esiwace
CENTRE OF EXCELLENCE IN SIMULATION OF WEATHER AND CLIMATE IN EUROPE

D4.2 New Storage Layout for Earth System Data

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Abstract

Making the best use of HPC in Earth simulation requires storing and manipulating vast quantities of data. Existing storage environments face usability and performance challenges for both domain scientists and the data centers supporting the scientists. These challenges arise from data discovery/access patterns, and the need to support complex legacy interfaces. In the ESiWACE project, we develop a novel I/O middleware targeting, but not limited to, earth system data. This deliverable sheds light upon the technical design of the ESD middleware, and the user perspective and implications when using the middleware. Its architecture builds on well established end-user interfaces but utilizes scientific metadata to harness a data structure centric perspective.

In contrast to existing solutions, the middleware maps data structures to available storage technology based on several parameters: 1) A data center specific configuration of available hardware with their characteristics; 2) The intended usage pattern explicitly provided by the user and implicitly by the structure of the data.

This allows to exploit performance characteristics of a heterogeneous storage environment more efficiently.

Contents

Chapter 1

Relation to the Project

The following text is the description of the project proposal for this task and deliverable:

> *I/O is being addressed at a number of levels within ESiWACE, since both current experience and projections have highlighted the performance/volume challenges ahead. The main goal of this task is to address performance and physical capacity issues associated with writing, accessing, and earth system data in the disk subsystem themselves. One key problem that can be addressed is separation of file metadata operations from the data access - this is the strategy some hybrid disk systems use to improve performance by putting file system metadata on SSD and data itself on spinning platters. However, with netCDF or GRIB data, the scientific relevant metadata and much of the information about actual data layout is invisible to the file system (whether parallel or serial), which cannot then exploit acceleration techniques. To address this, we propose and test an Earth System Data (ESD) middleware library which understands these key formats, and which is customizable for different hardware environments (as will occur in differing data center architectures). It will support, for example, writing the scientific metadata and possibly coordinate access to SSD systems, and the binary data fields to traditional systems potentially split into multiple files. Where in-memory storage backends are available, fast online data analytics will also become possible. [...] The layout components will decide the data placement and orchestrate data access on the storage characteristics. But blocking and non-blocking APIs will be supported to address typical use-cases. Tools will accompany the library so that data can be reconstructed as compatible with netCDF/GRIB and can be archived and exchanged.*

Chapter 2

Introduction

This section motivates the development of the new middleware and lists the challenges specifically for Numerical Weather Prediction (NWP) and climate.

2.1 Motivation

The development of the new middleware is motivated by two facts:

1. Firstly, the drastic changes in the storage landscape.
2. Secondly, the drawbacks of the current data management paradigm.

2.1.1 Changes in the Storage Landscape

With the emergence of new storage technologies such as NVRAM and cloud storage, the sea of options for storing data becomes increasingly complex. The storage architecture of novel systems deploys combinations of several technologies as a single solution. This is motivated by the fact that systems relying only on hard disk drives (HDDs) cannot deal with all the workloads efficiently. On the other hand, building systems that can serve different workloads by dynamically directing them to the storage media that serves their need best, can provide a better solution although it increases complexity.

TODO: Refer to outcomes of cost discussions (JJ: is this enough?)

Deliverable D4.1 investigated models for the data centre, focusing on the cost of providing services of the required QoS, e.g. with the required durability qualities, availabilities, etc.; in particular, services could be made up of different types of storage, and in general different kinds of storage are required also to support the processing of the data (e.g. scratch space, archiving, working repositories, space to share with other users, etc.) As climate and weather data volumes scale up, one needs to investigate which parts of the data centre and its operation need to scale up, and by how much. For example, operating the first tape library requires employing and training staff to look after it, but then operating another tape library does not require double the staff. Support for the users, though, is expected to scale approximately linearly with the number of users.

In particular, different types of services are needed to support different parts of the data processing – storage, archiving, possibly preservation, cache, fast disk for HPC/HTC, etc. No single storage "solution" meets all these requirements. Thus, systems consisting of multiple storage technologies are combined to provide various services, traditionally in a memory

hierarchy, because fast and expensive devices come with less capacity than slow and cheap(er) devices. Fast disk can then cache "hot" files which are being processed by many jobs, and slower storage with higher capacity can manage the rest of the data.

On many systems, data migration from one persistent storage hierarchy to another, e.g., disk based scratch to long term tape, is initiated by the user. This is an inconvenient additional step for the user but gives explicit knowledge about the data location. Depending on the usage, this may lead to a more efficient exploitation of the near-line storage, but only for educated users that know their workflow well.

An hierarchical storage system (HSM) extends this notion allowing administrators to define policies that describe how data is placed and potentially migrated between different storage tiers. However, HSMs operate at the file granularity (according to the definition of file systems). Block-based data migration can also be supported by some system. Both approaches have in common that they do not understand the data structures that are serialized to the 1D Byte array of a file.

Also the increasing use of object storage is relevant to this report. Currently, there are activities looking at the placements of slices of multidimensional HDF5 arrays into object stores, with a unified addressing and lazy loading in applications. Provided data is being indexed correctly, optimised storage of larger arrays can lead to a speed-up of processing of two orders of magnitude, so it will be worth investigating this topic further.

2.1.2 Data Management Paradigm

The file based data management paradigm forces users to define the hierarchical namespace in which store the experiments. From the user perspective, scientific file formats could store one or multiple variables in one file, which can be potentially partitioned and distributed across multiple physical files. Usually, the definition of the content of a file is driven by performance reasons and the initial originating process (i.e., the scientific program generating the data). In many cases, a portable data format that can be used to exchange data between working groups and scientists, is another important factor. However, a file format may not optimally support the workload or the storage system it is running on. The users could struggle to define a file system hierarchy that matches their workflow and is well performing on their system; indeed, some user communities overload the file paths with metadata to aid its discovery, but this also does not scale in the general case.

Once all data is ready, usually scientific databases are used to ingest the metadata and offer alternative views to the same data. They abstract from the actual hierarchical namespace used underneath and provide a flexible approach to query data.

TODO: More limitations later...

2.2 Challenges for NWP/Climate

Workloads from the domain of climate and weather face particular challenges in terms of data management and storage landscape[1].

1. **I/O intensity (volume and velocity)**. Multiple data sources can be used in one simulation or analysis. Observational sources such as satellites and sensor networks can produce large volumes of data. Simulations can produce data at any granularity:

[1]Note that other scientific domains have some overlap with the mentioned challenges, in that sense none of the challenges is unique for NWP/climate but in the combination the profile is unique.

Firstly, the resolution can be increased. Secondly, ensemble runs as mixes of multiple scenarios, number of experiments to be conducted and, thus, the data volume.

2. **Code portability**. Code is long-living, it can potentially live for decades, and excerpts of the code might be moved to newer code. Historically researchers used to optimize codes for specific supercomputers but with increasingly complex systems this approach is not feasible. Thus, data management needs to scale with future data volumes in a way which provides acceptable data access latencies and data durability, and is cost-effective. In this context the middleware hides specifics of the storage landscape and does not require users to change parameters specifically to a given system.

3. **There is no single perfect model**. The complexity of the physical processes that influence weather and climate is so immense that not all parameters are yet understood and can be quantified. This leads to a proliferation of predictive models. Each of them covers the processes slightly differently or covers alternative processes. Thus all of the models have some relevance and cannot be unified easily.

4. **Diversity of data formats and middleware**. In an effort to allow for easier exchange and inter-comparison of model and observations, data libraries for standardized data description and optimized I/O such as NetCDF, HDF5 and GRIB were developed but many more legacy formats exist. Since historical data is important, these formats must still be supported and maintained. Many I/O optimizations used in common libraries do not adequately reflect current data intensive system architectures, as they are maintained from domain scientists and not computer scientists.

5. **Sharing of data between many stakeholders**. Systems need to support multi-disciplinary research through shared, interoperable interfaces, based on open standards and deliver environmentally-responsible and flexible hybrid data and compute infrastructures.

6. **Time critical and guaranteed accuracy are mandatory**. Climate and weather applications can be used for the prediction of disasters such as tsunamis. This implies that the models must produce the well-defined and accurate output; and that in-situ and in-transit workflows are supported. It is also crucial that the runtime of such a prediction is short to react accordingly and mitigate the impact on society.

2.3 Outline

This deliverable is organized as follows:

TODO:

Chapter 3

Earth System Data

This chapter provides a high-level perspective on the data formats, middleware used for managing earth system data and how these are utilized by end-users and developers.

