~~The~~ Technology to aid the analysis of large-volume multi-institute climate model output at a Central Analysis Facility (PRIMAVERA Data Management Tool V2.10)

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Abstract. The PRIMAVERA project aimed to develop a new generation of advanced and well-evaluated high-resolution global climate models. As part of PRIMAVERA, seven different climate models were run in both standard and higher resolution configurations, with common initial conditions and forcings to form a multi-model ensemble. The ensemble simulations were run on high performance computers across Europe and generated approximately 1.6 pebibytes of output. To allow the data

5   from all models to be analysed at this scale, PRIMAVERA scientists were encouraged to bring their analysis to the data. All data was transferred to a Central Analysis Facility (CAF), in this case the JASMIN super-data-cluster, where it was catalogued and details made available to users using the PRIMAVERA Data Management Tool's (DMT's) web interface. Users from across the project were able to query the available data using the DMT and then access it at the CAF. Here we describe how the PRIMAVERA project used the CAF's facilities to enable users to analyse this multi-model data set. We believe that

10 PRIMAVERA's experience using a CAF demonstrates how similar, multi institute, big-data projects can efficiently share, organise and analyse large volumes of data.

1   Introduction

The PRIMAVERA project ran from 2015 until 2020 and aimed to develop a new generation of advanced and well-evaluated high-resolution global climate models. High-resolution simulations have been shown to better represent many different aspects of the climate, such as tropical cyclones (Roberts et al., 2020) and atmospheric blocking (Schiemann et al., 2020). Two "streams"

20 of simulations were performed within PRIMAVERA, each consisting of seven different climate models (AWI-CM-1-1, CMCC-

CM2, CNRM-CM6-1, EC-Earth3P, ECMWF-IFS, HadGEM3-GC31 and MPI-ESM1-2) that were run at their standard nominal resolution (Taylor et al., 2018) (typically 250 km in the atmosphere and 100 km in the ocean) and at a higher resolution (25 km atmosphere and 8-25 km ocean). All models were run with common initial conditions and forcings according to the High-ResMIP protocol (Haarsma et al., 2016). The simulations were run on high performance computers (HPCs) across Europe and the more than 100 scientists who analysed the data were based at 20 different institutes across Europe with assistance from other global scientists. Perhaps the most challenging aspect of working with global, high-resolution simulations is the volume of data produced~~. High-resolution simulations have been shown to better represent many different aspects of the climate, such as tropical cyclones (Roberts et al., 2020) and atmospheric blocking (Schiemann et al., 2020). The PRIMAVERA simulations generated~~, which in this case was a total of 1.6 pebibytes (PiB) of data[1].

A Data Management Plan (DMP) (Mizielinski et al., 2016) was developed to allow this data to be stored, analysed and archived at a Central Analysis Facility (CAF), which in PRIMAVERA's case was the JASMIN super-data-cluster. The Data Management Tool (DMT) software (Seddon and Stephens, 2020) was written to implement the ~~DMP and provides the~~ validate and analyse steps of the data workflow in the DMP and to assist with the ingest and disseminate steps. The DMT provided the ability to catalogue and then search the project's data. ~~The DMT~~ It tracked and controlled the movement of individual files as they ~~are~~ were moved between tape and disk, and allowed the data to be published to the global community for sharing at the end of the project.

~~If a CAF had not been available for PRIMAVERA to use then it would have been necessary for each modelling centre to make their own data available, typically on an Earth System Grid Federation (ESGF) node (Cinquini et al., 2014)(Petrie et al., 2021) or local File Transfer Protocol (FTP) server. Anyone wanting to analyse data would have needed to identify which variables were available and then download them from each modelling centre to their home institute. There would have been multiple copies of common datasets and each institute would have required significant volumes of storage, transfer bandwidth and compute resources.~~

In this paper we introduce the CAF and the PRIMAVERA project. We then describe the DMP and DMT and explain how they allowed the project's data to be managed. ~~Finally, we~~ We provide a summary of how the data was transferred to the CAF~~and~~, discuss the data that was accessed and users' views on the technology, and describe some of the hardware and software opportunities that may be suitable for managing similar projects in the future.

2 The Central Analysis Facility

The CAF used in the PRIMAVERA project is JASMIN, a super-data-cluster that was installed in 2012 (Lawrence et al., 2013). It is funded by the Natural Environment Research Council (NERC) and the United Kingdom (UK) Space Agency, and operated by the Science and Technology Facilities Council (STFC). It is located at the STFC Rutherford Appleton Lab (RAL), Harwell, UK. JASMIN's Phase 4 update in September 2018 added 38.5 PiB of new storage co-located with the existing 4000 cores of compute. The storage and compute are tied together with a low latency network. RAL has a fast connection to

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[1]Data volumes and rates in this paper use binary prefixes and so 1 PiB is 1024^5 bytes (IEEE, 2009).

