Analysis of parallel I/O use on the UK national supercomputing service, ARCHER using Cray's LASSi and EPCC SAFE

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***Abstract*—In this paper, we describe how we have used a combination of the LASSi tool (developed by Cray) and the SAFE software (developed by EPCC) to collect and analyse Lustre I/O performance data for all jobs running on the UK national supercomputing service, ARCHER; and to provide reports on I/O usage for users in our standard reporting framework. We also present results from analysis of parallel I/O use on ARCHER and analysis on the potential impact of different applications on file system performance using metrics we have derived from the LASSi data. We show that the performance data from LASSi reveals how the same application can stress different components of the file system depending on how it is run, and how the LASSi risk metrics allow us to identify use cases that could potentially cause issues for global I/O performance and work with users to improve their I/O use. We use the IO-500 benchmark to help us understand how LASSi risk metrics correspond to observed performance on the ARCHER file systems. We also use LASSi data imported into SAFE to identify I/O use patterns associated with different research areas, understand how the research workflow gives rise to the observed patterns and project how this will affect I/O requirements in the future. Finally, we provide an overview of likely future directions for the continuation of this work.**

***Index Terms*—Supercomputers, High performance computing, Parallel architectures, Data storage systems, Performance analysis**

I. Introduction

I/O technologies in supercomputer systems are becoming increasingly complex and diverse. For example, a recent trend has been to add a new kind of high-performance but limited capacity I/O to supercomputing systems—often referred to as *burst-buffer* technologies. Recent examples include Intel Optane [1] and Cray DataWarp [2]. These technologies typically provide orders of magnitude more performance, both in terms of I/O bandwidth and I/O operations per second, at the expense of total storage capacities.

To help establish the potential impact of such novel technologies within the HPC sphere, we need to revisit and update our data on the typical I/O requirements of modern applications.

There are many factors which affect the I/O behavioural requirements of any scientific application, and these factors have been changing rapidly in recent years. For example, the ratio of network performance to node-level performance tends to influence how much work each node needs to perform. As the node-level performance tends to grow faster than the network-level performance, the trend is for each node to be given more work, often implying larger I/O requirements per node. The complexity of the interactions between performance behaviour and system development are discussed by Lockwood et al [3]. They investigate the performance behaviour from the perspective of applications and the file system quantifying the performance development over the course of a year. Due to these changes, we cannot rely on conventional wisdom, nor even older results, when understanding current I/O requirements on HPC systems. Instead, we need up-to-date, good quality data with which to reason and inform our assumptions of current systems and predictions of future systems.

In this study, we have used ARCHER[1]—the UK's national supercomputer—as an example of a high-end supercomputer. ARCHER reached #19 in the Top500 upon its launch in 2013. It is a 4,920 node Cray XC30, and consists of over 118,000 Intel Ivy Bridge cores, with two 2.7 GHz, 12-core E5-2697 v2 CPUs per node. 4,544 of the 4,920 nodes have 64 GiB per node (2.66 GiB per core), while the remaining 376 'high memory'

This work was supported by the UK National Supercomputing Service, ARCHER (http://www.archer.ac.uk); funded by EPSRC and NERC.

[1] http://www.archer.ac.uk

nodes have 128 GiB each (5.32 GiB per core). The ARCHER production service has three Lustre file systems each based on a Cray Sonexion 1600 appliance. Two file systems have 12 OSS and one file system has 14 OSS. Each OSS is a Seagate Sonexion 1600 OSS controller module, 1 x Intel Xeon CPU E5-2648L @ 1.80GHz, 32GB memory. Each OSS has 40 discs, 4 OSTs per OSS, 10 discs per OST. These 10 discs are in RAID6, i.e. 8+2. There are also a number of hot spares and RAID and ext3 journaling SSDs on each OSS. Each disc is a 4TB SEAGATE ST4000NM0023 (Constellation ES.3 - 3.5" - SAS 6Gb/s - 7,200 rpm). There is one MDS and one backup MDS per file system. Each MDS is a Cary Sonexion 1600 MDS controller module, 2 x Intel(R) Xeon(R) CPU E5-2680 @ 2.70GHz Each of the 3 MDTs comprise 14 discs in RAID10. Each disc is a 600GB SEAGATE ST9600205SS (Enterprise Performance 10K 600 GB - 2.5" - SAS 6Gb/s - 10,000 rpm). Each client accesses the three file systems via 18 LNet router nodes internal to the ARCHER system. Each of the three file systems are attached to 10, 10 or 14 router nodes respectively; some router nodes service more than one path. This is complex, involving overlapping primary and secondary paths, however, the rule that affects performance is that the primary LNet path is configured so that all clients access 3 OSS nodes via 2 LNet router nodes. MDS nodes are accessed from the clients via 2 LNet router nodes each.

HPC applications scheduled to run on ARCHER have to share resources, in particular the file system and network. Even though these shared resources are built to scale well and provide high performance, they can become a bottleneck when multiple applications stress them at the same time. Occasionally the applications also use these shared resources inefficiently, which may impact other applications using the same resource.

Users expect applications to perform consistently in a time frame, i.e., the overall runtime for a given job does not vary excessively. Often time limits are chosen such that slowdown can cause jobs to fail. However, from time to time users would report that their applications were running slower than expected or interactive file system response was sub-optimal. Based on this feedback, we set out to analyse all of the applications running on ARCHER for their current I/O usage, to try to understand the variability of I/O performance on the system and its link to running applications. In contrast to other studies (that typically profile the I/O use of a small number of benchmark applications), we are sampling the I/O usage of *every* job run on ARCHER in the analysis period. Thus our data should complement those from previous studies.

Most monitoring tools [4], [5], [6], [7], [8] and [9] only provide raw I/O statistics of file systems or applications. UMAMI [10] and MELT [11] add features for slowdown analysis but require expertise. Previous work introduced metrics such as I/O severity [12] and File System Utilisation(FSU) [13] for studying I/O and application slowdown. We have developed a non-invasive framework where it is easy to identify applications with unusual I/O behaviour, and by targeting application interactions with the file system. The following sections describe this framework along with insights gained from running IO-500 benchmarks and detail the I/O patterns observed by the data analysis.

II. Tools and Methodology

This section first introduces the tools used to monitor the I/O utilisation and to relate them with user jobs. To validate the behavior of this approach on a well known pattern, we utilise the IO-500 benchmark.

A. LASSi

LASSi (Log Analytics for Shared System resource with instrumentation) [14] was developed by the Cray Centre of Excellence (CoE) for ARCHER to provide system staff with the ability to find and understand contention in the file system.

LASSi is a tool to analyse the slowdown of applications due to the shared Lustre file system usage. It provides HPC system support staff the ability to monitor and profile the I/O usage of applications over time. LASSi uses a metric-based approach to study the quantity and I/O quality. Metrics describe the risk of slowdown of applications at any time and also identifies the applications that cause such high risks. This information is then made available to the user or application developer as appropriate.

LASSi was originally planned to be an extension of work undertaken by Diana Moise of Cray on the HLRS system [15]. This work defined aggressor and victim jobs *running at the same time*. Grouping applications based on the exact command line used, the study defined slowdown as a deviation from the mean run times by 1.5 times or more. This study did not use any I/O or network statistics but was attempting to spot correlations in job runtimes.

Victim detection was based on observing applications that run slower than the average run time for an application group. *Aggressor* detection was based on applications that overlap with the *victims*. The *Victim* and *Aggressor* model based on concurrent running fails to provide useful insights when we move to a system like ARCHER, which is at a scale where there are always a large number of applications running.

In ARCHER, user reports of slowdown are usually addressed by analysing the raw Lustre statistics, stored in a MySQL database called LAPCAT (developed by Martin Lafferty from the onsite Cray systems team). LAPCAT provides the following Lustre I/O statistics from each compute node over time:

- **OSS:** *read_kb, read_ops, write_kb, write_ops, other*
- **MDS:** *open, close, mknod, link, unlink, mkdir, rmdir, ren, getattr, setattr, getxattr, setxattr, statfs, sync, sdr, cdr*

Before LASSi, mapping the Lustre statistics to application runs and looking for patterns using LAPCAT was a prohibitively long time to investigate.

We designed LASSi to use defined metrics that indicate problematic *behaviour* on the Lustre file systems. Ultimately, we have shown that there is less distinction between Victims and Aggressors. An alternative explanation, supported by the

LASSi-derived data, is that so-called Victims are simply using the Lustre file system more heavily than so-called Aggressors.

Application run time depends on multiple factors such as compute clock speed, memory bandwidth, I/O bandwidth, network bandwidth and scientific configuration (dataset size or complexity). LASSi aims only to model application run time variation due to I/O.

B. Risk-Metric Based Approach

These metrics are motivated by the fact that we expect users will report slowdown only when their application run takes longer than usual. We focus on I/O as the most likely cause of unexpected application slowdown and begin with the assumption that, in isolation, slowdown only happens when an application does more I/O than expected (for example, due to configuration or code change) or when an application has an unusually high resource requirement than normal at a time when the file system is busier than usual.

To characterise situations that cause slowdown means considering raw I/O rate, metadata operations and quality (size) of I/O operations. For example, Lustre file system usage is optimal when at least 1 MB is read or written for each operation (*read_ops* or *write_ops*).

The central metadata server can sustain a certain rate of metadata operations, above which any metadata request from any application or group of applications will cause slowdown. To provide the type of analysis required, LASSi must comprehend this complex job mix of different applications with widely different read/write patterns, the metadata operations running at the same time and how these interact and affect each other. This requirement informs the definition of the LASSi metrics.