3.1 Data Generated by Simulations

With the progress of computers and increase of observation data, numerical models were developed. A numerical weather/climate model is a mathematical representation of the earth's climate system, that includes the atmosphere, oceans, landmasses and the cryosphere. The model consists of a set of grids with variables such as surface pressure, winds, temperature and humidity. A numerical model can be encoded in a programming language resulting in an application that simulates the behavior based on the model. Inside an application, a grid is used to describe the covered surfaces of the model, which often is the globe. Traditionally, the globe has been divided based on the longitude and latitude into rectangular boxes. Since this produced unevenly sized boxes and singularities closer to the poles, modern climate applications use hexagonal and triangular meshes. Particularly triangular meshes have an additional advantage, that one can refine regions and, thus, can decide on the granularity that is needed locally – this leads to numeric approaches of the multi-grid methods. Grids that follow a regular pattern such as rectangular boxes or simple hexagonal grids are called structured grids. With partially refined grids or when covering complex shapes instead of the globe, the grids become unstructured, as they form an irregular pattern.

To create an hexagonal or triangular grid from the surface of the earth, the grid can be constructed starting from an icosahedron and repetitively refining the triangle faces until a desired resolution is reached. Variables contain data that can either describes a single value for each cell, the edges of the cells, or the vertices of the cells.

?? shows this localization – the scope of data – for the triangular and hexagonal grids.

Figure 3.1: Scope of variables inside the grids

Larger grids are shown in **??** and in (**??**). There are figures provided that illustrate the neighborhood between data points and for different data localization.

Triangular grid consists of cells shaped as a triangle (**??**). Values can be located at the centers of the primal grid hexagons **??**, and if we connect it to each other, we would see the grid of triangles **??**. If values are located at the edes (**??**) and they are connected with its neighbours, then the grid will be seen **??**. If the values are located at the vertices and they are connected with its neighbours, then the grid will be seen in **??**.

Hexagonal grid consists of cells shaped as a flat topped hexagon (**??**). Two ways can be used to map data to the grid: vertical or horizontal. Values can be located at the centers of the primal grid (hexagons **??**), and if we connect it to each other, we would see the grid of triangles **??**. If values are located at the edges (**??**) and edges are connected with those of the neighbours, then a grid emerges (**??**.) If the values are located at the vertices and vertices are connected with those of the neighbours, then a different grid emerges (**??**).

3.1.1 Serialization of Grids

The abstractions of grids need to be serialized as data structures for the programming languages and for persisting them on storage systems. In a programming language, regular grids can usally be addressed by n-dimensional arrays. Thus, a 2D array can be used to store the data of a regular 2D longitude/latitude-based grid.

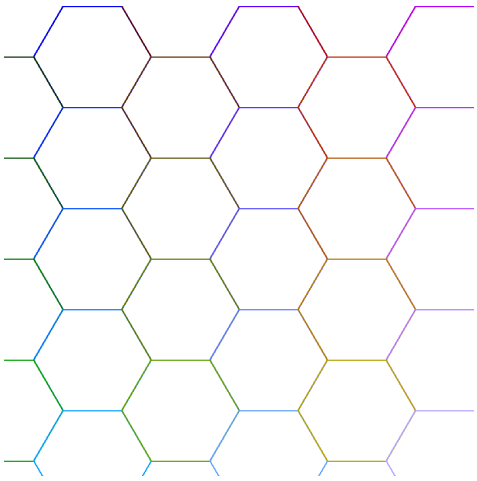
However, storing irregular grids is not so trivial. For example, a 1D array can be used to hold the data but then the index has to be determined. Staying with our 2D example, to map a 2D coordinate onto the 1D array, a mapping between the 2D coordinate and the 1D index has to be found. One strategy to provide the mapping are space-filling curves. These curves have the advantage that the indices to some extent preserve locality for points that are close together – which can be beneficial, as often operations are conducted on neighboring data (stencil operations, for example). A Hilbert curve is an example for one possible enumeration of a multi-dimensional space.

Hilbert curve is a continuous space-filing curve, that helps to represent a grid as n-dimensional-array of values. To visualize its behavior, a 2D grid is shown in **??**. In 2D, the basic element of the Hilbert curve is a square with one open side. Every such square has two end-points, and each of these can be the entry-point or the exit-point.

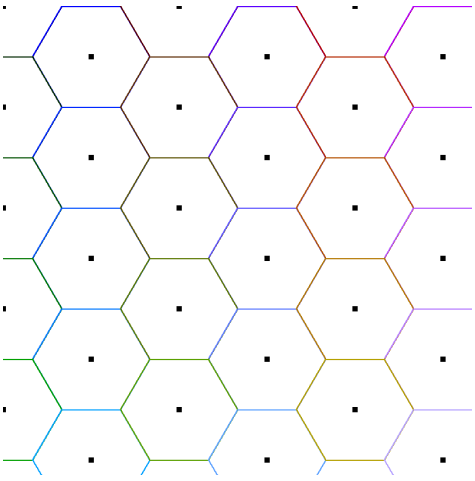
TODO: So, there are four possible varieties of open side. ... varieties are completely different mathematical objects ;-

So, there are four possible variations of an open side. A first order Hilbert curve consists of one basic element. It is a 2x2 grid. The second order Hilbert curve replaces this element by four (smaller) basic elements, which are linked together by three joins (4x4 grid). Every next order repeats the process by replacing each element by four smaller elements and three joins (8x8 grid). On the **??** is represented 5th level Hilbert curve for the 256x256 data, that is mapped to 32x32 grid.

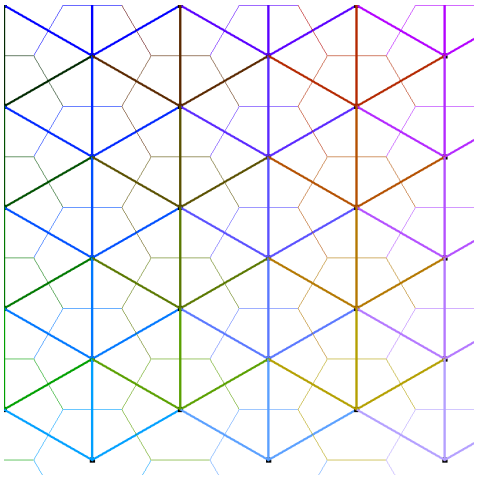
The characteristics of a Hilbert curve can be extended to more than two dimensions. The first step in the figure can be wrapped up in as many dimensions as is needed and the points/neighbours will be always saved.



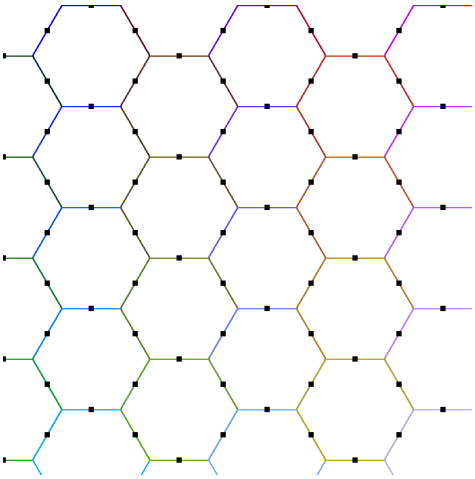
(a) Empty hexagonal grid



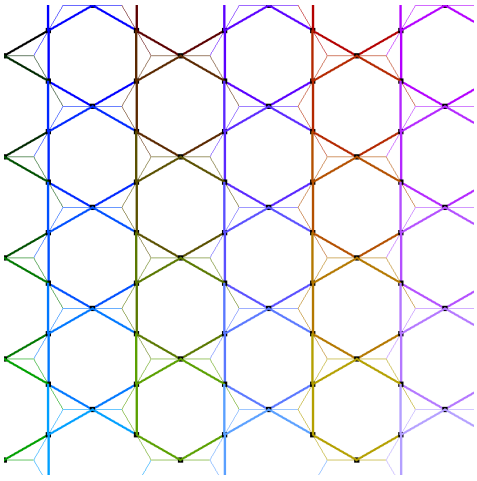
(b) Hexagonal grid with data at the cell centers



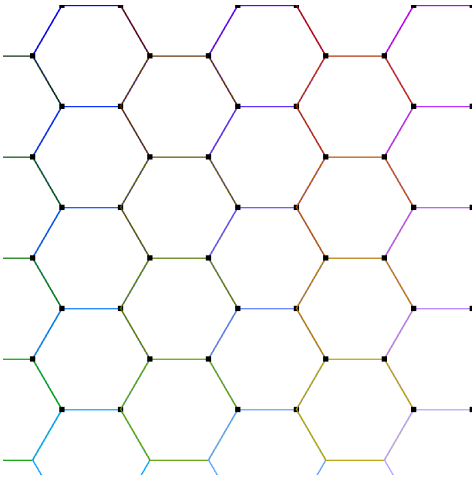
(c) Hexagonal grid with data at the cell's centers, connected neighbours