Janet, the UK's academic network, which in turn is connected to the GÉANT European network, allowing the fast transfer of data from the HPCs used to run the PRIMAVERA simulations to JASMIN. In addition, JASMIN is connected to an on-site tape library for the offline storage of data. Similar CAFs exist at Centro Euro-Mediterraneo sui Cambiamenti Climatici (CMCC) (CMCC, 2021), Deutsches Klimarechenzentrum (DKRZ, German Climate Computing Centre) (DKRZ, 2021)~~and at~~

5 ~~,~~ Lawrence Berkeley National Laboratory on the Cori supercomputer (LBNL, 2021) and at other sites.

The compute at JASMIN is split into interactive data analysis servers, the LOTUS batch processing system and some additional private cloud servers. During PRIMAVERA Intel Xeon processors were used. The compute is primarily designed for batch and parallel processing for scientific analysis, but it also has limited support for multi-node MPI jobs. Part of the storage is dedicated for the Centre for Environmental Data Analysis (CEDA) archive, which contains over 13 PiB of atmospheric

10 and earth observation data, and is connected to the UK's ~~ESGF~~ Earth System Grid Federation (ESGF) (Cinquini et al., 2014) (Petrie et al., 2021) node. The co-location of the storage, datasets in the archive and compute makes JASMIN a powerful facility to analyse climate simulations with.

All compute hosts at JASMIN run the Linux operating system and have a suite of modern software tools and programming languages installed for the analysis and manipulation of common Earth science data formats. The storage for individual projects

15 is split into allocations called group workspaces (GWS) each of which is up to 100 tebibytes (TiB).

3 PRIMAVERA

The Horizon 2020 funded PRIMAVERA project was made up of eleven work packages (WPs) (PRIMAVERA, 2015) covering a range of scientific, technical, management, communication and user engagement topics. The Stream 1 and 2 simulations described here were run and managed by two of the work packages. Several of the other WPs analysed these simulations and

20 compared them with existing simulations, observations and reanalyses. The remaining WPs carried out model development work or ran small simulations that did not need to be shared with other WPs. These WPs only required a small volume of storage on one of the GWS.

The Stream 1 and 2 simulations follow the HighResMIP protocol and have been submitted to the 6th phase of the Coupled Model Intercomparison Project (CMIP6) (Eyring et al., 2016). The Stream 1 simulations consist of a single ensemble member

25 from each model at a standard and a high resolution for six different experiments. The follow-on Stream 2 simulations contain additional ensemble members for the experiments performed in Stream 1, but with a reduced data output to minimise the volume of data generated plus some additional simulations to exploit the new physics modules (for example (Nurser et al., 2020)) that ~~have been~~ were developed in PRIMAVERA.

Due to the scientific complexity, data volumes and the geographical distribution of the project participants, it was ~~recognized~~

30 recognised that developing and implementing a data management plan would require a significant amount of time and effort. ~~Sufficient~~ 44 person months of leadership and developer resource was included in the four year project proposal to allow ~~for this development work~~ this work to take place.
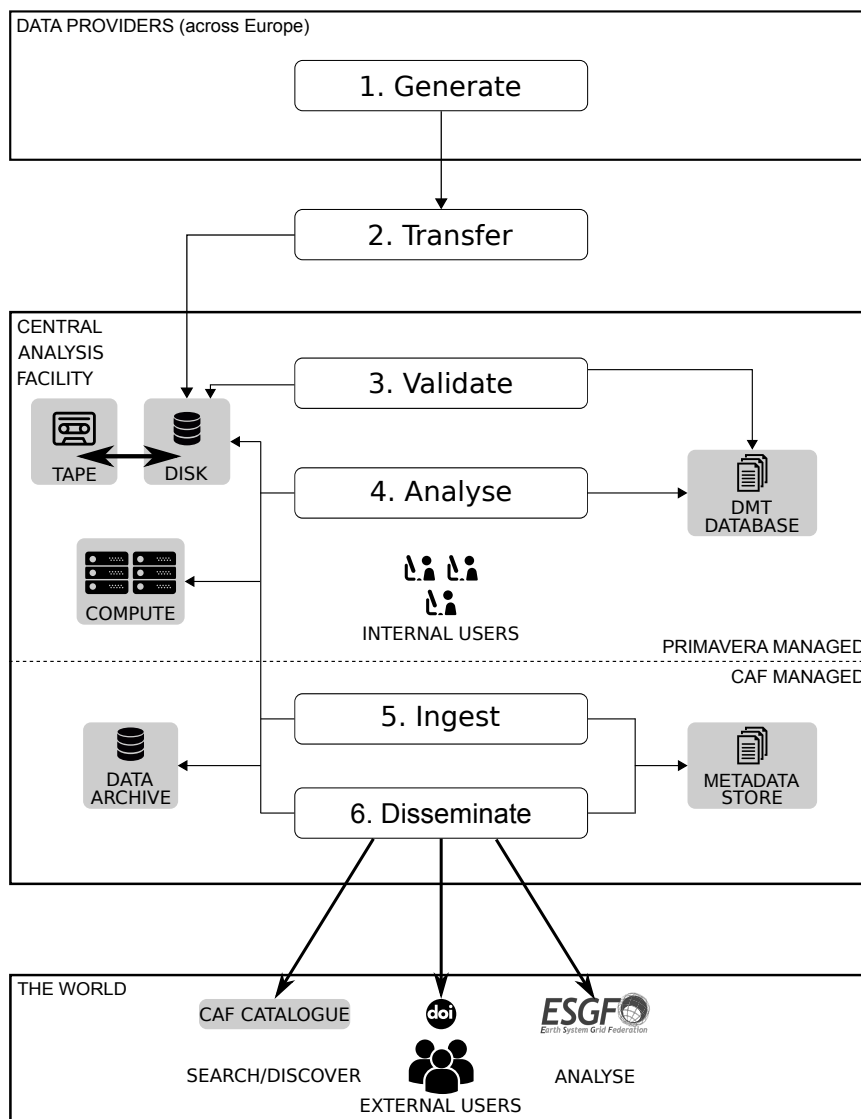
Figure 1. The workflow developed for PRIMAVERA in the Data Management Plan.

