, etc.) [12, 13, 19]. In this section, we examine user behavior from the standpoint of (i) the average user session length, (ii) misuses, and (iii) usage patterns of a complex class of applications such as scientific workflows.



**Fig. 9.** Users’ session lengths (in days) in relation to the number of jobs submitted and maximum number of nodes requested.

#### 4.1 User Sessions

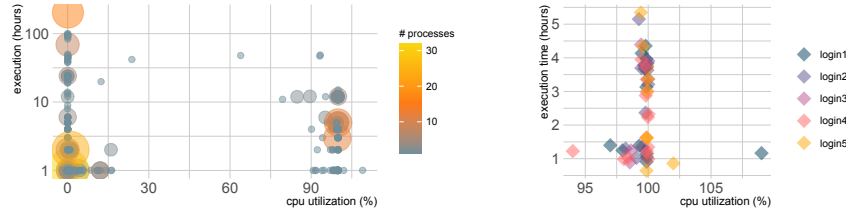
In this section, we investigate the length of user sessions in an attempt to characterize user behavior by relating the time users spend logged into the system with the number and size (in terms of number of nodes) of jobs submitted. We define a *session* as a time interval indicated by activity which begins and ends with inactivity. We use batch job submission as the indicator of activity, and for inactivity, we leverage *think time* [7], which quantifies the time between the completion of a job and the submission of the next job by the same user. Thus, a session is the time period that complements two subsequent think times for the same user. In this work, we assume that a think time is characterized by an interval of more than 24 hours. We do not consider weekends, holidays, or system downtimes or outages as think times.

We identified 27,789 sessions, the longest of which spans 123 days and runs 68 jobs over a maximum of 64 nodes. Most of the users (about 92%) established more than one session, and most of the user sessions (about 84%) span less than one day; also, more than 50% of these sessions request only 1 or 2 nodes per job. Sessions with large-scale jobs that use nearly all of Summit’s compute nodes span only a few hours, with only 3 spanning slightly more than one day. This supports the idea that user experience on login nodes significantly impacts user satisfaction, because users spend most of their time testing and debugging while using the login nodes.

Figure 9 shows the distribution of user sessions’ lengths in relation to the total number of nodes used by all jobs within a session.

#### 4.2 Misuse

Typically, HPC systems balance users across the set of login nodes to improve the overall user experience and limit any potential performance impact due to heavy user processes (see Section 3.1). To prevent low quality of service, most HPC systems provide guidance and best practices for operations that should not be performed on login nodes because they are shared resources. For instance, it is discouraged to run long-term and/or heavy services (e.g., databases) on such nodes. In this section, we examine whether users run processes that could harm the overall performance of these shared resources. To this end, we mined

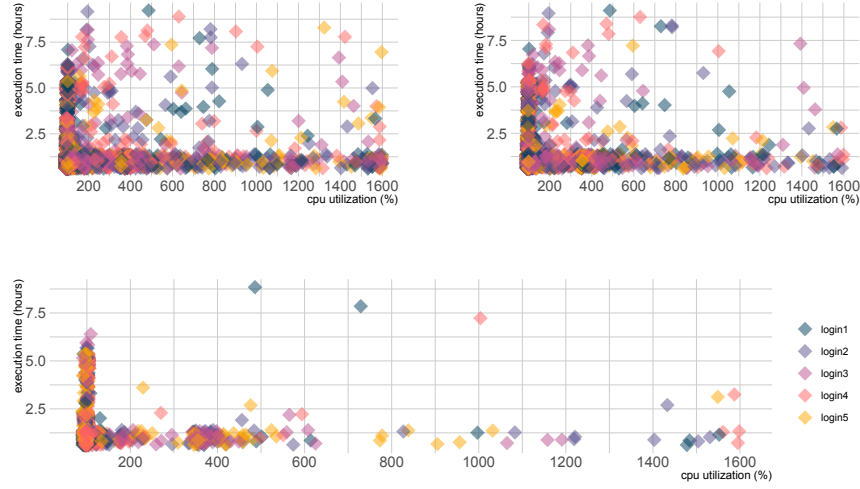


**Fig. 10.** *Left:* Execution of `mpirun` and `mpiexec` on login nodes (1,172 instances from 74 users). *Right:* 56 executions of GROMACS (`gmx.mpi`) on login nodes by two users. Each user runs instances of GROMACS on every login node, which occupy the available GPUs for several hours.