(d) Hexagonal grid with data on the edges

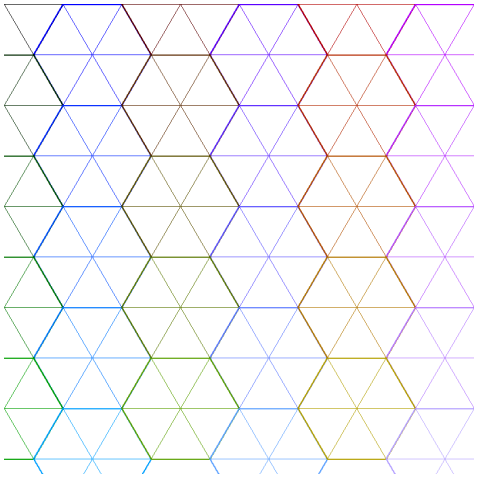


(e) Hexagonal grid with data on the edges, connected neighbours

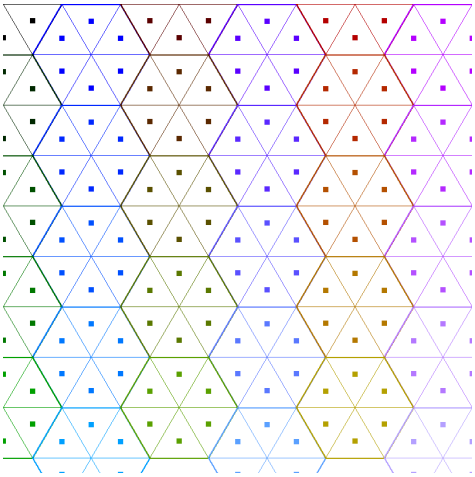


(f) Hexagonal grid with data at the vertices / connected neighbours

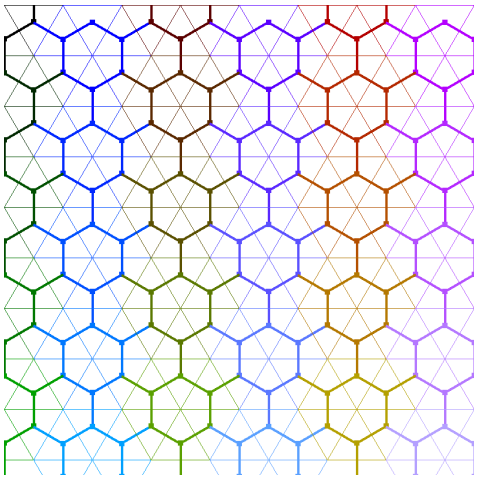
Figure 3.2: Hexagonal grid



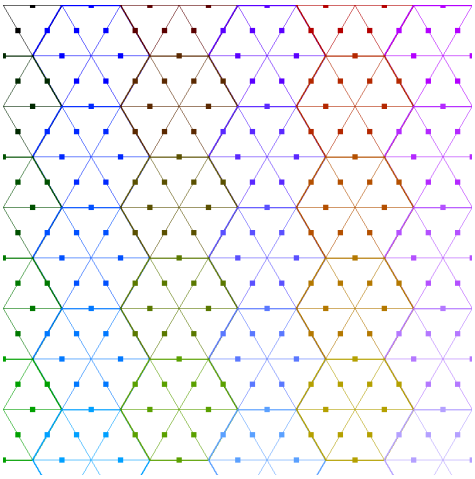
(a) Empty triangular grid



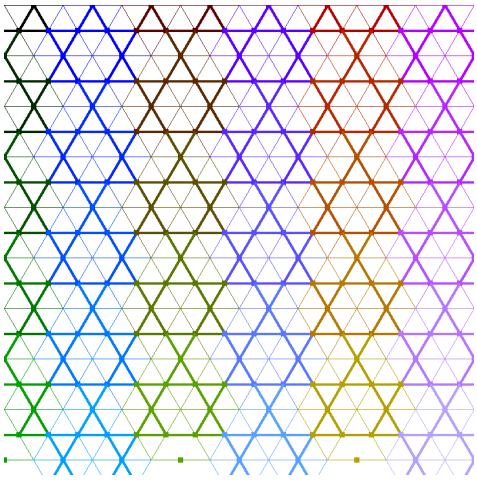
(b) Triangular grid with data at the cell centers



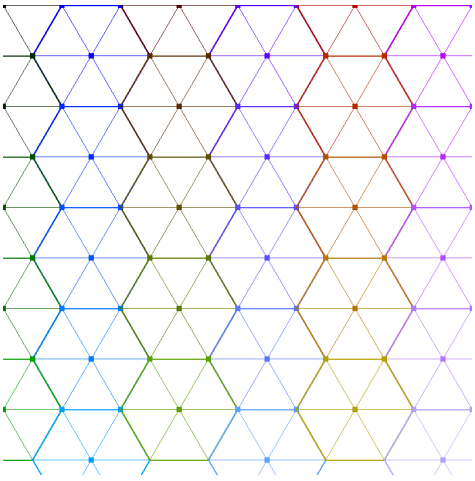
(c) Triangular grid with data at the cell centers, connected neighbours



(d) Triangular grid with data on the edges



(e) Triangular grid with data on the edges, connected neighbours



(f) Triangular grid with data on the vertices / connected neighbours

Figure 3.3: Triangular grid

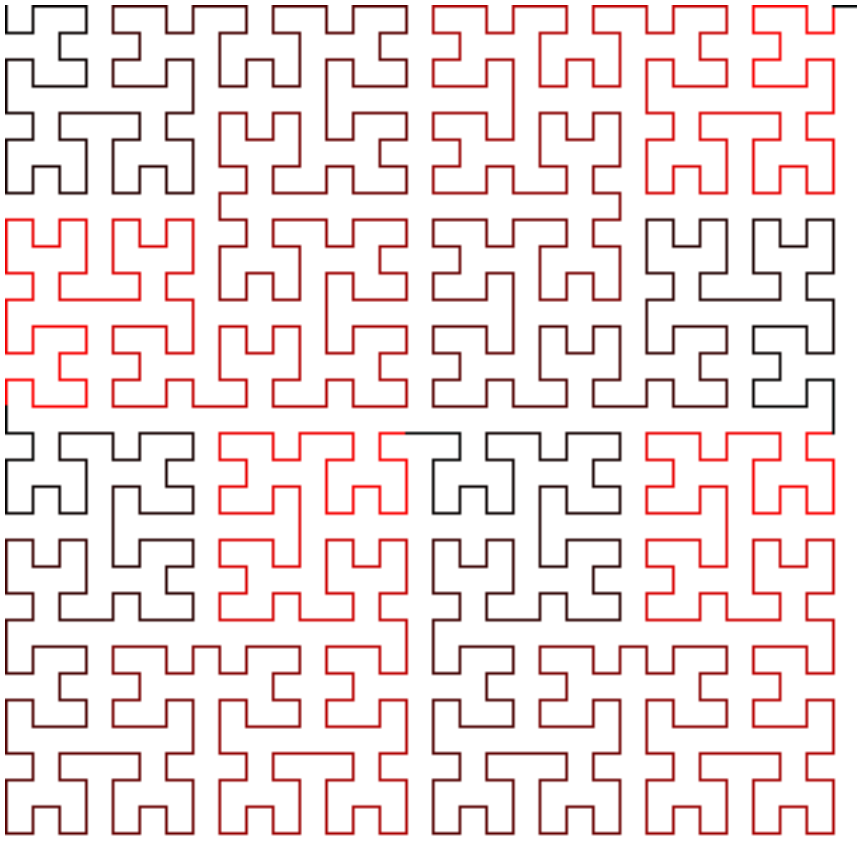


Figure 3.4: Hilbert fitting curve

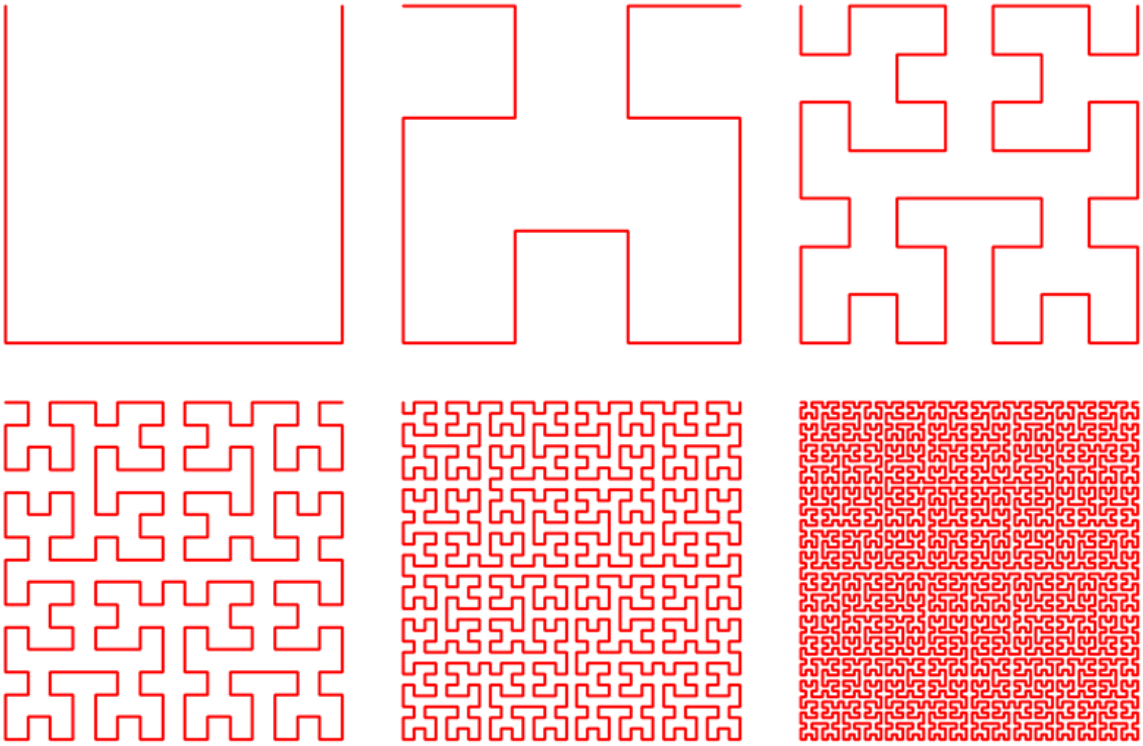


Figure 3.5: Hilbert fitting curve

Considerations when serializing to storage systems

TODO: JJ - What is meant here?