4 Data Management Plan

The PRIMAVERA Data Management Plan ~~(Mizielinski et al., 2016)~~ can be summarised as "taking the analysis to the data". Figure 1 shows the workflow developed in the DMP. All data files from the PRIMAVERA simulations were uploaded to the CAF and made accessible to project members, who were able to undertake their analysis of them. It has been common practise in many climate science projects to download the required data and perform analyses locally at users' home institutes.

Early analysis of the data requirements of the PRIMAVERA project, along with experience from prior projects, indicated that the downloading and local analysis of data would lead to significant technical challenges for each institute. As such, central analysis facilities such as JASMIN that provide data storage and compute are key to the exploitation of big data projects such as PRIMAVERA and CMIP6.

The first step in the DMP workflow is the generation of data by the modelling centres; simulations are run on a variety of HPCs across Europe and each model typically has its own proprietary output file format. As PRIMAVERA made up the majority of the European contribution to HighResMIP it was necessary to conform to the CMIP6 data standards (Balaji et al., 2018). These standards require data to be provided in CMOR3 (Climate Model Output Rewriter) (Nadeau et al., 2019) compliant netCDF files following the CMIP6 conventions. Where data had been generated in a proprietary format it was post-processed to comply with these standards.

The second step in the workflow is the transfer of the data from the HPCs or post-processing systems to the CAF. A discussion on the transfer techniques used and the rates achieved is given in Sect. 6. The data is uploaded to the PRIMAVERA storage volume at the CAF.

The data sets provided are passed through a quality control process in step 3, which includes checking that the data and metadata standards have been complied with, and the extraction of metadata to store in the DMT's database (Seddon, 2020a). After completion of the validation process, files are archived to tape and removed from the GWS to create space for other uploads. After the upload and validation of the data, users internal to the project analyse and work with it in ~~Step~~ step 4. The movement of files between tape and disk is fully automated by the DMT so that the consistency of file paths in the database is maintained.

The final steps in the workflow (steps 5 and 6 in Fig. 1) are managed by CEDA rather than the PRIMAVERA project as these relate to the use of shared facilities. Uploaded data is ingested into the CEDA archives (CEDA, 2020a) and is then available for dissemination to the global community using the CEDA Earth System Grid Federation node (CEDA, 2020b). Steps 5 and 6 do not have to be run immediately after the data has been validated. A delay before dissemination to the global community allows the project's users to have a period of sole access to the data and the opportunity to generate the first publications from the simulations.

4.1 CAF Resources

After reviewing the DMP, PRIMAVERA was allocated 440 TiB of storage at the CAF split across five volumes. A virtual machine in the internal cloud was provided, which was given a domain name and HTTPS access allowed to it from the Internet, and the DMT software and database were installed on this server.

The 440 TiB of storage at the CAF that was allocated to the project was 2.4 % of the almost 18 PiB of project storage allocated to all 242 group workspaces at JASMIN in March 2021 (Townsend et al., 2021). 100 PRIMAVERA users were 4.1 % of the total number of the CAF's users at the same time.