C. Definition of Metrics

Firstly, we define metrics that indicate quantity and I/O quality operations by an application run. We first define the risk for any *OSS* or *MDS* operation x on a file system *fs* as

$$risk_{fs}(x) = \frac{x - \alpha \cdot \text{avg}_{fs}(x)}{\alpha \cdot \text{avg}_{fs}(x)}$$

where the averages are over the raw file system statistics and α is a scaling factor, set to 2 for this analysis. The risk metric measures the deviation of Lustre operations from the (scaled) average on a file system. A higher value indicates higher risk of slowdown to a file system. To simplify the representation for the user, the risk for metadata and data operations aggregate various types of operations into one value:

$$\begin{aligned} risk_{oss} = \; & risk_{read\_kb} + risk_{read\_ops} + \\ & risk_{write\_kb} + risk_{write\_ops} + risk_{other} \end{aligned}$$

$$\begin{aligned} risk_{mds} = \; & risk_{open} + risk_{close} + risk_{getattr} + risk_{setattr} + \\ & risk_{mkdir} + risk_{rmdir} + risk_{mknod} + risk_{link} + \\ & risk_{unlink} + risk_{ren} + risk_{getxattr} + risk_{setxattr} + \\ & risk_{statfs} + risk_{sync} + risk_{cdr} + risk_{sdr} \end{aligned}$$

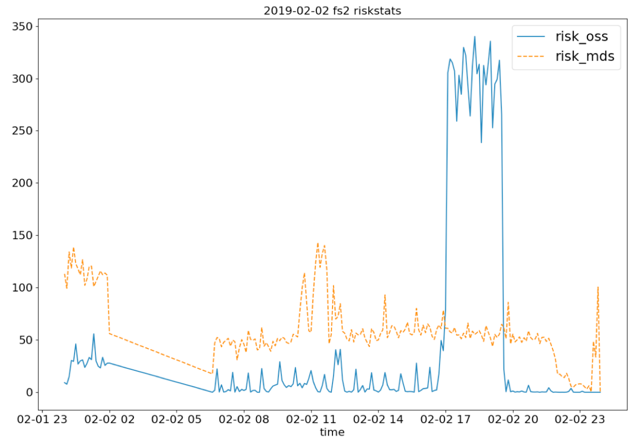


Fig. 1: Sample report showing the risk to file system fs2 over 24 hours.

Risks for individual operations are added only if the value is greater than zero; as any negative risks are ignored since this would correspond to the situation where the I/O was less than the average. The total risk on a file system at a given time is the sum of all application risks.

For some metadata operations, the averages are closer to zero and this can cause the *risk* metrics to become very large. We still want to measure and identify applications that do exceptional metadata operations like creating thousands of directories per second. For these metadata operations, we use β-scaled average of the sum of all metadata operations to measure risk, where β is usually set to 0.25. Both α and β are used to set the lower limit for defining the risks and this can be configured based on experience.

The above metric measures the quantity of I/O operations, but not the quality. On Lustre, 1 MB aligned accesses are the optimal size per operation. To define a measure of the quality reads and writes, we define the following metrics:

$$read\_kb\_ops = \frac{read\_ops \cdot 1024}{read\_kb} \tag{1}$$

$$write\_kb\_ops = \frac{write\_ops \cdot 1024}{write\_kb} \tag{2}$$

The read or write quality is optimal when (respectively) $read\_kb\_ops = 1$ or $write\_kb\_ops = 1$. A value of $read\_kb\_ops >> 1$ or $write\_kb\_ops >> 1$ denotes poor quality read and writes. The total ops metric on a file system at a given time is sum of all application ops metric with $risk_{oss} > 0$ (ignoring applications with low quantity of I/O). In general, *risk* metrics measures the quantity of I/O and *ops* metrics measures the quality.

A workflow has been established where Lustre statistics (collected in the LAPCAT database) and application data (from PBS) are exported and ingested by LASSi. Daily risk plots are generated and are available to helpdesk staff. LASSi uses Spark [16] for data analytics and matplotlib for generating reports. Custom risk plots and raw Lustre operation data plots can also be generated manually. Figure 1 shows the risk

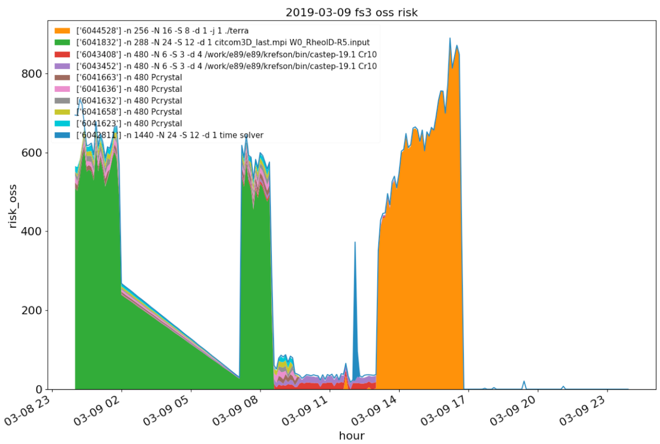


Fig. 2: Sample report showing the OSS risk to file system fs2 over 24 hours with applications that are contributing to the risk.

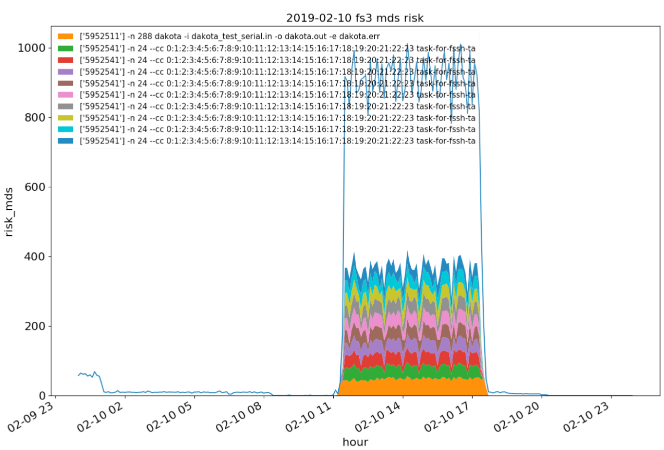


Fig. 3: Sample report showing the MDS risk to file system fs2 over 24 hours with applications contributing to the risk.

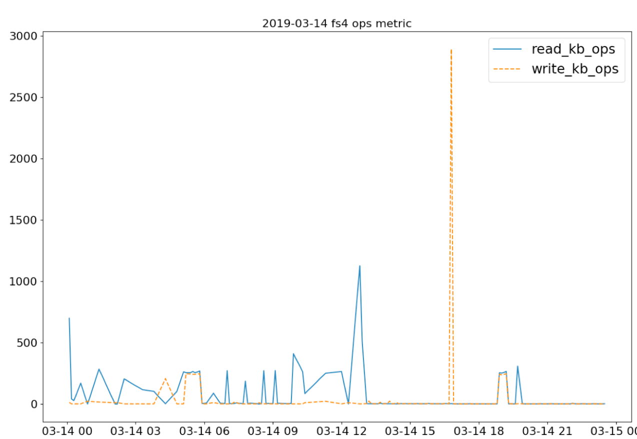


Fig. 4: Sample report showing the read and write quality to file system fs2 over 24 hours.

metrics for file system fs2 over a sample period of 24 hours. The *oss_risk* relates to actual data movement operations and the *mds_risk* to metadata operations, note the significant peak in the evening.

Figure 2 shows an example of the *oss_risk* metric over 24 hours attributed to the jobs that were running. These plots allow us to focus on particular applications. We have noticed a particular class of applications that can be problematic: *task farms* as is illustrated from Figure 3. Each individual application contributes to a significant metadata operation load from the whole job.

We have also found the read and write quality metrics to be useful, an example plot of this metric for fs2 over 24 hours is shown in Figure 4. The reason this is important is that small reads or writes to Lustre can keep the file system busy for (presumably) little benefit.

Figure 5 shows the variation in overall risk metric over many months and clearly there is a variation in workload during this time with a peak in March for fs2. We observe that fs2 and fs3 generally have higher risk than fs4. For the same period, we show the quality metrics (Figure 6) and we can see that reads on fs4 are generally of low quality. This file system has the most disparate workload and paradoxically we receive very few complaints over performance in this file system so it is likely that the user base are not heavily dependent on the file system performance.

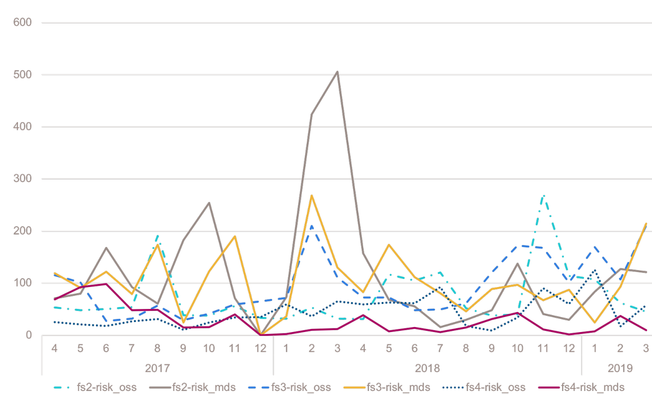


Fig. 5: Risk metric of file system averaged over months.