When serializing a data structure to a storage system, in essence this can be done similarly than in main memory. The address space exported by the file API of a traditional file system considers the file to be an array of bytes starting from 0. This is quite similar to the 1D structure from main memory. However, a general purpose language (GPL) uses variable names to point to the data in this 1D address space. A GPL offers means to access even multi-dimensional data easily. The user/programmer does not need to know the specific addresses in memory; addresses are calculated on within the execution environment or code of the application.

TODO: JJ - should we expand further on this? If so, I should add some diagrams... (or alternatively references)

The main concern here is consecutive or stride access through the array; if the programmer wishes the application to loop through a given dimension of the array, memory locations would be addressed which may not be close to each other in memory, thus leading to cache misses and hence poorer performance. The generalisation is the stride, which specifies steps through the different dimensions of the array (e.g. incrementing both dimensions of a 2D array, thus walking along the "diagonal"). Another special case is where the programmer needs to process the whole array, which would be done most efficiently by stepping through all the memory locations incrementally[1], whereas looping over the dimensions and incrementing them one at a time requires more calculation and may lead to inefficient memory access with cache misses if not done correctly[2].

TODO: problematic, as they = ? as they are implicitly known by the code and relatively defined by the execution environment of the application in form of stack and heap.

When storing data from memory directly on persistent media, then the original source code is necessary to understand this data. Similarly, the interpretation of the bytes in the data must be same when reading it back, thus, the byte order and size of the datatypes of the machine reading the data must be identical to those of the machine that wrote it. Floating point numbers must be encoded in the same byte formats. Since this is not always given, it threatens the longevity of our precious data, by hindering the portability and reusability of the data.

Therefore, portable data formats have been developed that allow to serialize and deserialize data regadless of the machine's architecture. To allow correct interpretation of a byte array, the library implementing the file format must know the data type the Bytes represent. This information must be stored besides the actual bytes representing the data to allow later reading and interpretation. From the user perspective, it is useful to also store further metadata describing the data. For instance, a name and description of the contained information. This eases not only debugging but also allows other applications to

[1] Assuming the whole array is stored in contiguous memory, as it is in these simple examples.

[2] Fortran historically stores 2D arrays in column-major order, whereas C and most other languages used in science store data in row-major order.

Name	Fullname	Version	Developer
GRIB1	GRIdded Binary	1	World Meteorological Organization
GRIB2	GRIdded Binary	2	World Meteorological Organization
NetCDF3	Network Common Data Form	3.x	Unidata (UCAR/NCAR)
NetCDF4	Network Common Data Format	4.x	Unidata (UCAR/NCAR
HDF4	Hierarchical Data Format	4.x	NCSA/NASA
HDF4-EOS2	HDF4-Earth Obseving System	2	
HDF5	Hierarchical Data Format	5.x	NCSA/NASA
HDF5-EOS5	HDF5-Earth Obseving System	5	

Table 3.1: Parallel data formats

read and process data in a portable way. File formats that contain this kind of semantical and structural metadata are called **self-describing file formats**.

Developers using a self-describing file format have to use an API to define the metadata. Such a format may support arbitrary complex data types, which implies that some kind of data description framework must be part of the API for the file format. See **??** for more information about data description frameworks.

3.2 File formats

Generally, parallel scientific applications are designed in such a way, they can solve complicated problems faster when running on a large number of compute nodes. This is achieved by splitting a global problem into small pieces and distributing it over the compute nodes; this is called domain decomposition. After each node has computed a local solution, they can be aggregated to one global solution. This approach can decrease time-to-solution considerably.

I/O makes this picture more complicated, especially when data is stored in one single file and is accessed by several processes simultaneously. In this case, problems can occur, when several processes access the same file region, e.g., two processes can overwrite the data of each other, or inconsistencies can occur when one process reads, while another writes. Portability is another issue: When transferring data from one platform to another, the contained information should still be accessible and identical. The purpose of I/O libraries is to hide the complexity from scientists, allowing them to concentrate on their research.

Some common file formats are listed in the **??**. All of these formats are portable (machine independent) and self-describing. Self-describing means, that files can be examined and read by the appropriate software without the knowledge about the structural details of the file. The files may include additional information about the data, called “metadata”. Often, it is textual information about each variable’s contents and units (e.g.,”humidity” and ”g/kg”) or numerical information describing the coordinates (e.g., time, level, latitude, longitude) that apply to the variables in the file.

GRIB is a record format, NetCDF/HDF/HDF-EOS formats are file formats. In contrast to record format, file formats are bound to format specific rules. For example, all variable names in NetCDF must be unique. In HDF, although, variables with the same name are allowed, they must have different paths. No such rules exist for GRIB. It is just a collection of records (datasets), which can be appended to the file in any order.

GRIB-1 record (aka, ’message’) contains information about two horizontal dimensions (e.g., latitude and longitude) for one time and one level. GRIB-2 allows each record to contain multiple grids and levels for each time. However, there are no rules dictating the order of the collection of GRIB records (e.g, records can be in random chronological order).

TODO: relate to chapter 4? "data description frameworks"

Finally, a file format without parallel I/O support, but still worth to mention, is CSV (comma-separated values). It is special due to its simplicity, broad acceptance and support by a wide range of applications. The data is stored as plain text in a table. Each line of the file is a data record. Each record consists of one or more fields, that are separated by commas (hence the name). The CSV file format is not standardized. There are many implementations that support additional features, e.g., other separators and column names.

3.2.1 NetCDF4

NetCDF4 with Climate Forecast (CF) metadata and GRIB evolved to the de-facto standard formats for convenient data access for the scientists in the domain of NWP and climate. For convenient data access, it provides a set of features, for example, metadata can be used to assign names to variables, set units of measure, label dimensions, and provide other useful information. The portability allows data movement between different possibly incompatible platforms, which simplifies the exchange of data and facilitates communication between scientists. The ability to grow and shrink datasets, add new datasets and access small data ranges within datasets simplifies the handling of data a lot. The shared file allows to keep the data in same file. Unfortunately, the last feature conflicts with performance and efficient usage of the state-of-art HPC. The files, which are accessed simultaneously by several processes, cause a lot of synchronisation overhead which slows down the I/O performance. Synchronization is necessary to keep the data consistent.

The rapid development of computational power and storage capacity, and slow development of network bandwidth and I/O performance in the last years resulted in imbalanced HPC systems. The application use the increased computational power to process more data. More data, in turn, requires more costly storage space, higher network bandwidth and sufficient I/O performance on storage nodes. But due to imbalance, the network and I/O performance are the main bottlenecks. The idea is, to use a part of the computational power for compression, adding a little extra latency for the transformation while significantly reducing the amount of data that needs to be transmitted or stored.

Before considering a compression method for HPC, it is a good idea to take a look at the realization of parallel I/O in modern scientific applications. Many of them use the NetCDF4 file format, which, in turn, uses HDF5 under the hood.

3.2.2 Typical NetCDF Data Mapping

?? gives an example for scientific metadata stored in a NetCDF file. Firstly, between Line 1 and 4, a few dimensions of the multidimensional data are defined. Here there are longitude, latitude with a fixed size and time with a variable size that allows to be extended (appending from a model). Then different variables are defined on one or multiple of the dimensions. The longitude variable provides a measure in "degreees east" and is indexed with the longitude dimension; in that case the variable longitude is an 1D array that contains values for an index between 0-479. It is allowed to define attributes on variables, this scientific metadata can define the semantics of the data and provide information about the data provenance. In our example, the unit for longitude is defined in Line 7. Multidimensional variables such as `sund` (Line 45) are defined on an 2D array of values for the longitude and latitude over various timesteps. The numeric values contain a scale factor and offset that has to be applied when accessing the data; since the data is here stored as short values, it should be converted to floating point data in the application. The `_FillValue` indicates a default value for missing data points.

Finally, global attributes such as indicated in Line 54 ff. describe that this file is written with the NetCDF-CF schema and its history describes how the data has been derived / extracted from original data.