It was originally estimated that around 2.4 PiB of data would be generated by the project, and therefore only a subset of data could be held on disk at once. The remaining data would have to be held on tape and moved to the GWS as required. The DMP describes how the DMT would allow data to be efficiently and reliably moved between tape and GWS and its location tracked.

4.2 Typical Analysis Workflow
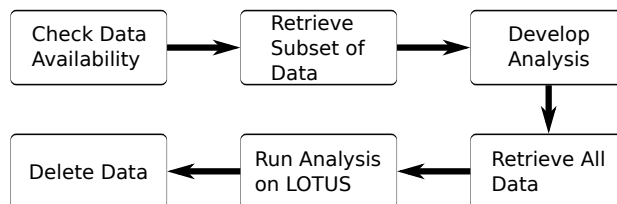
Figure 2. The workflow used by users working with the PRIMAVERA data at the CAF.

Figure 2 shows the workflow that users working with the PRIMAVERA data at the CAF were required to follow. Users began by using the DMT's web interface to identify what data had been uploaded. If the data they required was not available on disk then they used the DMT's web interface to request that a subset of their data was restored from tape to disk. The DMT sent them an email when this requested sample dataset was available on disk and they could then work on the CAF's interactive servers to develop and test their analysis code. After testing and validating their analysis code, they could then use the DMT to request that all of the data they required was restored from tape to disk. Once the full dataset was available on the GWS then the analysis was run on the LOTUS batch processing cluster. When their analysis was complete, users then marked the data as finished in the DMT's web interface and the DMT would then delete the data from disk to create space for other data. This workflow allowed for the efficient use of disk space; PRIMAVERA generated over 1.6 PiB of data but the upload of data, analysis and some storage of additional observations and reanalyses was able to fit into the 440 TiB of ~~allocated disk space~~ disk space that was available to the project.

5 Data Management Tool

The DMT was developed to track and control the flow of PRIMAVERA data around the CAF and to allow users to query the available data and its location. It was built upon a PostgreSQL database and custom software written in the Python programming language, using the Django web framework (Django, 2019). The database was installed on a dedicated server, along with web server software and the DMT application, and was accessible to users across all hosts at the CAF. Access to the database from the compute cluster allowed the batch submission of validation processes to the compute cluster allowing significant parallelisation of the work.

A typical screenshot from a user querying the DMT's web interface is shown in Fig. 3. In this example the variable "rsut", the top of atmosphere outgoing shortwave radiation, from the "highres-future" coupled future experiment is being queried. A

Figure 3. A screenshot from the DMT's web interface showing the data available for one variable from the coupled future experiment.

value of "offline" in the "Online Status" column shows that the files for this simulation are currently only available on tape, a
25 value of "partial" shows that some files are on disk, but others are only available on tape and "online" shows that all files are available on disk. The "Request Retrieval?" column allows users to indicate that they want to work with this variable. If the variable's files need to be restored from tape to disk then they are queued for retrieval and the user is emailed when the data becomes available. The DMT contains a similar page to allow users to view the data that they have requested and to mark it as used, so that it can be deleted from disk to release storage.

5 The DMT software ~~(Seddon and Stephens, 2020)~~ is distributed under an open source license. Development of the DMT began in April 2016 and the first data was made available via the DMT in May 2017, requiring the full time work of one developer. Development work ~~has~~ continued as required ~~since then~~ to improve the flow of data through the system and to facilitate the publication of data to the ESGF.

5.1 DMT Internal Structure

Figure 4 shows a simplified UML class diagram ~~showing~~ illustrating how data is represented as Django models, implemented as Python classes in the DMT. Internally, the DMT's primary data object is a DataRequest. A DataRequest object consists of a VariableRequest object along with details of the institute, climate model, experiment and variant label. The VariableRequest object specifies a CMIP6 variable and MIP table along with additional metadata. VariableRequest objects are created program-
5 matically from the CMIP6 HighResMIP data request (Juckes et al., 2020). During the development of the data management plan, a shared spreadsheet was created from the HighResMIP data request and each institute edited the spreadsheet to indicate the variables that they would generate. The DataRequest objects were created programmatically from this spreadsheet. A facility to allow ~~institutes~~ data providers to update the data requests that they would provide ~~during the project~~ was developed to allow for changes to ~~institutes~~providers' plans.
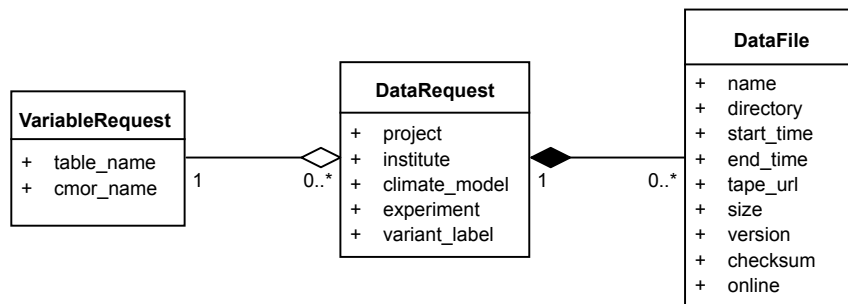
Figure 4. A simplified UML class diagram showing how data requests and data files are implemented as Django models in the DMT.