D. SAFE

SAFE is an integrated service administration and reporting tool developed and maintained by EPCC [17]. For this work, it is important to note that SAFE is able to take data feeds from a wide variety of sources and link them in such a way that enables reporting across different system aspects.

We have developed a data feed from LASSi into SAFE that provides the following *aggregated* I/O metrics on a *per job* basis for every job that is run on the ARCHER system:

- Total amount of data read.
- Total amount of data written.
- Total number of read operations.
- Total number of write operations.

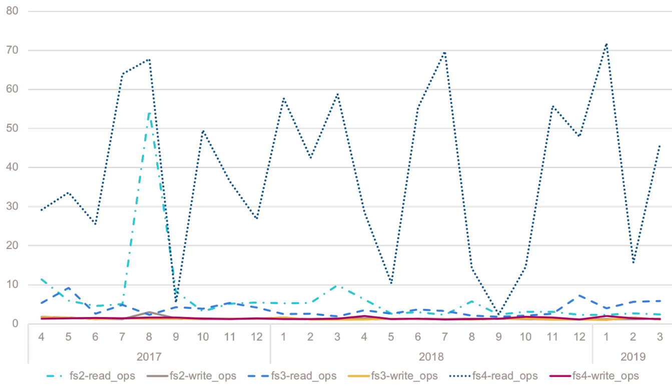


Fig. 6: Ops metric of file systems averaged over months.

Once ingested into SAFE, these records can then be linked to any other aspects of the job to enable different reporting queries to be performed. For example, we can summarise the I/O data based on all jobs that belong to a particular research area (by linking with project metadata linked to the job) or we can report on I/O associated with a particular application (by linking with application metadata provided by the Cray Resource Usage Reporting data feed). We have used the first of these linkages in the analysis presented below.

We measure the amount of data written and read by each job in GiB and use this value, along with the job size and the amount of core hours (core-h) spent in the job to compute a two-dimensional heatmap that reveals in which categories of job size and data size the most ARCHER resource is spent. The core-h correspond directly to cost on ARCHER and so using this value as the weighting factor for the heatmaps allows us to assess the relative importance of different I/O patterns.

E. IO-500

The IO-500[2] is a benchmark suite that establishes I/O performance expectations for naive and optimised access; a single score is derived from the individual measurements and released publicly in a list to foster the competition. Similarly to Top500, a list is released on each ISC-HPC and Supercomputing conference [18].

The design goals for the benchmark were: representative, understandable, scalable, portable, inclusive, lightweight, and trustworthy. The IO-500 is built on the standard benchmarks MDTest and IOR[3]. The workloads represent:

- IOREasy: Applications with well optimized I/O patterns.
- IORHard: Applications that require a random workload.
- MDEasy: Metadata and small object access in balanced directories.
- MDHard: Small data access (3901 bytes) of a shared directory.
- Find: Locating objects based on name, size, and timestamp.

[2]https://github.com/vi4io/io-500-dev
[3]https://github.com/hpc/ior

The workloads are executed in a script that first performs all write phases and then the read phases to minimise cache reuse.

a) Performance Probing: To understand the response times for the IO-500 case further, we run a probe every second on a node that measures the response time for accessing a random 1 MB of data in a 200 GB file and for a create, stat, read, delete of one file in a pool of 200k files. The I/O test uses the `dd` tool for access while the metadata test uses MDWorkbench [19] which allows for such regression testing. The investigation of the response times enables a fine-grained investigation of the system behavior and to assess the observed risk.

III. Results and Analysis

A. LASSi Application Analysis

In this section we show recent analysis of the application I/O on ARCHER for the period April 2017 to March 2019 inclusive (*i.e.* two full years) by characterising them with the *risk* and *ops* metrics.

1) Applications Slowdown Analysis: LASSi was originally developed to analyse events of slowdown, reported by users. In the case of a slowdown event, the time window of the event is mapped to the file system risk and ops profile. This will easily tell us if I/O is responsible for slowdown and which application was causing the slowdown. LASSi has historical run time data of all application runs and user reports of application slowdown is always validated to check for actual slowdown.

High *risk_oss* usually corresponds to a more than average quantity of reads and writes. This is generally not concerning since the shared file systems are configured to deliver high I/O bandwidth. In such cases, attention should be given more to the I/O quality as denoted by ops metric. In case of high MDS risk, the application should be carefully studied for high metadata operations that contribute to the risk.

In LASSi, applications are grouped by the exact run time command used. Usually a user reports jobs that ran normally and which ran slower. Sometimes this detailed information is not provided. In such cases, LASSi analysis will consider all jobs in the group for analysis. Slowdown is a function of the I/O profile of the application and the risk and ops profile of the file system that the application encounters. For instance, an application that does not perform I/O will not be impacted by the risk in the file system. Similarly, application with high metadata operations will be impacted by the $risk\_mds$ and not $risk\_oss$.

This slowdown analysis used to take around a day or two and LASSi has made this process simple and such analysis are usually done in minutes using the automated daily reports. Further development is in progress to automatically identify application slowdown and identify the causes.

2) Applications Usage Analysis: A useful way to view the risk to the file system from a mix of applications is a scatter plot showing *OSS* and *MDS* risk for a set of applications. Using the scatter plots, we can identify general trends in file system usage and identify main issues or usage patterns. This study of the profile of the *risk* and *ops* metrics across file

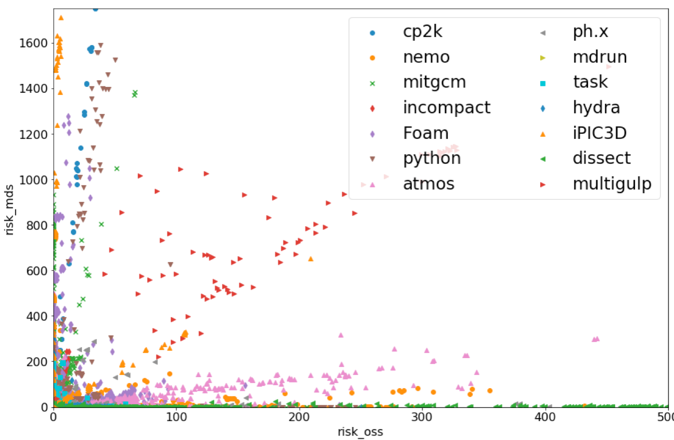


Fig. 7: Scatter plot of *risk_oss* vs *risk_mds* for applications.

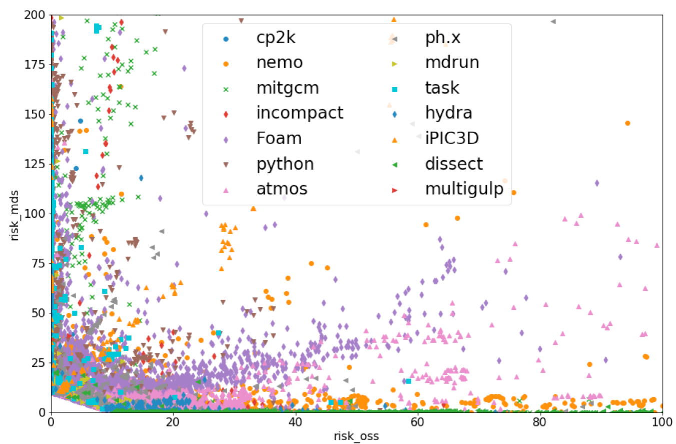


Fig. 8: Scatter plot of *risk_oss* vs *risk_mds* for applications at high resolution.

system over a long period is helpful for system architects and service staff to improve operational quality and plan for future. Even though we can characterize different file systems based on the metrics, there is usually not a strict direct mapping from applications to file system. A more interesting analysis is to study the metrics of each application group. In this section we will look at the *risk* and *ops* profile of application groups based on their run command.

We use previous experience gained by the site support team, to map the run command to the application being run. Figure 7 shows the scatter plot of *risk_oss* vs *risk_mds* for different application groups. Figure 8 shows the same metric for applications zoomed in to the bottom-left corner. For simplicity, 14 application groups are shown and we ignore applications with $(risk\_oss + risk\_mds) < 25$. The $risk\_oss$ and $risk\_mds$ in the plots refer to the average value of any application run over its run time.

The first thing to note from Figure 7 is a pattern of risks mostly clustered around the axis for most applications except *multigulp*. The points scattered around the $risk\_oss$ indicates application doing more reads and write using lesser metadata

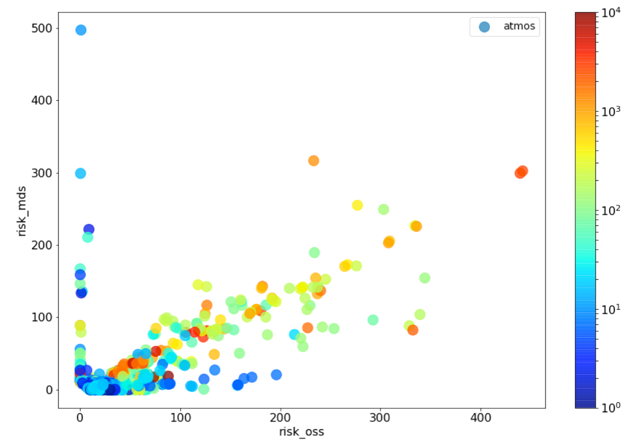


Fig. 9: Scatter plot of *risk_oss* vs *risk_mds* for Atmos, with color map indicating the I/O quality ($read\_kb\_ops$ + $write\_kb\_ops$).

operations. *dissect*, *atmos* and *nemo* applications follow this pattern Similarly, the points scattered around the $risk\_mds$ indicates application using more metadata operations to complete lesser quantity of reads or writes. This pattern is seen in *iPIC3D*, *Foam*, *cp2k*, *python* and *mitgcm* applications.