Listing 3.1: Example NetCDF metadata

```
1  dimensions:
2    longitude = 480 ;
3    latitude = 241 ;
4    time = UNLIMITED ; // (1096 currently)
5  variables:
6    float longitude(longitude) ;
7      longitude:units = "degrees_east" ;
8      longitude:long_name = "longitude" ;
9    float latitude(latitude) ;
10     latitude:units = "degrees_north" ;
11     latitude:long_name = "latitude" ;
12   int time(time) ;
13     time:units = "hours since 1900-01-01 00:00:0.0" ;
14     time:long_name = "time" ;
15     time:calendar = "gregorian" ;
16
17   short t2m(time, latitude, longitude) ;
18     t2m:scale_factor = 0.00203513170666401 ;
19     t2m:add_offset = 257.975148205631 ;
20     t2m:_FillValue = -32767s ;
21     t2m:missing_value = -32767s ;
22     t2m:units = "K" ;
23     t2m:long_name = "2 metre temperature" ;
24   short sund(time, latitude, longitude) ;
25     sund:scale_factor = 0.659209863732776 ;
26     sund:add_offset = 21599.6703950681 ;
27     sund:_FillValue = -32767s ;
28     sund:missing_value = -32767s ;
29     sund:units = "s" ;
30     sund:long_name = "Sunshine duration" ;
31
32 // global attributes:
33     :Conventions = "CF-1.0" ;
34     :history = "2015-06-03 08:02:17 GMT by grib_to_netcdf-1.13.1:
       ↪ grib_to_netcdf /data/data04/scratch/netcdf-atls14-
       ↪ a562cefde8a29a7288fa0b8b7f9413f7-lFD4z9.target -o /data/data04/
       ↪ scratch/netcdf-atls14-a562cefde8a29a7288fa0b8b7f9413f7-CyGl1B.nc -
       ↪ utime" ;
35 }
```

3.3 Typical Workflows

3.3.1 NWP

TODO: UC: ask for DWD Weather use cases; ....

WUC1: Incoming Stream of Observations

satellites radar weather stations ships

WUC2: Pre-Processing

insufficient sampling makes preprocessing necessary so models can be intialised correctly

WUC3: Now Casting (0-6h)

directly inffered from satellite data and weather stations
most importantly extrapolation of radar echos
usually for warnings

WUC4: Numeric Model Forecasts (0-10+ Days)

1. Read-Phase to intialise simulation
2. periodic snapshots (write) for time evolution

WUC5: Post-Processing

nowcasting: multi sensor integration classification ensembles impact models
model: statistical interpretation model-combination
generation of GRIB files as services to customers of weather forecasts

WUC6: Visualisation

of many variables available in a simulation only a view are read and visualised
timeseries

3.3.2 Characteristics of Workload Mix

The systems are shared so it is distinguished between emergent system behaviour and workload of individual applications.

How are the shares for different workloads on the system?
e.g. 10% of applications are CUC1, 20% WUC1, ...

We assume that in principle this mix changes over time, but a specialized data centre makes only sense as long some things are somewhat stable...

TODO: Discuss with DKRZ/App team, there should be a paper or something as the workload mix is also considered for procurements

E.g. DKRZ...regular load at every point in time is about 20 GByte/s

3.3.3 Climate

CUC1: Writing Data from a Parallel Program

We have P processes utilizing PPN cores per node. Iterative program. Asynchronous communication and I/O ? Every I iterations, a subset of memory capacity C_I should be persisted. After T iterations, the program terminates and writes C_T capacity for a snapshot. This process may be repeated, restarting from a snapshot to simulate 100 or 1000 of years of climate.

What people do right now: - store AND Keep every checkpoint, may be used for later analysis and for re-computation. - Some people only keep every 10th of a checkpoint (as the costs to recompute 9 other checkpoints is less than storing 10).

ICON I/O coordinators, write out groups of variables.. variables at different intervals individual variables are not yet parallel

CUC2: Post-Processing Data

A scientist reads a time series produces from multiple runs of the parallel program (see **??**). He/she may want to read a subset of data points (i.e., an area of interest) across all time steps.

CUC3: Post-Processing: Partial CDO

TODO: What kind of user behaivor is common? Is the same user, applying the same CDO to many many records?

CUC4: Visualisation

TODO: are the challenges for climate visualisation different from weather?

vtk paraview
of many variables available in a simulation only a view are read and visualised
timeseries average e..g temperature anomaly
expensive cloud visualisation..

3.4 Use cases from a data access perspective

TODO: JL: Decide where this fits best.

Chapter 4

Background and Related Work

This chapter gives an overview to related work in the area of I/O research for HPC and Big Data. Then, alternative approaches for defining data structures within scientific middleware are introduced.

4.1 Exascale I/O

The advent of exascale computing is exacerbating the gap between computational performance (measured in FLOPS) and the capability of the storage system to feed data into the computational pipelines at a sufficient speed (measured in GB/s). Indeed, today's storage infrastructures still heavily rely on spinning disk drives, which performance have not scaled at the same pace of the compute components. Along with the computing power also grows the amount of data that can be generated/analysed, and thus the size of the corresponding datasets in the storage system. This aspect also affects the complexity of scientific workflows that nowadays need to account for the generation (simulation codes or sensor), analysis (extraction of meaningful information), and finally sharing of large datasets with the research community. All these requirements have been driving many different research projects and efforts to build efficient I/O libraries. Weather and Climate communities have used some of these libraries for years and have also relied on them to decouple data view at the application level (multidimensional arrays) from data representation in the storage backend (one dimensional array). NetCDF [**?**] and GRIB [**?**] are the I/O libraries of choice for the Climate and Weather communities respectively. The NetCDF library relies on additional I/O service libraries to work. In particular NetCDF4 exploits the HDF5 [**?**] library to organise as well as to read/write data from/to the file system. We will explore some ESDM relevant aspects of these libraries in the rest of this section. The HDF5 library is modular and allows for different implementations of the I/O transfer mechanism, as well as for different I/O optimisations.

The Distributed Shared Memory driver, HDF5dsm [**?**], takes advantage of the HDF5 modularity in the Virtual File Layer (VFL) to transparently redirect data from disks to staging nodes that will later use this data for post processing analysis, thus making the building of computing pipelines simpler and more efficient (reduced total time to solution). On the same line the Adaptable I/O System, ADIOS [**?**], provides an interface independent I/O middleware in which specific I/O transports (e.g. HDF5, NetCDF, POSIX) and optimisations (N-1, N-M, N-N) are encoded in a separate XML file. The ADIOS code at the application level remains fairly simple, just declaring what variables should be written and how big they are. All the details about how these variables are effectively transfered are hidden in the XML file, making the middleware adaptable. Similarly to HDF5dsm, ADIOS provides mechanisms to stage data in apposite nodes for later indexing construction, compression, and/or post processing. Unlike the HDF5dsm driver, which uses the same familiar HDF5 API at the user level, ADIOS requires modifications of the application source, making its adoption in

legacy codes not feasible. Besides data staging and indexing the library also supports data provenance and advanced techniques for data mining to drive, e.g., effective pre-fetching. Nevertheless, the ADIOS library still relies on the legacy POSIX-IO interface and does not give the user the flexibility to distribute his data to different backends according to data characteristics.

The Fast Forward I/O project [**?**], from the U.S. Department of Energy (DOE), has built an Exascale ready storage infrastructure called Distributed Application Object Storage (or DAOS) based on a Lustre file system with object storage extensions (as the storage backend) and the HDF5 library as the data format interface for manipulating/storing/retrieving data. In this context, the HDF5 library has been extended with a Virtual Object Layer (VOL) to support the new object storage capabilities offered by the extended Lustre [**?**] and to support new NVM technologies to burst buffer data at intermediate nodes (Burst Buffer I/O Nodes) before writing it to Lustre. Additionally, a VOL plug-in for the Parallel Log-structured File System (PLFS) has been developed to allow HDF5 to store data on PLFS [**?**] using alternative mappings [**?**]. Dong et al [**?**] have used the HDF5 VOL to build the Scientific Data Service (SDS) framework, adapting the layout of stored data to the specific I/O pattern of applications retrieving it. Similarly to Fast Forward I/O the EC funded SAGE (percipient StorAGe for Exascale data centric computing) [**?**] project aims at building a Big Data Extreme Computing (BDEC) storage infrastructure based on the Mero object store [**?**] and new 3D-Xpoint memory technology. One of the most interesting features of the SAGE system is the ability to offload parts of the computation to the storage nodes and retrieve the results of the computation afterwards, thus minimising data movement and energy consumption. The SAGE project is also exploring advanced analytics techniques on the storage system performance metadata, opening the possibility for automatic tuning of the storage parameters.

The Dynamic Exascale Entry Platform Extended Reach (DEEP-ER) project is building an extreme scale platform based on the BeeGFS file system and the integration of NVM and Network Attached Memory (NAM) technologies in the storage hierarchy [**?**]. In DEEP-ER exascale level fault tolerance is achieved by combining the Scalable Checkpoint Restart (SCR) [**?**] buddy checkpointing capabilities withe the SIONlib library, which takes care of storing the checkpoint data using a unified file format. At the data format library level the HDF group is also working on the ExaHDF5 project to provide efficient parallel I/O handling for the movement of massive amounts of data and extending the HDF5 API with a query API that can be used by other tools to selectively extract information from datasets [**?**].