the dataset for processes that did not represent typical, system-related tasks, that consumed a substantial amount of resources (CPU / GPU / memory), or that ran for a long period of time. We limit our discussion in this section to two representative use cases: (i) execution of tightly coupled applications using `mpirun` and `mpiexec`, and (ii) execution of high-throughput applications.

***Tightly Coupled Applications*** – In the dataset, we have identified 1,172 uses of `mpirun` and `mpiexec` by 74 users for running tightly coupled applications in the login node. (Our filtering process removed mentions to compiling operations and flags, environment variables, etc.) By further investigating the dataset, we noticed that 816 out of the 1,172 instances of `mpirun` and `mpiexec` spawned only a single process for less than one hour – which suggests that those executions were simple tests. Figure 10-*left* shows execution times for the `mpirun` and `mpiexec` instances, their associated CPU utilization, and the number of processes spawned. The longest execution runs for 204 hours and spawns 16 processes, followed by a dozen of executions that run for about 100 hours. There is also a cluster of instances that consume more than 90% of CPU for an average of 12 hours, with two instances running for 47 and 49 hours each. A detailed investigation of these instances unveiled that they use up to 4 cores from the login nodes and up to 4 GB of RAM each, which could then considerably impact the performance of sound processes (compilation, (de)compression, file synchronization, etc.) from other users.

Figure 10-*right* shows a subset of the executions shown in Figure 10-*left*, which corresponds to executions of GROMACS [17], a widely used molecular dynamics package, on GPUs in the login nodes. Specifically, we highlight a use case in which two users attempt to “game the system” by launching concurrent executions of the GPU-enabled version of GROMACS (`gmx.mpi`), configured to spawn one CPU process and as many GPU processes as available in the system. To prevent such behaviors, Summit enforces limits on the login nodes to ensure resource availability by leveraging the Linux kernel feature `cgroups`: each user is limited to 16 hardware threads, 16 GB of memory, and 1 GPU; and after 4 hours of CPU-time all login sessions are limited to 0.5 hardware threads; after 8 hours, the process is automatically killed. These limits are reset as new login



**Fig. 11.** *Left:* Execution of user processes (high-throughput applications) on login nodes. *Right:* Execution of Python programs on login nodes. *Bottom:* Execution of Python programs by users that have never submitted a batch job to the system. (Note that 1600% CPU utilization means that a process comprising 16 threads consumed 100% CPU utilization each.)

sessions are started. These two users consumed 50% of all GPU resources across login nodes for about 84 consecutive hours, however, through a synchronized process in which each of them re-initiated a session periodically, so the limits would be reset. This behavior is not only substantially harmful to other users by preventing a fair share of resources, but also it conflicts with best practices of not running scientific applications within login nodes.

**High-Throughput Applications** – We have identified a substantial number of executions of high-throughput applications on the login nodes. Here, we focus on a subset of these executions that consumes more than 90% of CPU per process, which comprises 8,014 instances executed by 549 users (27.9% of total users). Figure 11-*left* shows the distribution of user processes *vs.* their length, in hours, that run user codes (i.e., scientific applications) on the login nodes. As for the tightly-coupled applications above, we have filtered out all instances related to sound processes (compilation, (de)compression, file synchronization, etc.). Users ran a wide range of codes—495 unique programs—in which  $\sim 78\%$  of them run for less than an hour; thus, we consider them as execution tests. Some instances span 16 threads (`cgroups` limit) and run up to 7 hours, while others (about 7% of the dataset) use more than 8 threads and run between 3 and 8 hours. We then consider these instances as misuse of the login nodes. Due to the limits imposed by Summit, we do not observe any attempt to “game the system”; these processes are mostly evenly distributed across login nodes, with a slightly higher number for login3 (405 instead of 330 on average for the other login nodes).