The zoomed-in view (in Figure 8) shows a similar pattern of risks mostly clustered around the axis. We can see clustering of *hydra* near both the $risk\_oss$ and $risk\_mds$ axis. *incompact* and few instances of *mdrun* application clustered near the $risk\_mds$ axis. The *ph.x* application show no clear pattern but have many runs with considerable $risk\_oss$ and $risk\_mds$ like the *multigulp* applications. There are many instances of *task-farm* like applications that have smaller risk. The risks from *task-farm* get amplified as individual tasks are scheduled to run in huge numbers at the same time.

3) Application profile: In this section, we will take a more in depth look at the detailed risk and ops profile of four application groups. Figures 7 and 8 show the risk profile of multiple application groups but does not include the I/O quality (ops profile).

Figures 9, 10, 11 and 12 show the risk and ops profile of the *atmos*, *python*, *incompact* and *iPIC3D* applications respectively. All plots show scatter of $risk\_oss$ vs $risk\_mds$, with the color map showing the I/O quality ($read\_kb\_ops$ + $write\_kb\_ops$). Blue denotes best I/O quality and red, worse I/O quality.

The clusters in Figure 9, the *atmos* applications reveal three different I/O patterns. Clusters near the axis show good I/O quality whereas the cluster away from the axis shows poor I/O quality. Clusters of *python* applications in Figure 10, show both high metadata and *OSS* usage, but in general suffer from poor I/O quality, whereas some application with low risk perform good I/O quality.

Most *incompact* applications in Figure 11 show good I/O quality whereas a cluster of application runs away from the axis show very bad I/O quality. Many *iPIC3D* application are characterised by high metadata usage and bad I/O quality as

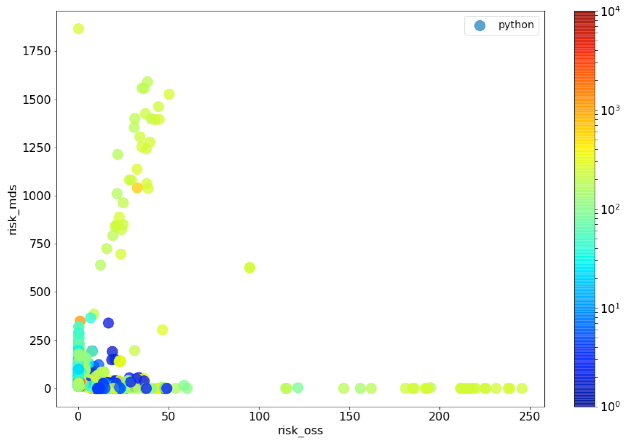


Fig. 10: Scatter plot of *risk_oss* vs *risk_mds* for Python, with color map indicating the I/O quality (*read_kb_ops* + *write_kb_ops*).

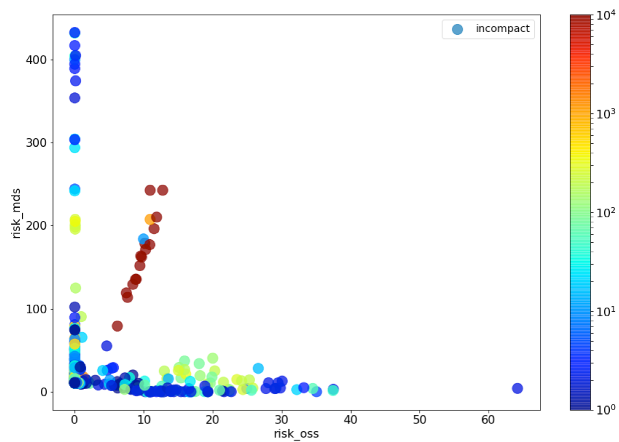


Fig. 11: Scatter plot of *risk_oss* vs *risk_mds* for Incompact, with color map indicating the I/O quality (*read_kb_ops* + *write_kb_ops*).

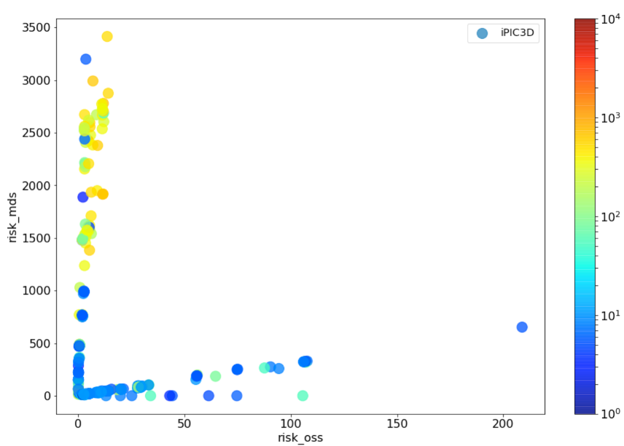


Fig. 12: Scatter plot of *risk_oss* vs *risk_mds* for *iPIC3D*, with color map indicating the I/O quality (*read_kb_ops* + *write_kb_ops*).

shown in Figure 11. A cluster of *iPIC3D* application with high OSS risk have good I/O quality.

We see a general trend in application profiles that there is variance in both the quantity and I/O quality but they all show clear trends as seen by the clustering. This clearly points to different application configurations used by researchers. It is encouraging to see many application runs showing good I/O quality and high amounts of I/O. Understanding why different application runs in the same scientific community have lower I/O quality or use more metadata operations is important and we plan to investigate this further in the future.

B. IO-500 Probes and LASSi

To investigate the behavior of the risk for running applications, we executed the IO-500 benchmark on 100 nodes on ARCHER. The benchmark reported for the different phases the following performance values: (IOREasy_write: 12.973 GB/s, MDEasy_write: 58.312 kiops, IORHard_write: 0.046 GB/s, MDHard_write: 34.324 kiops, find: 239.300 kiops, IOREasy_read: 9.823 GB/s, MDEasy_stat: 64.173 kiops, IORHard_read: 1.880 GB/s, MDHard_stat: 63.166 kiops, MDEasy_delete: 13.195 kiops, MDHard_read: 20.222 kiops, MDHard_delete: 10.582 kiops) with a total IO-500 score of 8.45.

The observed risk is shown in Figure 13(a). Be aware that due to the reporting interval, the data points cover the 6 minute period left of them (*i.e.* the previous 6 minutes). We can see that the OSS risk is high during the IOR easy phases, reaching 2000 for the read phase. The value is around 500 during the MDHard Read phase. The IOHard values cannot be recognized from the OSS risk.

Looking at the metadata risk, the MD workloads can be identified; high peaks are seen in the hard workloads towards the end.

To understand the impact on the user perspective, we also run the periodic probing and reported the response time in Figure 13(b) for metadata rates and I/O. The data response time correlates well with the risk for IOREasy patterns, the response times are high compared to the risk for the MD hard write and MD delete. The metadata risk and the metadata shows some correlation particularly to md.delete, but small I/O (md.read) is also delayed significantly for some patterns.

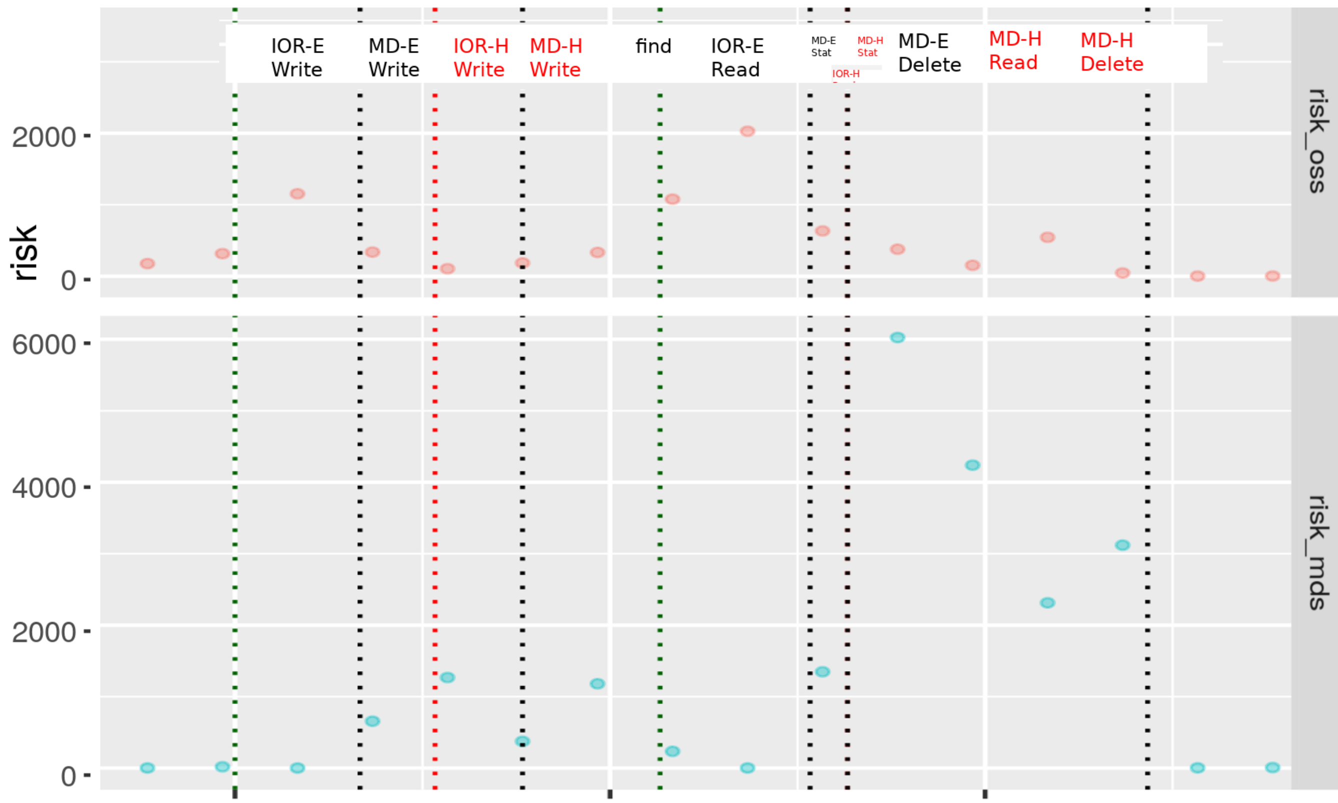
This analysis gives us confidence that the LASSi risk metrics correspond to real, observable effects on the file systems studied.