All the works mentioned so far solve some of the well known I/O pain points typically found when moving to extreme scale. Nevertheless, none of these works has addressed the problem of format independent data access. Every I/O library can only access data that has been stored using that particular format and cannot, on the other hand, understand the format of other libraries. This makes the use of data in scientific workflows cumbersome, since data may need to be stored in one format and then transformed to be fed to the next stage of processing (e.g. store a dataset into a HDFS file system to be processed by a Hadoop cluster). Sharing also becomes very complex since data has to be converted to the target format before it can be used, causing a waste of compute and storage resources. The ESD middleware addresses this problem and takes advantage of the lessons learned by other projects to optimise I/O performance at the same time.

4.2 Data Description Frameworks

Many application developers rely on data description frameworks or libraries to manage datatypes[1]. Different libraries and middlewares provide mechanisms to describe data using

[1] A datatype is a collection of properties, all of which can be stored on storage and which, when taken as a whole, provide complete information for data conversion to or from the datatype.

basic types and to construct new ones using dedicated APIs. Datatypes are provided as a transparent conversion mechanism between internal representation (as data is represented in memory) and external representation (how data is transmitted over the network or saved to permanent storage). This section gives an overview of datatypes provided by different software packages. Starting from existing middlewares' datatype definitions, we will propose a list of basic datatypes to be supported by the ESD middleware.

4.2.1 MPI

The Message Passing Interface supports derived datatypes for efficient data transfer as well as compact description of file layouts (through file views). MPI defines a set of basic datatypes (or type class) from which more complex ones can be derived using appropriate data constructor APIs. Basic datatypes in MPI resemble C atomic types as shown in **??**.

Datatype	Description
MPI_CHAR	this is the traditional ASCII character that is numbered by integers between 0 and 127
MPI_WCHAR	this is a wide character, e.g., a 16-bit character such as a Chinese ideogram
MPI_SHORT	this is a 16-bit integer between -32,768 and 32,767
MPI_INT	this is a 32-bit integer between -2,147,483,648 and 2,147,483,647
MPI_LONG	this is the same as MPI_INT on IA32
MPI_LONG_LONG_INT	this is a 64-bit long signed integer, i.e., an integer number between -9,223,372,036,854,775,808 and 9,223,372,036,854,775,807
MPI_LONG_LONG	same as MPI_LONG_LONG_INT
MPI_SIGNED_CHAR	same as MPI_CHAR
MPI_UNSIGNED_CHAR	this is the extended character numbered by integers between 0 and 255
MPI_UNSIGNED_SHORT	this is a 16-bit positive integer between 0 and 65,535
MPI_UNSIGNED_LONG	this is the same as MPI_UNSIGNED on IA32
MPI_UNSIGNED	this is a 32-bit unsigned integer, i.e., a number between 0 and 4,294,967,295
MPI_FLOAT	this is a single precision, 32-bit long floating point number
MPI_DOUBLE	this is a double precision, 64-bit long floating point number
MPI_LONG_DOUBLE	this is a quadruple precision, 128-bit long floating point number
MPI_C_COMPLEX	this is a complex float
MPI_C_FLOAT_COMPLEX	same as MPI_C_COMPLEX
MPI_C_DOUBLE_COMPLEX	this is a complex double
MPI_C_LONG_DOUBLE_COMPLEX	this is a long double complex
MPI_C_BOOL	this is a _Bool
MPI_INT8_T	this is a 8-bit integer
MPI_INT16_T	this is a 16-bit integer

MPI_INT32_T	this is a 32-bit integer
MPI_INT64_T	this is a 64-bit integer
MPI_UINT8_T	this is a 8-bit unsigned integer
MPI_UINT16_T	this is a 16-bit unsigned integer
MPI_UINT32_T	this is a 32-bit unsigned integer
MPI_UINT64_T	this is a 64-bit unsigned integer
MPI_BYTE	this is an 8-bit positive integer
MPI_PACKED	-

Table 4.1: MPI Datatypes

Datatypes from Table **??** can be used in combination with the constructor APIs shown in Table **??** to build more complex derived datatypes.

Datatype Constructor	Description
MPI_Type_create_hindexed	create an indexed datatype with displacement in bytes
MPI_Type_create_hindexed_block	create an hindexed datatype with constant-sized blocks
MPI_Type_create_indexed_block	create an indexed datatype with constant-sized blocks
MPI_Type_create_keyval	create an attribute keyval for MPI datatypes
MPI_Type_create_hvector	create a datatype with constant stride given in bytes
MPI_Type_create_struct	create a MPI datatype from a general set of datatypes, displacements and block sizes
MPI_Type_create_darray	create a datatype representing a distributed array
MPI_Type_create_resized	create a datatype with a new lower bound and extent from an existing datatype
MPI_Type_create_subarray	create a datatype for a subarray of a regular, multidimensional array
MPI_Type_contiguous	create a contiguous datatype

Table 4.2: MPI Derived Datatypes Constructors

Before they can be actually used, MPI derived datatypes (created using the constructors in Table **??**) have to be committed to memory using the `MPI_Type_commit` interface. Similarly, when no longer needed, derived datatypes can be freed using the `MPI_Type_free` interface. Unlike data format libraries, MPI does not provide any permanent data representation (MPI-IO can only read/write binary data), therefore derived datatypes are not used to store any specific data format on stable storage and are instead used only for data transfers or file layout descriptions.

An example code for defining a derived data structure for a structure is shown in **??**. The structure is defined in Lines 5-9. The function in Lines 12-22 registers this datatype in MPI. This requires to define the beginning and end of each array, its type and size. Once a datatype is defined, it can be used as memory type in subsequent operations. In this example, on process sends this datatype to another process (Line 38 and Line 45).

Since MPI datatypes were initially designed for computation and, thus to define memory

regions, it does not offer a way to name the data structures.

Listing 4.1: Example construction of an MPI datatype for a structure

```
#include <stdio.h>
#include <string.h>
#include <mpi.h>

typedef struct student_t_s {
    int id[2];
    float grade[5];
    char name[20];
} student_t;

/* create a type for the struct student_t */
void create_student_datatype(MPI_Datatype * mpi_student_type){
    int   blocklengths[3] = {2, 5, 20};
    MPI_Datatype types[3] = {MPI_INT, MPI_FLOAT, MPI_CHAR};
    MPI_Aint     offsets[3];

    offsets[0] = offsetof(student_t, id) ;
    offsets[1] = offsetof(student_t, grade);
    offsets[2] = offsetof(student_t, name);
    MPI_Type_create_struct(3, blocklengths, offsets, types,
    ↪ mpi_student_type);
    MPI_Type_commit(mpi_student_type);
}

int main(int argc, char **argv) {
    const int tag = 4711;
    int size, rank;

    MPI_Init(&argc, &argv);
    MPI_Comm_size(MPI_COMM_WORLD, &size);
    MPI_Comm_rank(MPI_COMM_WORLD, &rank);

    MPI_Datatype mpi_student_type;
    create_student_datatype(& mpi_student_type);

    if (rank == 0) {
        student_t send = {{1, 2}, {1.0, 2.0, 1.7, 2.0, 1.7}, "Nina
    ↪ Musterfrau"};
        const int target_rank = 1;
        MPI_Send(&send,   1, mpi_student_type, target_rank, tag,
    ↪ MPI_COMM_WORLD);
    }
    if (rank == 1) {
        MPI_Status status;
        const int src=0;
        student_t recv;
        memset(& recv, 0, sizeof(student_t));
        MPI_Recv(&recv,   1, mpi_student_type, src, tag, MPI_COMM_WORLD,
    ↪  &status);
        printf("Rank %d: Received: id = %d grade = %f student = %s\n",
    ↪ rank, recv.id[0], recv.grade[0], recv.name);
    }

    MPI_Type_free(&mpi_student_type);
    MPI_Finalize();

    return 0;
}
```

4.2.2 HDF5

HDF5 is a data model, library, and file format for storing and managing data. It supports an unlimited variety of datatypes, and is designed for flexible and efficient I/O and for high volume and complex data. HDF5 is portable and is extensible, allowing applications to evolve in their use of HDF5. The HDF5 Technology suite includes tools and applications for managing, manipulating, viewing, and analyzing data in the HDF5 format. Like MPI, HDF5

also supports its own basic (native) datatypes reported in **??**.