In spite of the large variation of user programs, we have identified that 4,478 instances (from 329 users) are running Python programs (Figure 11-*right*). These instances represent 72.6% of the instances shown in Figure 11-*left*, which run for more than an hour. This result indicates that some users may tend to use these login nodes as additional computing resources, or even as their sole computing node. In order to assert the latter, we attempted to isolate the list of users that ran any of these codes without ever submitting a single job to the batch queue. Astonishingly, we identified 41 users that fall into this category, which comprises 1,012 instances, i.e., 12.6% of the original dataset (Figure 11-*bottom*). Although running user programs on login nodes as an extension of computing resources is against best practices, using a leadership-class HPC system for running user-based codes uniquely on login nodes must be prevented—strict policies and processes should then be defined to impede similar misuse of resources.

While the `cgroups` mechanism protects the overall login node resources, it falls short in “low key” and “gaming the system” misuse, as shown above. Several steps may be taken to mitigate these issues which not only will lead to an improved system usage but also benefit the other users with faster execution on compute nodes. One such measure could be to use the data collected as part of this work to identify the users of the misuse reported here and educate them of best practices. Another measure might be to introduce punitive actions, but we will not conjecture about potential new policies in this work.

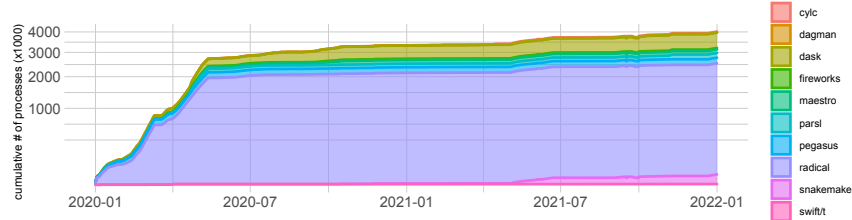
### 4.3 Scientific Workflows

Scientific workflows are used almost universally across scientific domains for solving complex and large-scale computing and data analysis problems. The importance of workflows is highlighted by the fact that they have underpinned some of the most significant discoveries of the past few decades [3]. Many of these workflows have significant demands for computation, storage, and communication, and thus they have been increasingly executed on large-scale computer systems [14]. In this section, we seek to identify how and to what extent workflows have been used on Summit. Typically, workflow systems run a coordinator process that manages workflow tasks’ dependencies, launches jobs to the batch queue as their dependencies are satisfied, monitors their jobs’ execution, and performs data movement operations on behalf of the user. Table 2 shows the total number of processes run by workflow systems in Summit login nodes. In total, 71 users utilized workflow technologies for automating the execution of their scientific applications. These processes often refer to agents that manage the workflow execution and they can take several formats: from single orchestration components (e.g., Swift/T) to the management of ensembles (e.g., RADICAL/EnTK). The former leverages batch jobs for defining workflows within a parallel, tightly coupled application (thus the lower number of processes), while the latter manages sets of tasks as high-throughput applications, i.e. the so-called *pilot jobs* [2].

Figure 12 shows the cumulative number of workflow-related processes across Summit login nodes for our dataset. Overall, workflow technology adoption has

**Table 2.** Total number of workflow management systems’ processes observed across Summit login nodes (Jan 2020–Dec 2021).

	parsl	swift/t	pegasus	fireworks	dask	maestro	cylc	dagman	snakemake	radical
processes	3,807	88	5,399	319	40,875	2,225	106	4	15,797	2,113,192
users	7	3	3	5	27	6	1	1	5	13

**Fig. 12.** Cumulative number of workflow management systems’ processes observed across Summit login nodes (Jan 2020–Dec 2021), shown with square root scale.

gradually increased throughout these past two years. A notable growth in workflow usage is observed in the first two quarters of 2020, which coincides with research conducted to understand the COVID-19 pandemic through the use of HPC. Specifically, this research leveraged the RADICAL/EnTK framework for investigating spike dynamics in a variety of complex environments, including within a complete SARS-CoV-2 viral envelope simulation [5]. This research has been awarded the 2020 ACM Gordon Bell Special Prize for High Performance Computing-Based COVID-19 Research.