C. SAFE Analysis of LASSi Data

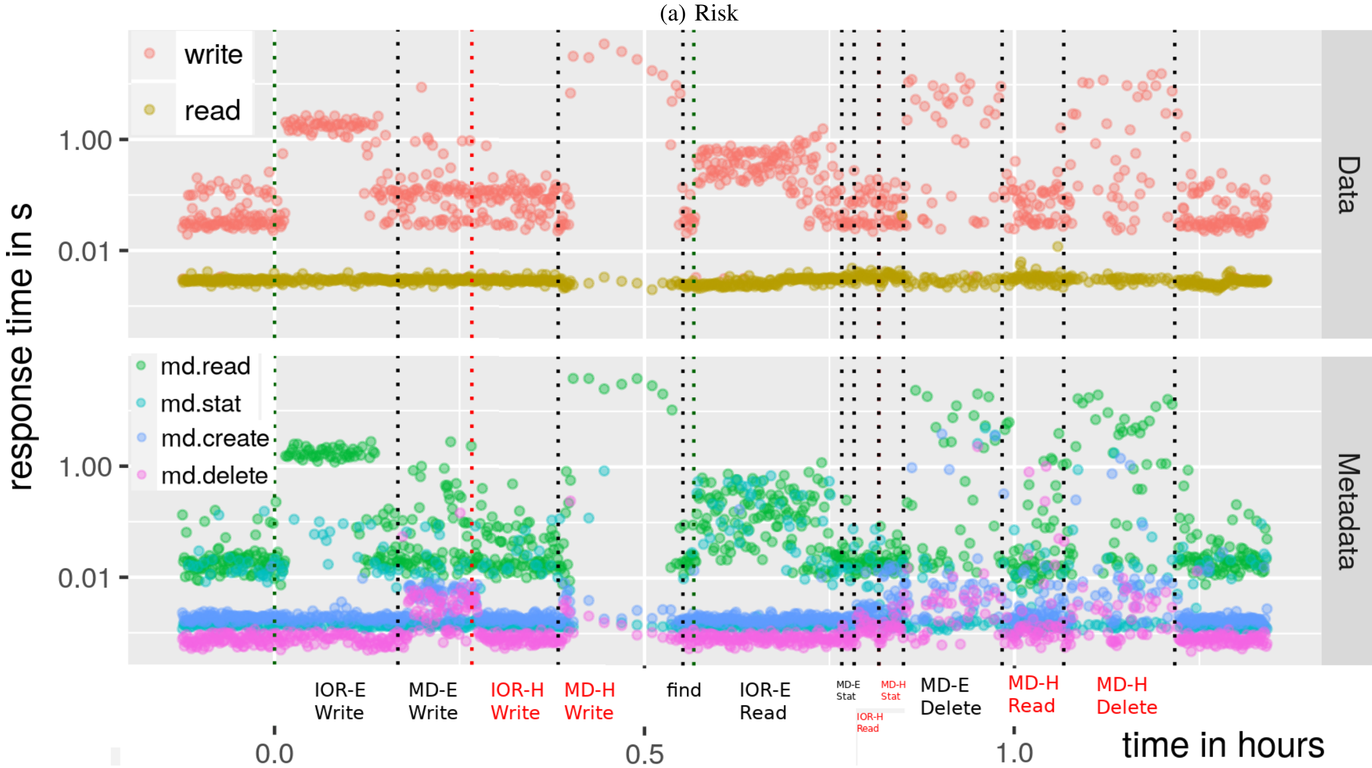
For the SAFE analysis of LASSi data we considered all jobs that ran on ARCHER in the 6-month period July to December 2018.

1) Overall view: Figures 14 and 15 show I/O heatmaps for data read, data written, mean read ops/s and mean write ops/s for all jobs on ARCHER during the analysis period (Jul-Dec 2018 inclusive).

Table I summarises the percentage use by amount of data read or written per job for the same period.



(a) Risk



(b) Response time as measured by the probing

Fig. 13: Observed behavior of the IO-500 on 100 ARCHER nodes.

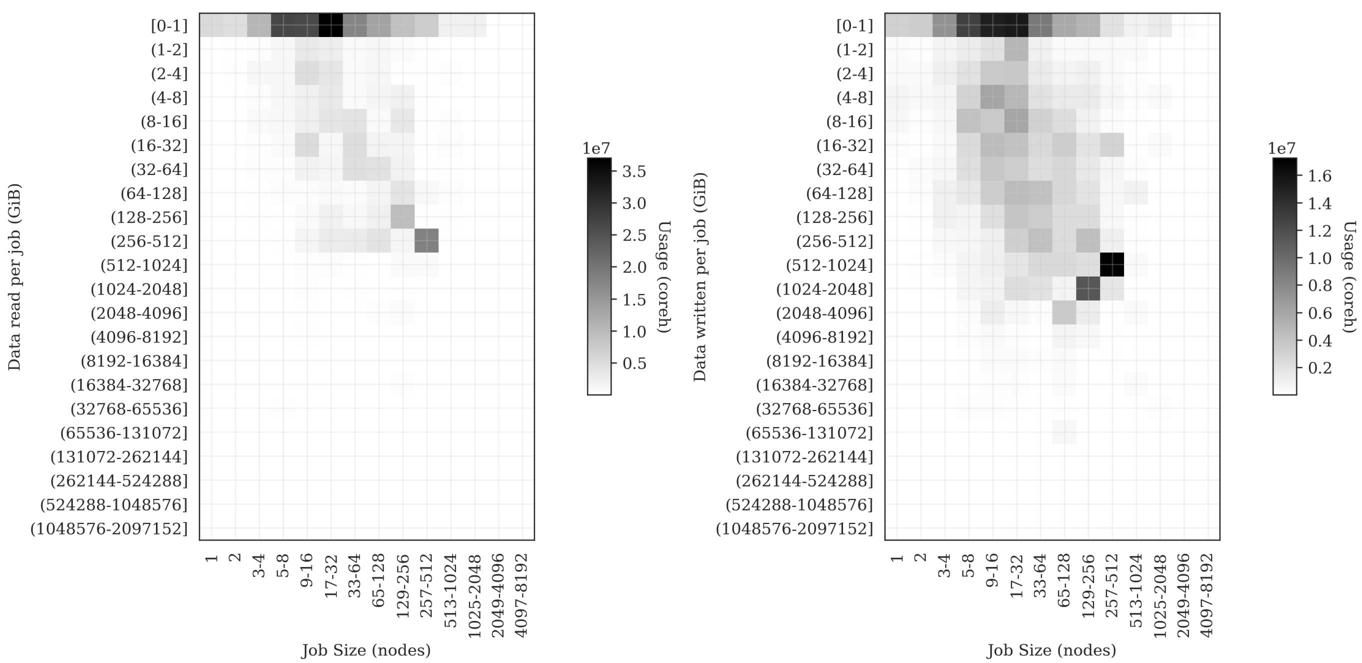


Fig. 14: Heatmaps of data read per job and data written per job vs job size. Weights correspond to total core-h spent in a particular category.

In total, 11,279.4 TiB of data were read and 22,094.3 TiB of data were read by all jobs on ARCHER during the six month analysis period.

TABLE I: % usage breakdown by data read and written for all jobs run on ARCHER during the analysis period.

Total data per job (GiB)	Usage Read	Usage Write
(0,4)	59.8%	34.8%
[4, 32)	14.7%	21.5%
[32, 256)	13.4%	17.8%
[256, 2048)	11.1%	21.4%
[2048,)	1.0%	4.5%

The table and heatmaps reveal that a large amount of resources are consumed by jobs that do not read or write large amounts of data (less than 4 GiB read/written per job). We can also see that there are large amounts of use in some categories with large amounts of data written per job - particularly at 129-256 nodes with 1-2 TiB written per job and 257-512 nodes with 0.5-1 TiB written per job. There is a broad range of use writing from 2 to 512 GiB per job in the job size range from 8 to 512 nodes. We note that the analysis shows that user jobs on ARCHER generally read less data than they write by roughly a factor of two.