Datatype	Corresponding C Type
H5_NATIVE_CHAR	char
H5_NATIVE_SCHAR	signed char
H5_NATIVE_UCHAR	unsigned char
H5_NATIVE_SHORT	short
H5_NATIVE_USHORT	unsigned short
H5_NATIVE_INT	int
H5_NATIVE_UINT	unsigned int
H5_NATIVE_LONG	long
H5_NATIVE_ULONG	unsigned long
H5_NATIVE_LLONG	long long
H5_NATIVE_ULLONG	unsigned long long
H5_NATIVE_FLOAT	float
H5_NATIVE_DOUBLE	double
H5_NATIVE_LDOUBLE	long double
H5_NATIVE_B8	8-bit unsigned integer or 8-bit buffer in memory
H5_NATIVE_B16	16-bit unsigned integer or 16-bit buffer in memory
H5_NATIVE_B32	32-bit unsigned integer or 32-bit buffer in memory
H5_NATIVE_B64	64-bit unsigned integer or 64-bit buffer in memory
H5_NATIVE_HADDR	haddr_t
H5_NATIVE_HSIZE	hsize_t
H5_NATIVE_HSSIZE	hssize_t
H5_NATIVE_HERR	herr_t
H5_NATIVE_HBOOL	hbool_t

Table 4.3: HDF5 Native Datatypes

Besides the native datatypes just described, the library also provides so called standard datatypes, architecture specific datatypes (e.g., for i386), IEEE floating point datatypes, and others. Datatypes can be built or modified starting from the native set of datatypes using the constructors listed:

Datatype Constructor	Description
H5Tcreate	Creates a new datatype of the specified class with the specified number of bytes. This function is used only with the following datatype classes: H5T_COMPOUND, H5T_OPAQUE, H5T_ENUM, H5T_STRING. Other datatypes, including integer and floating-point datatypes, are typically created by using H5Tcopy to copy and modify a predefined datatype

H5Tvlen_create	Creates a new one-dimensional array datatype of variable-length (VL) with the base datatype. The base type specified for the VL datatype can be any HDF5 datatype, including another VL datatype, a compound datatype, or an atomic datatype
H5Tarray_create	Creates a new multidimensional array datatype object
H5Tenum_create	Creates a new enumeration datatype based on the specified base datatype, dtype_id, which must be an integer datatype
H5Tcopy	Copies an existing datatype. The returned type is always transient and unlocked. A native datatype can be copied and modified using other APIs (e.g. changing the precision)
H5Tset_precision	Sets the precision of an atomic datatype. The precision is the number of significant bits
H5Tset_sign	Sets the sign property for an integer type. The sign can be unsigned or two's complement
H5Tset_size	Sets the total size in bytes for a datatype
H5Tset_order	Sets the byte order of a datatype (big endian or little endian)
H5Tset_offset	Sets the bit offset of the first significant bit
H5Tset_fields	Sets the locations and sizes of the various floating-point bit fields. The field positions are bit positions in the significant region of the datatype. Bits are numbered with the least significant bit number zero

Table 4.4: HDF5 Datatypes Constructors

HDF5 constructs allow the user a fine grained definition of arbitrary datatypes. Indeed, HDF5 allows the user to build a user-defined datatype starting from a native datatype (by copying the native type) and then change datatype characteristics like sign, precision, etc, using the supported datatype constructor API. However, since these user defined data types have often no direct representation on available hardware, this can lead to performance issues.

TODO: concept of dataspaces?

4.2.3 NetCDF

NetCDF as important alternative popular within the climate community. NetCDF provides a set of software libraries and self-describing, machine-independent, data formats that support

Datatype	Description
NC_BYTE	8-bit signed integer
NC_UBYTE	8-bit unsigned integer
NC_CHAR	8-bit character byte
NC_SHORT	16-bit signed integer
NC_USHORT	16-bit unsigned integer
NC_INT	32-bit signed integer
NC_UINT	32-bit unsigned integer
NC_INT64	64-bit signed integer
NC_UINT64	64-bit unsigned integer
NC_FLOAT	32-bit floating point
NC_DOUBLE	64-bit floating point
NC_STRING	variable length character string

Table 4.5: netCDF Atomic External Datatypes

the creation, access, and sharing of array-oriented scientific data. In the version 4 of the library (NetCDF4), the used binary file representation is HDF5. Like MPI and HDF5, NetCDF also defines its own set of atomic datatypes as shown in **??**

Similarly to HDF5 and MPI, in addition to the atomic types the user can define its own types. NetCDF supports four different user defined types:

1. **Compound**: are a collection of types (either user defined or atomic)
2. **Variable Length Arrays**: are used to store non-uniform arrays
3. **Opaque**: only contain the size of each element and no datatype information
4. **Enum**: like an enumeration in C

Once types are constructed, a variables of the new type can be instantiated with nc_def_var. Data can be written to the new variable using nc_put_var1, nc_put_var, nc_put_vara, or nc_put_vars. Data can be read from the new variable with nc_get_var1, nc_get_var, nc_get_vara, or nc_get_vars. Finally, new attributes can be added to the variable using nc_put_att and existing attributes can be accessed from the variable using nc_get_att.

Table **??** shows the constructors provided to build user defined datatypes.

Type	Constructor	Description
Compound	nc_def_compound	create a compound datatype
	nc_insert_compound	insert a name field into a compound datatype
	nc_insert_array_compound	insert an array field into a compound datatype
	nc_inq_{compound,name,...}	learn information about a compound datatype
Variable Length Array	nc_def_vlen	create a variable length array
	nc_inq_vlen	learn about a variable length array
	nc_free_vlen	release memory from a variable length array
Opaque	nc_def_opaque	create an opaque datatype
	nc_inq_opaque	learn about an opaque datatype

Enum	`nc_def_enum`	create an enum datatype
	`nc_insert_enum`	insert a named member into an enum datatype
	`nc_inq_{enum,...}`	learn information about an enum datatype

Table 4.6: NetCDF Datatypes Constructors

4.2.4 GRIB

GRIB is a library and data format widely used in whether applications. It differs from previously described libraries in the sense that it does not define datatypes that can be used to store a wide range of different data. Instead, GRIB very clearly defines the sections of every – so called – message which is the unit sent across a network link or written to permanent storage. Every message in GRIB has different sections, each of which contains some information. GRIB defines the units that can be represented in every message and thus does not specifically need datatypes to represent them. But a library supporting these formats needs to know the mapping from a message type to the contained data fields and their data types. In that sense, GRIB is not a self-describing file format but requires code to defines the standardized content. GRIB messages contain 32-bit integers that can be scaled using a predefined data packing schema. The scaling factor is stored along with the data inside the message.

TODO: Do we cover grib in the prototype? If yes this should be similar in detail to HDF5 etc.

TODO: Relate to chapter 3, "File formats"

4.3 Big Data Storage

In the context of Big Data, there are many (typically Java based) technologies that address storing and processing of large quantities of data.

4.3.1 Hadoop File System

The Hadoop File System (HDFS) is a distributed file system that is designed to work with commodity hardware. It provides fault tolerance via data replication and self healing. One limitation of its design is its consistency semantics which allows concurrent reads of multiple processes but only a single writer (WORM Model, write-once-read-many). The data stored on HDFS are replicated in the cluster to ensure fault tolerance. HDFS ensures data integrity and can detect loss of connectivity when a node is down. The main concepts:

- Datanode: nodes that own data;
- Namenode: node that manages the file access operations.

The supported interfaces and languages are: HDFS Java API, WebHDFS REST API and libhdfs C API, as well as a Web interface and CLI shells. Security is based on file authentication (user identity). However, HDFS accepts network protocols like Kerberos (for users) and encryption (for data). HDFS was designed in Java for Hadoop Framework, therefore any machine that supports Java is able to run it. It can be considered as the "source" of many processing systems (especially in the Apache eco-system) like Hadoop and Spark. All data stored into HDFS become "sequencefile" files. However, its sub-optimal performance on high-performance storage and assumption to work on cheap hardware makes it no optimal choice for HPC environments. Therefore, many vendors support HDFS adapters on top of high-performance parallel file systems such as GPFS and Lustre.

4.3.2 HBase

Apache HBase is a distributed, scalable, big data store. HBase is an open-source, distributed, versioned, non-relational database modeled after Google's "Bigtable: A Distributed Storage System for Structured Data" by Chang et al. [R19]. Similarly to Bigtable, which leverages the distributed data storage provided by GFS, Apache HBase provides Bigtable-like capabilities on top of Hadoop and HDFS (https://hbase.apache.org/). It can be used to perform random, realtime read/write access to large volumes of data. HBase's goal is the hosting of very large tables, on top of clusters of commodity hardware. As in the case of HDFS this is not the optmital choise for HPC infrastructures.

4.3.3 Hive

Apache Hive is a data warehouse software facilitating reading, writing, and managing of large datasets residing in distributed storage using SQL (https://hive.apache.org/). It is built on top of Apache Hadoop and provides:

- tools to enable easy access to data via SQL, allowing data warehousing tasks such as ETL, reporting, and data analysis;
- access to files stored directly in Apache HDFS or in other data storage systems like Apache HBase;
- support for query execution via various frameworks (i.e. Apache Tez, Apache Spark or MapReduce).
- a convenient SQL interface (including many of the later 2003 and 2011 features for analytics) to this data. This allows users to explore data using SQL at a fine grain scale by accessing data stored on the file system.

4.3.4 Drill

Drill [2] also provides an SQL interface to existing data. Similar to Hive existing data can be adjusted, but in the case of Drill, data may be stored on various storage backends such as simple JSON file, on Amazon S3, or MongoDB.