A DataFile object was created for each file uploaded to the CAF during the validation process and a checksum was calculated for each file submitted to the DMT. The checksums were used throughout the workflow as ~~files were moved~~ the DMT moved files from tape to disk to ensure their integrity. Each DataFile is related to a DataRequest and all views in the DMT's web interface are generated from these DataRequest objects. All objects are mapped to database tables using Django's object-relational mapper.

~~The DMT worked well, although some~~

5.2 Design Considerations

An agile (Beck et al., 2001) methodology was used for the development of the DMT. Releases were regularly made available to users and their feedback was incorporated into additional functionality and performance improvements in future releases. The initial releases of the DMT provided the functionality for the validate and analyse steps in the workflow shown in Figure 1. Further development provided the functionality for the ingestion and dissemination steps later in the project. The choice of an agile approach was partly necessary because of the limited amount of developer resource available and so the need to concentrate the available resource on releasing functionality to the users as soon as possible.

The DMT's users were not formally involved in the initial design of the tool. The developers used their experience of working with previous climate modelling projects to include the search and browsing functionality that they thought would be the most useful to the users. This functionality was then refined in future releases based on informal feedback from users.

The underlying data structures used in the DMT were designed at the start of the project during the development of the DMP and were documented in there. The data structures were designed to hold enough information to uniquely identify each file and data request and their design was based on experience gained during previous projects. The structures evolved as experience was gained during the initial DMT development. The Django framework allows the underlying data structures to be changed as a project evolves using "migrations"; this flexibility worked well with the agile methodology.

The data structures used in the DMT were based on the metadata attributes in the netCDF files specified by the CMIP6 data standards. The existing DMT software could be reused by other projects using the same data standards. The current version

of the DMT is not immediately generalisable to other data standards as the search facilities rely on these CMIP6 metadata attributes. However, the DMT can be generalised to a wider range of file standards by either reducing the number of metadata attributes extracted from data files, or by making the attributes extracted optional. Reduced metadata extraction would limit the usefulness of the current search fields, which may need to be removed from the search interface. Such changes would be relatively trivial. Some of the functionality to restore data from tape to disk is specific to the structure of the current CAF and would need to generalised for use at other CAFs.

Users had to use the DMT's web interface as no alternative was available. Several solutions are available to add a web Application Programming Interface (API) to applications written in the Django framework. A web API should be added to future versions of the DMT to provide users with alternative methods to access the DMT. One user used web scraping technology to extract information from the DMT to automate their own workflows, which could have been avoided had an API been available. Additionally, an API would allow command line software to interface with the DMT, which some existing users may prefer to the web based interface.

The DMT worked well, although some manual effort was required to maintain the set of expected data requests. The data request objects in the database that were planned to be produced by each modelling centre were created programmatically at the start of the project. As each modelling centre gained more experience with their model, and as scientists requested additional data, modelling centres generated additional output variables. Additional data request objects then had to be created manually by the system administrator. Programmatically creating data ~~requests~~ request objects when each file is validated and added to the DMT would have been more efficient than creating them at the start of the project and then having to manually handle such changes.

The upload of data, analysis and storage of additional observations was all able to fit into the 440 TiB of CAF disk storage allocated to the project. As discussed in Sect. 4.2 users marked their data as finished so that it could be deleted from disk if no other users had requested that data. All data requests were given equal priority for retrieval and deletion. Occasionally, the amount of free disk space became low and so targeted emails were sent to high volume users reminding them to mark any completed data as finished. If targeted emails had not worked then the next step would have been to develop a utility that deleted the lowest priority data requests. However, demand never exceeded the available resource and so no prioritisation algorithm had to be developed.

6 Data Transfer

Table 1 shows the sustained rates achieved when transferring data from the data providers to the CAF in mebibytes per second (MiB s^{-1}). JASMIN contains several servers in a data transfer zone, whose connection to the Internet and to the rest of the CAF has been designed for maximum data throughput. At the start of the project it had been assumed that parallel transfer protocols such as BBCP (Hanushevsky, 2015) or GridFTP (Foster, 2011)(Globus, 2019) would provide the best transfer rates and data providers were encouraged to use these. In reality, most data providers used the techniques that they were most familiar with as long as they gave sufficiently fast transfer rates. The rates achieved depend on many factors including the file systems, the

Table 1. The rates achieved while transferring data from the data providers to the CAF.