## 5 Related Work

Analyzing and characterizing HPC workloads is a common practice for measuring system and application performance metrics and thus identifying potential bottlenecks and atypical behaviors [7]. For example, the National Energy Research Scientific Computing Center (NERSC) has profiled and characterized three generations of their supercomputing systems [11]. In these studies, HPC benchmarks are used to obtain performance measurements, which are then used for the procurement process of machines. Similarly, a characterization of the workload of Tianhe-1A at the National Supercomputer Center in Tianjin presents equivalent system-level metrics [8]. In [10], a characterization of a parallel filesystem unveils I/O bottlenecks for different classes of applications. Conversely, our analyses in this paper target users’ experience and behavior on login nodes—the interface to HPC systems.

In [13], user behavior is studied with regards to think time, the time between the completion of a job and the submission of the next job by the same user. Although this work leverages this same concept for defining user sessions, the



study conducted in [13] attempted to understand and characterize patterns of job submissions. Our work, instead, seeks to understand user behavior on login nodes and relate their actions to misuses of the system or performance issues. To the best of our knowledge, this is the first work that conducts such a study.

## 6 Conclusion and Future Work

We examined observation data from the login nodes of the leadership-class Summit supercomputer at OLCF. We analyzed traditional system performance metrics such as user access, I/O throughput, and job characteristics, as well as user behavior regarding session lengths, misuse of login nodes, and how users have leveraged workflows to perform complex, distributed computing. Our findings identified key usage patterns that we believe will shed light on the usage of login nodes on contemporary clusters and supercomputers. As immediate future work, we will continue to collect this observation data for the rest of the life of Summit, and we will start data collection for the upcoming exascale Frontier supercomputer at OLCF. We also intend to analyze the data further into other dimensions, including resource usage balancing and correlation of external events (e.g., conference deadlines, call for proposals deadlines, etc.), as well as the impact of the COVID-19 pandemic on the user behavior.

**Acknowledgments.** This research used resources of the Oak Ridge Leadership Computing Facility at the Oak Ridge National Laboratory, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC05-00OR22725. We acknowledge Suzanne Parete-Koon for early brainstorming of some of the ideas presented here. We thank Sarp Oral, Scott Atchley and Bronson Messer for their thorough revision of this paper.

## References

1. IP Geolocation API. <https://www.abstractapi.com/ip-geolocation-api> (2022)
2. Ananthraj, V., De, K., Jha, S., Klimentov, A., Oleynik, D., Oral, S., Merzky, A., Mashinistov, R., Panitkin, S., Svirin, P., Turilli, M., Wells, J., Wilkinson, S.: Towards exascale computing for high energy physics: The atlas experience at ornl. In: 2018 IEEE 14th International Conference on e-Science (e-Science). pp. 341–342 (2018). <https://doi.org/10.1109/eScience.2018.00086>
3. Badia Sala, R.M., Ayguadé Parra, E., Labarta Mancho, J.J.: Workflows for science: A challenge when facing the convergence of hpc and big data. *Supercomputing frontiers and innovations* **4**(1) (2017). <https://doi.org/10.14529/jsfi170102>
4. Bang, J., Kim, C., Wu, K., Sim, A., Byna, S., Kim, S., Eom, H.: Hpc workload characterization using feature selection and clustering. In: *Proceedings of the 3rd International Workshop on Systems and Network Telemetry and Analytics* (2020). <https://doi.org/10.1145/3391812.3396270>
5. Casalino, L., Dommer, A.C., Gaieb, Z., Barros, E.P., Sztain, T., Ahn, S.H., Trifan, A., Brace, A., Bogetti, A.T., Clyde, A., et al.: Ai-driven multi-scale simulations illuminate mechanisms of sars-cov-2 spike dynamics. *The International Journal of High Performance Computing Applications* (2021). <https://doi.org/10.1177/10943420211006452>