Figure 15 heatmaps of I/O operations provide less useful information. As the data ingested into SAFE only contains the total number of operations over the whole job, the computed mean I/O rate is generally small and we would expect that it is the peak rate (in terms of operations per second) that would be required to provide additional insight. For this reason, we constrain our remaining analysis of the LASSi data in SAFE to the total amounts of data read and written per job. We do plan, in the future, to import the peak ops/s rate into SAFE to facilitate useful analysis of this aspect of I/O.

As demonstrated by the LASSi application use analysis, the data for all jobs within the analysis period will be a overlay of many different I/O use patterns. In order to start to understand and identify these different use patterns, the following sections analyse the I/O patterns for different research communities on ARCHER. In this initial analysis, we consider four different communities that make up a large proportion of the core hours used on the service in the analysis period:

- Materials science.
- Climate modelling.
- Computational fluid dynamics (CFD).
- Biomolecular modelling.

Together, these communities typically account for around 60% of the total usage on the ARCHER service. Our initial analysis has focussed on communities with large amounts of core-h use in the analysis period as core-h use corresponds directly to how resources are allocated on the service. Future analyses will examine use cases which use large amounts of I/O resource without a corresponding large amount of core-h use to allow us to distinguish other I/O use patterns.

2) Materials science: Materials science research on ARCHER is dominated by the use of periodic electronic structure applications such as VASP, CASTEP, CP2K and Quantum Espresso. The I/O heatmap for this community can be seen in Figure 16 and the breakdown of data read and written in Table II. In the six month analysis period, the materials science community read a total of 1,219.0 TiB and

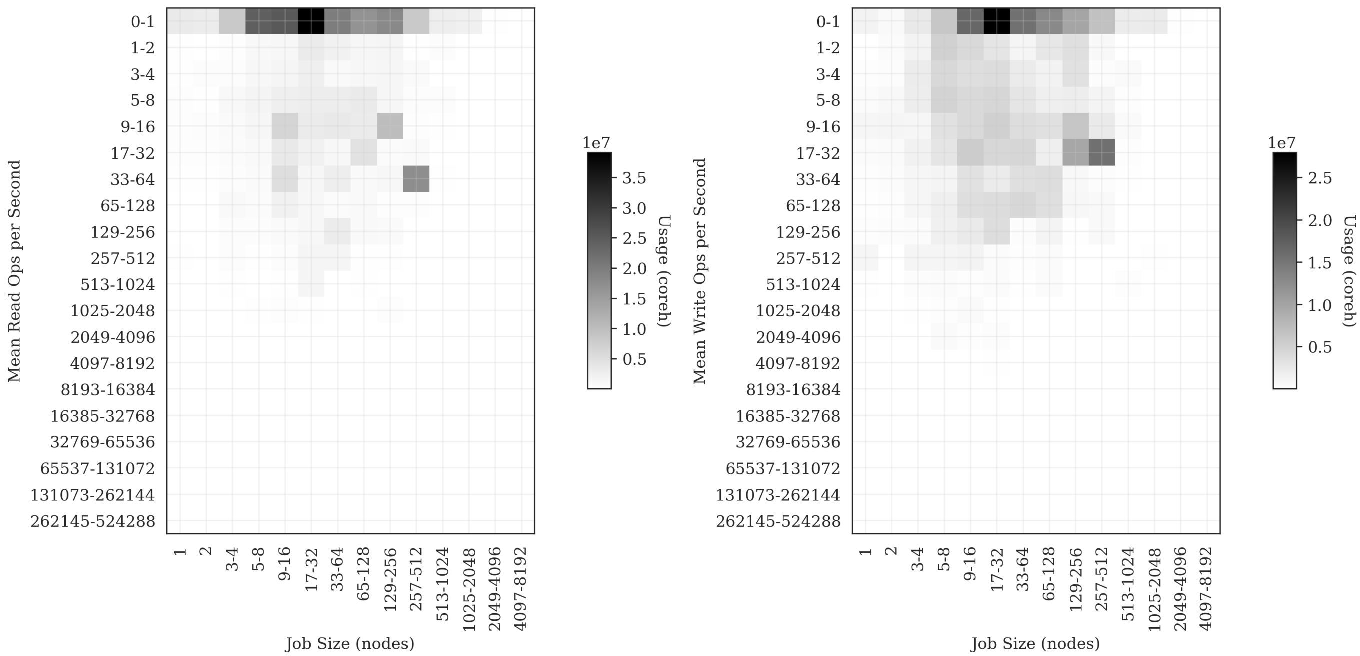


Fig. 15: Heatmaps of mean read ops/s per job and mean write ops/s per job vs job size. Weights correspond to total core-h spent in a particular category.

wrote a total of 3,795.1 TiB. Note that the total disk quota for this community on the ARCHER Lustre file systems is 244 TiB so much of the data read/written is transient in some way.

TABLE II: Percent usage breakdown by data read and written for all jobs run by materials science community on ARCHER during the analysis period.

Total data per job	Usage	
(GiB)	Read	Write
(0,4)	94.3%	55.4%
[4, 32)	4.2%	25.0%
[32, 256)	1.1%	12.3%
[256, 2048)	0.4%	5.1%
[2048,)	0.2%	2.2%

It is obvious that the vast majority of materials science research on ARCHER does not have large requirements on reading or writing large amounts of data *on a per job basis*. However, due to the large amount of use associated with this community, they still manage to read and write large amounts of data in total even though the amount per job is small. In most cases, for the applications used and research problems treated by this community this I/O pattern can be understood as:

- the input data is small: often just a description of the initial atomic coordinates, basis set specification and a small number of calculation parameters;
- the output data is also small: including properties of the modelled system such as energy, final atomic coordinates and descriptions of the wave function.

Closer inspection of the data shows that there is significant usage (37.3%) for jobs that write larger amounts of data ([4, 256) GiB). We expect these jobs to correspond mostly to cases where users are running dynamical simulations where the time trajectories of properties of the system being modelled are captured for future analysis.

In the future, we expect the size of systems modelled in this community to stay largely static and so the I/O requirement for individual jobs will not increase significantly. However, the drive to more statistically-demanding sampling of parameter space in this community will drive an overall increase in I/O requirements going forwards.

3) Climate modelling: This research is dominated by the use of applications such as the Met Office Unified Model, WRF, NEMO and MITgcm. The I/O heatmap for this community can be seen in Figure 17 and the breakdown of data read and written in Table III. The climate modelling community read a total of 503.5 TiB and wrote a total of 2,404.5 TiB in the six month analysis period. The disk quota for this community on the ARCHER Lustre file systems is 541 TiB.

TABLE III: Percent usage breakdown by data read and written for all jobs run by climate modelling community on ARCHER during the analysis period.

Total data per job	Usage	
(GiB)	Read	Write
(0,4)	30.0%	6.3%
[4, 32)	22.4%	24.0%
[32, 256)	39.8%	21.1%
[256, 2048)	7.8%	46.4%
[2048,)	0.0%	2.2%

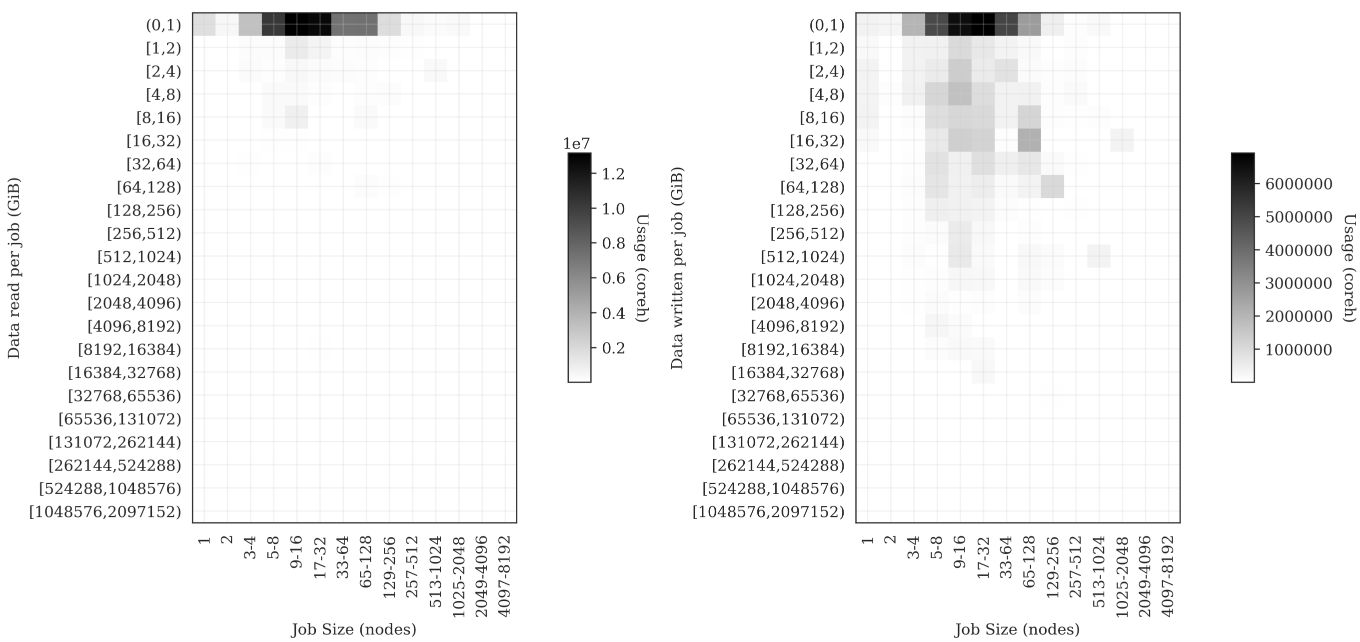


Fig. 16: Heatmaps of data read per job and data written per job vs job size for the materials science community. Weights correspond to total core-h spent in a particular category.