Transfer from	Rate achieved	Protocol used
Toulouse, France	13 MiB s^{-1}	4 BBCP jobs in parallel, with 4 streams each
Hamburg, Germany	20 to 55 MiB s^{-1}	globus-url-copy
Lecce, Italy	34 MiB s^{-1} average, 69 MiB s^{-1} peak	gridftp, with 4 concurrent FTP connections 8 process in parallel
Bologna (Cineca), Italy	200 to 300 MiB s^{-1}	5 parallel `rsync -av -e "ssh -c arcfour"`
Barcelona, Spain	13 MiB s^{-1}	rsync
Exeter, UK	30 MiB s^{-1}	5 groups of 3 FTP connections over dedicated link
Reading, UK	85 MiB s^{-1}	4 parallel `rsync -rvz -rsh="ssh -c arcfour"`

load on the servers and the network between the servers. The fastest transfer rate from a site was over 200 MiB s^{-1}, equivalent to 16.5 TiB per day. Typical rates were 30 MiB s^{-1} (2.5 TiB per day). These rates were sufficient to complete the project on time. It is hoped that with further optimisation work a sustained minimum transfer rate of 5.0 TiB per day could be achieved.

The collection of all of PRIMAVERA's data at the CAF was only possible because of the magnitude of the transfer rates that were achieved. If data transfer rates between the HPC centres and the CAF had been insufficient then the scientific analysis performed by PRIMAVERA would have been significantly impacted.

7   Data Access and Analysis

Because the DMT was used to restore data from tape to disk it ~~is~~ was possible to analyse the fraction of data produced by the project that was analysed. As of 20th July 2020, 31,048 data requests had been uploaded to JASMIN containing 1.5 PiB of data. 6,070 ~~unique~~ data requests had been restored from tape to disk at least once, which is 20 % of the data requests by number. However, these ~~unique~~ restored data requests contained 426 TiB of data, which is 27 % of the volume of data that had been uploaded (Seddon, 2020b). One reason that more data by volume than by number of data requests was requested could be because users were analysing the larger volume variables, which tend to be variables with a higher temporal frequency.

The number of downloads of each variable was published (Seddon et al., 2020) as this information may be useful when designing the data requests in future projects. This information was used when developing the DMP for a successor project to PRIMAVERA (Savage and Wachsmann, 2023).

All of the data from the PRIMAVERA simulations was added to the CEDA archives and published to the ESGF. Because of the need to restore the data from tape, publication took over one year to complete.

In PRIMAVERA, users accessed the data using a variety of tools such as CDO (Schulzweida, 2022), Python, Iris (Met Office, 2010 - 2022), Jupyter Notebooks (Kluyver et al., 2016) and ESMValTool (Righi et al., 2020). PRIMAVERA provided some resource for the development of ESMValTool, therefore much scientific analysis was completed before ESMValTool was available. ESMValTool may allow for the more efficient analysis of multi-model datasets in future projects.

8 User Feedback

Table 2. Number of responses for each score from the users of the PRIMAVERA facilities at the CAF with 1 being very difficult and 7 being very easy.

		Querying the data request to see which variables were scheduled to be produced.	Use of the DMT to discover and query the PRIMAVERA data available at JASMIN.	Retrieving data from tape to group workspace / disk.	Accessing the data on the JASMIN group workspaces.	Analysing the data at JASMIN?
Score	1	0	1	1	1	1
	2	1	1	0	1	0
	3	0	0	0	2	1
	4	0	0	1	0	2
	5	3	1	1	0	0
	6	7	11	10	7	8
	7	4	7	6	10	4
# Responses		15	21	19	21	16
Mean		5.8	5.9	5.9	5.8	5.5

A survey of all PRIMAVERA users of the CAF (approximately 100 users) was conducted and responses were received from 24 users (Seddon et al., 2020). Users of the data were asked to rate five aspects of the process out of seven with 1 being very difficult and 7 being very easy and the results are shown in Table 2. The response to all of the questions was midway between neutral and very easy to use. Four users did indicate that they had various levels of difficulty accessing the data and two users indicated some levels of difficulty analysing the data at the CAF; no additional feedback was provided explaining the difficulties that these users had encountered. The remaining 17 and 14 users respectively answered these two questions with neutral to very positive answers. These largely positive responses indicate that users had few problems performing their analyses at the CAF.