6. Dongarra, J., Gottlieb, S., Kramer, W.T.: Race to exascale. *Computing in Science & Engineering* **21**(1) (2019). <https://doi.org/10.1109/MCSE.2018.2882574>
7. Feitelson, D.G.: Looking at data. In: 2008 IEEE International Symposium on Parallel and Distributed Processing (2008). <https://doi.org/10.1109/IPDPS.2008.4536092>
8. Feng, J., Liu, G., Zhang, J., Zhang, Z., Yu, J., Zhang, Z.: Workload characterization and evolutionary analyses of tianhe-1a supercomputer. In: International Conference on Computational Science (2018). [https://doi.org/10.1007/978-3-319-93698-7\\_44](https://doi.org/10.1007/978-3-319-93698-7_44)
9. Liu, Z., Lewis, R., Kettimuthu, R., Harms, K., Carns, P., Rao, N., Foster, I., Papka, M.E.: Characterization and identification of hpc applications at leadership computing facility. In: Proceedings of the 34th ACM International Conference on Supercomputing (2020). <https://doi.org/10.1145/3392717.3392774>
10. Lockwood, G.K., Snyder, S., Wang, T., Byna, S., Carns, P., Wright, N.J.: A year in the life of a parallel file system. In: Proceedings of the International Conference for High Performance Computing, Networking, Storage, and Analysis. IEEE Press (2018). <https://doi.org/10.1109/SC.2018.00077>
11. Nersc benchmarking and workload characterization. <https://www.nersc.gov/research-and-development/benchmarking-and-workload-characterization> (2021)
12. Rodrigo, G.P., Östberg, P.O., Elmroth, E., Antypas, K., Gerber, R., Ramakrishnan, L.: Towards understanding hpc users and systems: a nersc case study. *Journal of Parallel and Distributed Computing* **111** (2018). <https://doi.org/10.1016/j.jpdc.2017.09.002>
13. Schlagkamp, S., Ferreira da Silva, R., Deelman, E., Schwiegelshohn, U.: Understanding user behavior: from hpc to htc. *Procedia Computer Science* (2016). <https://doi.org/10.1016/j.procs.2016.05.397>, international Conference on Computational Science 2016, ICCS 2016
14. Ferreira da Silva, R., Filgueira, R., Pietri, I., Jiang, M., Sakellariou, R., Deelman, E.: A characterization of workflow management systems for extreme-scale applications. *Future Generation Computer Systems* **75** (2017). <https://doi.org/10.1016/j.future.2017.02.026>
15. Ferreira da Silva, R., Rynge, M., Juve, G., Sfiligoi, I., Deelman, E., Letts, J., Würthwein, F., Livny, M.: Characterizing a high throughput computing workload: The compact muon solenoid (CMS) experiment at LHC. *Procedia Computer Science* **51** (2015). <https://doi.org/10.1016/j.procs.2015.05.190>, international Conference On Computational Science, ICCS 2015 Computational Science at the Gates of Nature
16. Top 500. <https://www.top500.org> (2021)
17. Van Der Spoel, D., Lindahl, E., Hess, B., Groenhof, G., Mark, A.E., Berendsen, H.J.: Gromacs: fast, flexible, and free. *Journal of computational chemistry* **26**(16) (2005). <https://doi.org/GROMACS: fast, flexible, and free>
18. Vazhkudai, S.S., De Supinski, B.R., Bland, A.S., Geist, A., Sexton, J., Kahle, J., Zimmer, C.J., Atchley, S., Oral, S., Maxwell, D.E., et al.: The design, deployment, and evaluation of the coral pre-exascale systems. In: SC18: International Conference for High Performance Computing, Networking, Storage and Analysis. pp. 661–672. IEEE (2018)
19. Wolter, N., McCracken, M.O., Snively, A., Hochstein, L., Nakamura, T., Basili, V.: What’s working in hpc: Investigating hpc user behavior and productivity. *CTWatch Quarterly* **2**(4A) (2006)
20. Zhang, S., Zhang, C., Yang, Q.: Data preparation for data mining. *Applied artificial intelligence* **17**(5-6) (2003). <https://doi.org/10.1080/713827180>