The climate modelling community typically read and write large amounts of data per job with the largest use in the per-job read interval $[32, 256)$ GiB and the largest use in the per-job write interval $[256, 2048)$ GiB. This pattern can be understood as:

- most jobs read in large amounts of observational data and model description data;
- most jobs write out time-series trajectories of the model configuration and computed properties for a number of snapshots throughout the model run. These trajectories are archived and used for further analysis.

The size of the output trajectories is intrinsically linked to the resolution of the model being used for the research and so we would expect the I/O requirements of *individual jobs* from this community to increase as the resolution of models increases.

4) Computational fluid dynamics (CFD): CFD research on ARCHER is dominated by the use of applications such as SBLI, OpenFOAM, Nektar++ and HYDRA. The I/O heatmap for this community can be seen in Figure 18 and the breakdown of data read and written in Table IV. The CFD community read a total of 205.2 TiB and wrote a total of 1,016.7 TiB in the six month analysis period. The disk quota for this community on the ARCHER Lustre file systems is 352 TiB.

Table IV shows a very similar high-level profile to that for the climate modelling community (Table III) however, there is a larger difference in the distribution of usage shown in Figure 18 when compared to that for the climate modelling community (Figure 17). The high-level similarity can be understood due to the similarity in technical setup between the two communities: jobs for both communities use grid-based modelling approaches, need to read in large model descriptions and write out time-series trajectories with large amounts of data. The difference in the distribution of use can be understood due to the wider range of modelling scenarios used within the CFD community compared to the climate modelling community. Climate models have a small range of scales (in terms of length and timescale) when compared to CFD models, where the systems being studied can range in size from the tiny (e.g. flow in small blood vessels) to the very large (e.g. models of full offshore wind farms) and also encompass many different orders of magnitude of timescales.

TABLE IV: Percent usage breakdown by data read and written for all jobs run by CFD community on ARCHER during the analysis period.

Total data per job (GiB)	Usage Read	Usage Write
(0,4)	27.6%	7.7%
$[4, 32)$	30.7%	19.5%
$[32, 256)$	32.8%	28.4%
$[256, 2048)$	8.5%	37.9%
[2048,)	0.4%	8.5%

Going forwards, we expect the diversity of modelling scenarios to remain for the general CFD community with, similarly to the climate modelling community, a corresponding drive to higher resolution in most use cases leading to an increase in the I/O requirements on a *per job* basis.

5) Biomolecular modelling: Biomolecular modelling research on ARCHER is dominated by the use of applications such as GROMACS, NAMD and Amber. The I/O heatmap for

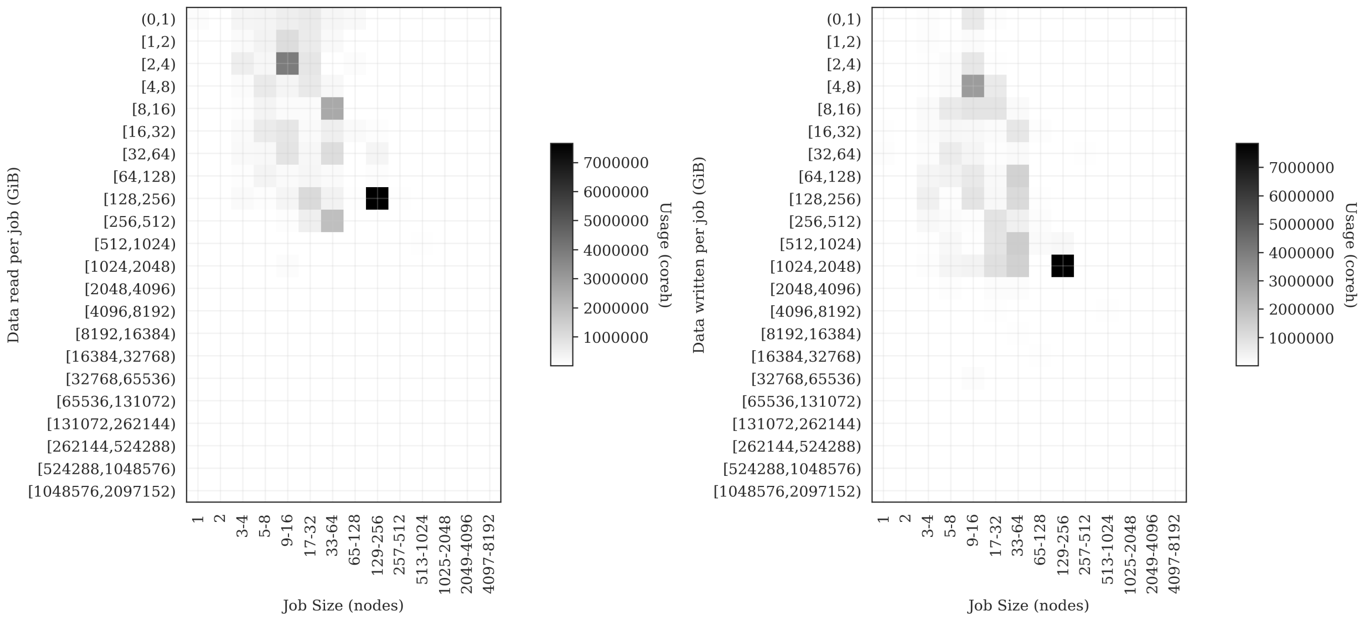


Fig. 17: Heatmaps of data read per job and data written per job vs job size for the climate modelling community. Weights correspond to total core-h spent in a particular category.

this community can be seen in Figure 19 and the breakdown of data read and written in Table V. The biomolecular modelling community read a total of 1.4 TiB and wrote a total of 197.0 TiB in the six month analysis period. The disk quota for this community on the ARCHER Lustre file systems is 26 TiB.

TABLE V: Percent usage breakdown by data read and written for all jobs run by biomolecular modelling community on ARCHER during the analysis period.

Total data per job (GiB)	Usage Read	Usage Write
(0,4)	97.9%	30.5%
[4, 32)	2.1%	34.4%
[32, 256)	0.0%	32.6%
[256, 2048)	0.0%	2.8%
[2048,)	0.0%	0.9%

The overall I/O use profile seen for the biomolecular modelling community differs from those already seen for the other communities investigated: in particular, jobs in this community read in small amounts of data (similar to the materials science community) but write out larger amounts of data (though not generally as large as the climate modelling and CFD communities which use grid-based models). In addition, the usage heatmaps reveal that this community uses smaller individual jobs than the communities using grid-based models and that the amount of data written is roughly correlated with job size. We interpret the I/O use profile in the following way:

- The small amount of data that is read in corresponds to the small amount of data required to specify the model system and parameters. In a similar way to jobs in the materials science community, all that is required to describe the model system are initial particle positions and a small number of model parameters.
- The larger amount of data written when compared to the materials science community is because the majority of jobs produce trajectories with the model system details saved at many snapshots throughout the job to be used for further analysis after the job has finished.

In the future we do not expect the I/O requirements for individual jobs to change very much (as the size of biomolecular systems to be studied will not change dramatically); however, as for the materials science jobs, we expect the overall I/O requirements to increase as more jobs need to be run to be able to perform more complex statistical analyses of the systems being studied.

IV. Summary and Conclusions

We have outlined our approach to gaining better understanding of how applications on ARCHER interact with the file systems using a combination of the Cray LASSi framework and the EPCC SAFE software. The LASSi framework takes a risk-based approach to identifying behaviour likely to cause contention in the file systems. This risk based approach has not only been successful in analysing all reported incidents of slowdown but also incidents where a reported slowdown was not related to I/O but had another cause. LASSi has been used to deliver faster triage of issues and provide a basis for further analysis of how different applications are using the file systems.