9 Future Opportunities

9.1 Platforms

9.1.1 Central Analysis Facility

Access to the CAF has been essential to the success of PRIMAVERA. JASMIN has a finite capacity and so may not be able to support all further projects that would benefit from having access to it. ~~Central Analysis Facilities~~ CAFs similar to JASMIN providing additional capacity would be incredibly useful for collaborative projects like PRIMAVERA as they would reduce the need for all institutes participating in a project to have their own large data storage and data analysis facilities. Such facilities also reduce the volume of data that needs to be transferred, which is important as climate simulations increase in resolution and complexity, and therefore increase in size.

Access to a CAF also allows scientists from some countries that do not currently have access to high-performance data analysis facilities locally to analyse large cutting-edge data sets. Some of these countries are on the front-line of climate change and access to a CAF would allow them to further contribute to climate science. For example, the CP4-Africa (Stratton et al., 2018) convection-permitting regional climate simulations over Africa are now available at JASMIN (Senior, 2019) and have been analysed at JASMIN by scientists working from Africa. Tools to access CAFs must be robust to the potentially slow and unreliable Internet connections that may be encountered in some countries. For example Secure Shell (Ylonen, 1996) (SSH) sessions do not retain state when they disconnect from unreliable connections (Senior et al., 2020). Further work is required to choose the most appropriate tools to allow all users to reliably access CAFs.

9.1.2 Public Cloud

Public cloud computing technologies could provide an alternative to a facility such as JASMIN. As users have been using local Unix based computers to analyse data for many years, the change from working locally to working remotely at JASMIN was therefore only a small change for users. The change was assisted by the CAF's comprehensive documentation (CEDA, 2020c) and the development of additional documentation and demonstration videos by the PRIMAVERA project. The CAF's mix of interactive servers and the batch processing cluster allowed for the easy development of analysis software and its running on the full multi-model datasets. Moving the analyses to the cloud would be a larger change for users, and significant development and support would be required. However, the use of public cloud technology would allow the compute to be easily scaled to the amount required at any one time, and potentially provide large volumes of data storage and remote access to the data for all users.

STFC were PRIMAVERA project partners and received £141,000 of funding for the provision of the CAF and support services over the course of the project (Townsend and Bennett, 2020). STFC receive an annual grant from NERC to cover the remainder of their running costs. If a project decided to use the public cloud rather than an existing facility such as JASMIN then funding for the provision of the public cloud resources would need to be included in the project proposal. Compute in the public cloud is billed per second per processor core, storage is billed per unit of storage and there can be a charge for moving

data into and out of the ~~the~~ storage. A typical cost for storage using Amazon Web Service's S3 storage service ~~is~~ in September 2022 was $0.022 per ~~gigabyte~~gibibyte, resulting in a charge of $~~10,643~~ 9,912 per month for 440 TiB of storage, or $~~510,877~~ 475,791 for disk storage over the course of the four year project~~.~~ (AWS, 2022). Some discounts are available for the advanced and bulk purchase of cloud resource. Additional costs on top of this would be required for data upload and download, tape storage and compute.

Determining the level of funding required for public cloud computing in a proposal will be difficult, but important to correctly

5   determine so that the project does not overspend or run out of compute or storage before the end of the project. No record of the compute time used at the CAF was made for the PRIMAVERA project. However, data sharing outside of the project could be made easier in a public cloud based solution as external users could fund their own processing costs, whereas in PRIMAVERA they had to be invited onto the CAF.

Significant architectural design and software development is required before projects like PRIMAVERA can move their data

10   storage and analysis to the public cloud.

9.2   Software

The DMT was a significant component in the success of the PRIMAVERA project and appears to be a novel tool in projects of this scale. The current implementation of the DMT for PRIMAVERA makes some assumptions about the layout of the storage allocated to PRIMAVERA at JASMIN~~and about the structure of the PRIMAVERA data~~. Applying the DMT to other

15   projects and using it at other CAFs may require ~~adjustment and/or redesign~~code modifications to remove these assumptions, but this implementation has demonstrated the value of such a tool. The current PRIMAVERA DMT implementation relies on the presence of CMIP6 metadata attributes in data files and may not work with other data standards. Development of a more generic version has begun in an alternative repository (Seddon, 2023) and the community has been invited to use and contribute to the new version.

20   ~~New software technologies such as Pangeo offer further benefits if a public cloud solution was used or if external access was available to multiple CAFs around the world (Pangeo, 2020). Pangeo is a~~ In PRIMAVERA all analysis was performed at a single CAF. Multiple CAFs (perhaps called distributed analysis facilities) coupled together by improved software tools could reduce the need for data transfers in future projects. Pangeo (Pangeo, 2020) is an example of such a tool and is a collection of software packages to enable Earth science research in cloud and HPC environments. It allows data to be distributed across

25   different storage areas and it schedules processing on the compute attached to each storage area. ~~Pangeo could reduce the volume of data needing to be transferred in future projects.~~ Model output data would be uploaded to a storage location close to the data provider. Just the metadata would be uploaded to a ~~central (or distributed) catalogue . Tools such as Pangeo~~ catalogue such as the DMT. These tools would then run users' analysis software on the compute where each dataset is stored and only the small volume of analysis results would need to to transferred back to the user. ~~Two tools have been implemented at JASMIN~~

30   ~~since the end of~~ Such technologies would be a further extension to the DMP's aim of "taking the analysis to the ~~PRIMAVERA project to improve collaboration and data sharing, including a Jupyter notebook service to allow web based access to compute and visualisation (?) and an object store including external access to data in the store (?)~~data".

10   Conclusions

PRIMAVERA's Data Management Tool and access to the Central Analysis Facility have been essential to the success of the PRIMAVERA project. The DMT and CAF have allowed over 100 researchers to collaboratively analyse a multi-model high-resolution set of climate simulations. Over 1.6 PiB of data was collected in a single location where users were able to analyse the data via both interactive analysis servers and a batch processing cluster. The Data Management Tool minimised the volume of expensive disk storage in use at any one time by allowing data to be seamlessly moved between tape and disk under the control of data users.

If a CAF had not been available for PRIMAVERA to use then it would have been necessary for each modelling centre to make their own data available, typically on an ESGF node or local File Transfer Protocol (FTP) server. Anyone wanting to analyse data would have needed to identify which variables were available and then download them from each modelling centre to their home institute. There would have been multiple copies of common datasets and each institute would have required significant volumes of storage, transfer bandwidth and compute resources.

The use of the CAF and the DMT have laid down a marker for future projects and their adoption is recommended. The DMT allowed the project to manage its storage resources to the best of its ability. The DMT's ability to allow users to move data between tape and disk minimised the use of expensive disk storage. A user survey indicated that project members found this solution ~~straight forward~~ straightforward to integrate into their working practises.

Access to the CAF has been essential for analysing data in the PRIMAVERA project but continued expansion of the storage and compute of CAFs such as at JASMIN, CMCC, DKRZ and Cori is necessary to allow them to continue supporting such projects and to support additional projects in the future. In each CMIP era the data volume has increased by an order of magnitude (Balaji et al., 2018). The Earth sciences community would benefit from the development of additional CAFs, or the expansion of existing CAFs, to allow even more projects and a wider range of users to take advantage of such facilities and to handle the inevitable increase in future data volumes.

The tools developed by the PRIMAVERA project have successfully demonstrated the feasibility of such techniques. The tools have been made freely available, but require some development before they can be seamlessly adopted by other projects. The inclusion in the project proposal of dedicated time resource for data management and development of the DMT contributed to the success.

Code availability. The PRIMAVERA Data Management Tool's source code can be found in a Zenodo repository at https://doi.org/10.5281/ZENODO.4011770 distributed under a BSD 3-Clause license (Seddon and Stephens, 2020). Additional code is similarly available in the validation tool at https://doi.org/10.5281/ZENODO.3596772 (Seddon, 2020a) and MIP tables at https://doi.org/10.5281/ZENODO.1245673 (Nadeau et al., 2018) with similar licenses. Development of a more generic version of the Data Management Tool has begun under the same license at https://doi.org/10.5281/zenodo.8273457 (Seddon, 2023) and the community is invited to contribute there.

Author contributions. MM and AS developed the PRIMAVERA data management plan. JS then developed and implemented the DMT, with input from AS, and managed the data upload and data availability. JS prepared the manuscript with contributions from all co-authors.

Competing interests. The authors declare that they have no conflict of interest.

Acknowledgements. The PRIMAVERA project is funded by the European Union's Horizon 2020 programme, Grant Agreement no. 641727. MM received additional funding from the EU Horizon 2020 CRESCENDO project, Grant Agreement no. 641816 and by the Newton Fund through the Met Office Climate Science for Service Partnership Brazil (CSSP Brazil). This work used JASMIN, the UK's collaborative data analysis environment (https://jasmin.ac.uk). The IS-ENES3 project has provided funding from the European Union's Horizon 2020 research and innovation programme under grant agreement no. 824084 to support continued access for the PRIMAVERA project to JASMIN. The authors would like to thank all of the STFC staff who design and maintain JASMIN, without whom this work would not have been possible. The data providers from the PRIMAVERA modelling centres should also be thanked for their hard work complying with the metadata standards and their enthusiasm to use the workflows developed in the project, along with all of PRIMAVERA's users.

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