LASSi provides automated daily reports that are available to helpdesk staff. We demonstrated how LASSi provides holistic I/O analysis by monitoring file system I/O, generating coarse I/O profile of file systems and application runs along

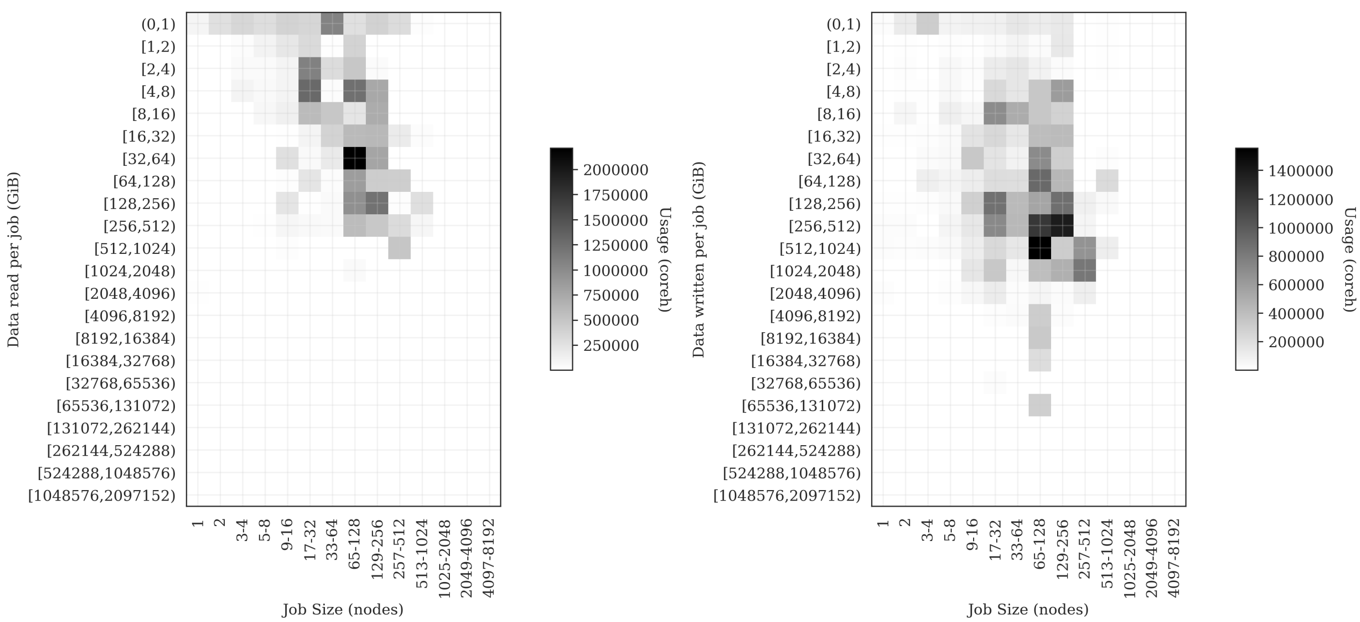


Fig. 18: Heatmaps of data read per job and data written per job vs job size for the CFD community. Weights correspond to total core-h spent in a particular category.

with analysis of application slowdown using metrics. This application-centric, non-invasive, metric-based approach has been used successfully in studying application I/O patterns and could be used for better management of file system and application projects. We have also shown how a file system probing approach using IO-500 complements the risk-based approach and validates it. Here, from the user perspective, the single risk metric provides a good indicator but does not reflect the observed slowdown in all cases.

SAFE provides a way to combine data and metrics from LASSi with other data feeds from the ARCHER service allowing us to understand I/O use patterns by analysing the I/O use of *all* jobs on the service in a six month period broken down by different research communities. The statistics generated by LASSi have been further analysed to gain an understanding of how particular application areas use the file system.

Our analysis of LASSi I/O data linked to other service data using SAFE allowed us to investigate the overall I/O use pattern on ARCHER and has revealed four distinct I/O use patterns associated with four of the largest research communities on ARCHER:

- **Overall:** The overall I/O use pattern on ARCHER reveals the overlay of a range of different patterns with the major ones described below. Over 50% of the use in the analysis period was for jobs that read less than 4 GiB and wrote less than 32 GiB. Overall, twice as much data was written than was read on ARCHER in the analysis period.
- **Materials science:** Job I/O use is characterised by small amounts of data read and written on a *per job* basis but overall high amounts of data read and written due to the very large number of jobs. Approximately three times as much data was written as was read by the materials science community.
- **Climate modelling:** Job I/O use is characterised by large amounts of data read and written on a *per job* basis with a small range of per-job read/write behaviours due to the natural constraint of size of scenarios modelled. Approximately five times as much data was written as was read by the climate modelling community.
- **Computational fluid dynamics:** Job I/O use is characterised by large amounts of data read and written on a *per job* basis with a wide range of per-job read/write behaviours due to the wide range of sizes of scenarios modelled. Approximately five times as much data was written as was read by the CFD community.
- **Biomolecular modelling:** Job I/O use is characterised by small amounts of data read and medium amounts of data written on a *per job* basis with a wide range of per-job write behaviours due to the variety of modelling scenarios. Approximately ten times as much data was written as was read by the biomolecular modelling community.

Based on our analysis, we were also able to qualitatively predict how the I/O requirements of each of the communities will change in the future: communities that use grid-based models (climate modelling, CFD) will see an increase in per-job I/O requirements as the resolution of the modelling grids increases; the materials science and biomolecular modelling would expect to see less change in the per-job I/O requirements (due to scientific limits on the size of systems to be studied) but would see an overall increase in I/O requirements as more sophisticated statistical methods and larger parameter sweeps

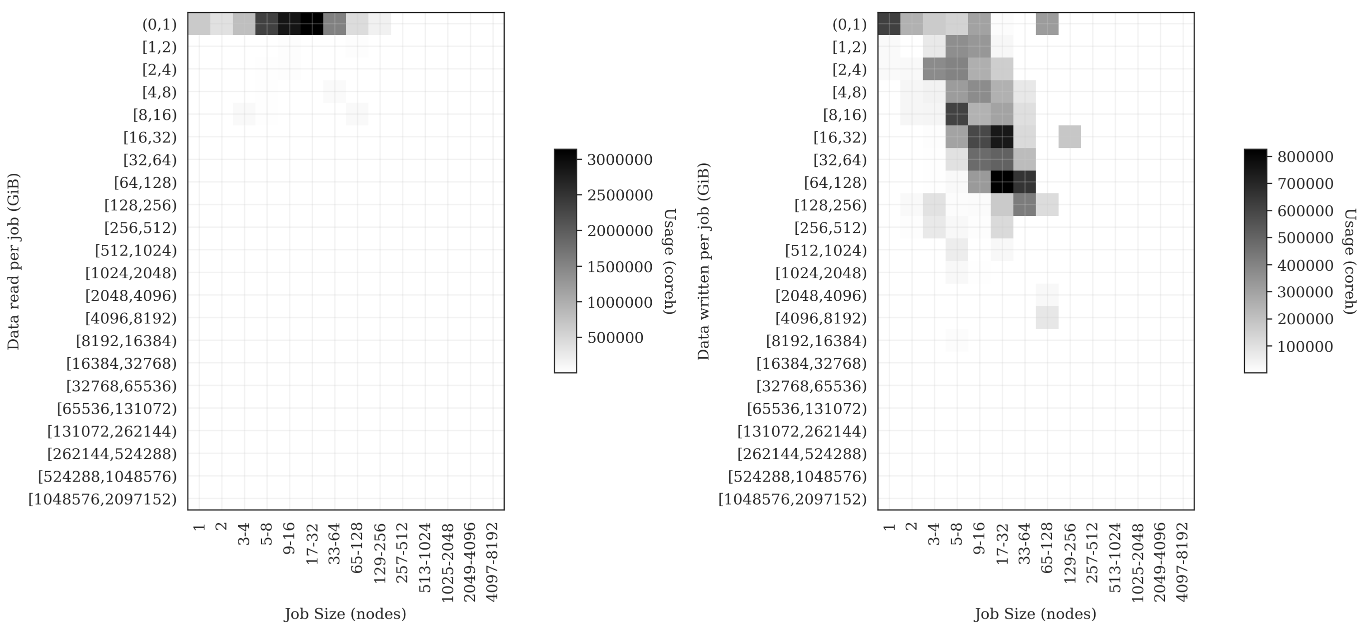


Fig. 19: Heatmaps of data read per job and data written per job vs job size for the biomolecular modelling community. Weights correspond to total core-h spent in a particular category.

require more individual jobs per research programme. Future national services serving these communities will need to take these requirements into account in their design and operation.

V. Future Directions

We are in the early stages of analysing the data obtained so far and plan to continue our analysis to learn more about application requirements for I/O. We expect to find more situations of applications that do not use the file system in an optimal way. As we find more incidents of application slowdown we will refine and augment the metrics used by LASSi. We also plan to automate detection of application slowdown so that we do not have to wait for individual incident reports to allow us to correlate LASSi metrics and actual incidents on the system.

We found that the current I/O operations metrics imported into SAFE (total number of I/O ops over the whole job) are not particularly useful for understanding this aspect of the I/O use on the system. Importing the peak I/O ops rate (for different operations) for each job should prove more useful and we plan to develop this functionality so we can analyse the I/O operations across the service using the powerful combination of LASSi and SAFE in the same way as we have been able to for data volumes.

This initial analysis has looked at I/O patterns for four of the largest research communities on the UK National Supercomputing Service, ARCHER (in terms of core-h use in the analysis period) but this approach neglects research communities that may have low resource use overall (measured in core-h) but high or different demands of the I/O resources. We plan to modify our analysis to reveal which communities are making different demands of the I/O resources by altering the weighting factor for the heatmaps produced from core-h to both data volume read/written and I/O operations.

We are also working to identify other HPC facilities that routinely collect per-job I/O statistics to allow us to compare the use patterns on ARCHER and understand how similar (or different) patterns are for similar communities on different facilities.

In addition to future research directions, we have the following activities planned to increase the impact and utility of the I/O data and metrics we are collecting:

- Integrate LASSi into the data collection framework provided by Cray View for ClusterStor[4] so that sites with this software can take advantage of the alternative view that LASSi can provide.
- Develop an I/O score chart that can be used as part of the ARCHER resource request process to give the service a better way to anticipate future I/O requirements and improve operational efficiency.
- Develop a machine learning model for application run time and its I/O to potentially allow the scheduler to make intelligent decisions on how to schedule different job types to reduce I/O impact between jobs and on the wider service.

Acknowledgments

This work used the ARCHER UK National Supercomputing Service. We would like to acknowledge EPSRC, EPCC, Cray, the ARCHER helpdesk and user community for their support.

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