4.3.5 Alluxio

Alluxio [3] offers a scalable in-memory file system. An interesting feature is that one can attach (mount) data from multiple (even remote) endpoints such as S3 into the hierarchical in-memory namespace. It provides control to the in-memory data, for example, to trigger a flush of dirty data to the storage backend and an interface for pinning data in memory (similar to burst buffer functionality). Data stored on Alluxio can be used on various big data tools.

4.3.6 MongoDB

The MongoDB[4] is an open-source document database. Its architecture is high-performant and horizontally scalable for clusters systems. MongoDB offers a rich set of interfaces, e.g., RESTful access, C, Python, Java.

The data model of MongoDB provides three levels:

[2] `https://drill.apache.org`
[3] `https://www.alluxio.com/docs/community/1.3/en/`
[4] `https://docs.mongodb.com/`

- Database: follows our typical notion; permissions are defined on the database level.
- Document: This is a BSON object (binary JSON) – consisting of subdocuments with data. An example as JSON is shown in **??**. Each document has the primary key field: _id. The field must be either manually set or it will be automatically filled.
- Collection: this is like a table of documents in a database. Documents can have individual schemas. It supports indices on fields (and compound fields).

To access data, one has to know the name of a database (potentially secured with a username and password), collection name. All documents within the collection can be searched or manipulated with one operation.

In the example of **??**, it would also be possible to create one document for each person and use the $_id$ field with a self-defined unique ID such as a tax number.

Listing 4.2: Example MongoDB JSON document

```
"_id" : ObjectId("43459bc2341bc14b1b41b124"),
"people" : [ # subdocuments:
    { "name" : "Max", "id" : 4711, "birth" : ISODate("2000-10-01")},
    { "name" : "Lena", "id" : 4712, "birth", ... }
  ]
```

MongoDB's architecture uses sharding of document keys to partition data across different servers. Servers can be grouped into replica sets to provide high availability and fault tolerance.

Query documents A query document is a BSON document that is used to search all documents of a collection for data that matches the defined query. The example in **??** specifies documents that contain the subdocument people with an id field that is bigger than 4711. Complex queries can be defined. In combination with indices on fields, MongoDB can search large quantities of documents quickly.

Listing 4.3: Example MongoDB Query document

```
{ "people.id" : { $gt : 4711 } }
```

TODO: if we use mongo for metadata storage, maybe a short piece about why its particular suitable for this? also: relate to chapter 6 "mapping with mongo"

4.4 Community Specific Work: Climate / Weather

The highly scalable data storage project

TODO: Is this supposed to be related work section?

TODO: Also what tools are considered here? sionlib, FTI, some of the formats developed at dkrz/mpi or stfc earlier?

Chapter 5

Design

Goal of this chapter is to describe the requirements for an earth-system data (ESD) middleware and the resulting user experience. This leads to the high-level design for interfaces the application developers use to access and manipulate data stored using the ESD middleware.

5.1 Requirements

Based on software engineering techniques, the requirements are grouped into functional requirements and non-functional requirements. Additionally, we add specific requirements from the perspective of the data centers. We provide a list with a short explanation and importance for the NWP/climate communities.

5.1.1 Deployment Requirements

The ESD demonstrator...

TODO: Deployment Requirements

5.1.2 Functional Requirements

TODO: Functional Requirements, only list right now

- Handling of scientific/structural metadata as first class citizen
- Appending data ...
- Reading data ...
- Searching for data based on the scientific metadata
- Exporting/Importing data to/from standardized file formats
- Exposing data via existing interfaces
- Accessing data via POSIX tools

- Exposing data via the WWW
- Access control
- System wide configuration of available storage resources
- Notifications, Publish Subscribe

5.1.3 Access Control

TODO: changed acces control to section, though it is a function requirement, the headline nesting has to be discussed for this section

Actors

There are three actors who can interact with the ESIWACE storage resource:

- Unprivileged Users
- Priviliged Users
- Administrators

In the following, we use the term object to refer primarily to something with equivalent semantics to an HDF file. A more fine grained object access will also be available via the HDF API exposed by the service.

Unprivileged User

An unprivileged user is someone who has only readonly access. These users can:

- navigate content, using faceted browse against public tags, so what does that require?
- list all (public) tags to which they have access.
- given a tag, list all tags carried by objects with the first tag.
- given a list of tags, list all tags carried by objects with all members of that list,
- given a tag list, list all objects with the union set of all those tags.
- retrieve any visible object from the list of objects presented by any tag list.
- interact with any visible object via the HDF API limited to read only operations.

Privileged Users

A privileged user is someone who has CRUD access to (their) content within the archive as well as all the abilities of an unprivileged user applied to their own content. They can:

- create, retrieve, update, and delete content within prescribed quotas.
- control access to their objects (see below)
- assign tags to objects

- navigate both public or (own) private tags.

Controlling access:

- Users can create "group" identifiers, and associate user identifiers with that group.
- They must themselves be a member of any group they create.
- They can add/remove any other user identifiers known to them to that group.
- How users find the identifiers of other users is not defined here.
- If they use the identifier "public" for a group, then users in this group (who may also include the special identifier "anonymous"), then users in this group will have readonly access to these objects.
- Users can assign any group identifer of which they are a member to any object they create. In doing so, they make "their" objects into "shared" objects (except for the public group as defined above, where they are simply making the object readonly to that group).
- Any user with "shared" access has the same privileges for that object as the original owner, except that of modifying or removing the group tag.
- (With the This means they can delete, update, and retreive the object. Of course deleting it does disassociate the group tag in a
- Users can list the groups of which they are members, and list the members of any of those groups.

(Note that this usage of group is not identical to the concept of UNIX groups, not least, because users control their definition.)

Adminstrators

Can

- Start and Stop the service.
- Access all data held by all priviledged users
- Manage privileged users:
- Create, Update, Delete Users
- Allocate Quotas
- Retreive usage information
- Configure the layout of content in the service against available storage resources.
- Migrate content within the storage resources (a process that might temporarily disable user access).
- Configure any required compute, cache, and network services.

Consequences

- HDF API needs to reflect some sort of access token to limit some users to readonly operations.
- All operations need to be logged, in particular, all creations, retrievals, and updates discriminated by users.

5.1.4 Non-functional Requirements

TODO: What is a non functional requirement? If it does not meet the performance its not fit to fill the function.. if the data is not reliable.. it neglects a the function to ensure data safety?

- Efficiency
- Utilization of heterogeneous storage
- Fault-tolerance
- High-availability
- Data integrity
- Easy to maintain
- Deployable on existing storage technology
- Support for BigData storage (e.g., HDFS)

Access patterns: basic data transfer, data access (reference to D4.1 on tier 0 storage, burst buffers, HSM?). Note that this section covers only *read* access to data; write semantics would be different.

Data access presumes the ability to:

- identify the file or object which contains interesting data, possibly by consulting meta-data catalogues, and eventually obtaining an identifier for the object and an endpoint through which it can be accessed;
- to ask to have the object made available
  - This step may require obtaining permissions to access the data, and/or acceptance of a licence;
  - The object may need to be brought up from lower tier storage (e.g. tertiary);
  - For some more advanced uses of data, endpoints may also be dynamically allocated.
- Either transfer the whole file, or,
- Identify sections of interest in the file/object and remotely access those sections.

5.2 Data Model

The data model describes how data is represented at the application level and supports several **logical objects** that might be linked together. References between the objects allow re-use and reduce the storage footprint.

Container A container contains references to one or multiple variables together with their metadata. Similar to the concept of views in databases, it is a virtual entity. It can be considered as a handle to a single NetCDF/HDF5 file that contains all the data needed for the application run. It is usually constructed by the middleware based on the requests of the application at runtime but can also be saved to provide convenient access to the data. This allows scientists to define the scope for data access dynamically.

For example, during one runtime a scientist may request to read data of one particular variable created by different models to compare the quality of these models. Next time, a time series of various variables are analyzed.

The notion of these dynamic containers allows users to abstract from the regular file system semantics that required them to determine the mapping from logical data structures to files and directories manually.

TODO: Are the examples stubs? Can we collpase it into a single paragraph?

Variable We partition a multidimensional variable dynamically based on the participating processes across the available storage devices. A variable covers a domain such a 3D data space with the dimensions of 100x50x10. Potentially, a subset of the domain is replicated and stored in alternative representations. We call one piece of the variable a **shard**.

Metadata Metadata describes the semantics and technical aspects of data further. Internally, we distinguish between scientific metadata, that contains all the information about the data relevant for domain scientists, and technical metadata that is used for internal data management purpose.

Uses can set arbitrary scientific metadata onto variables and containers. Metadata can refer to other variables or provide the actual scope of the data. Metadata attached to a container will be automatically embedded into newly created variables.

Shard A shard is a piece (subdomain) of a variable that is written by exactly one process. Shards are also the entities that are distributed across available storage systems. For example, a variable is split into two shards, one is stored in a parallel file system, while the other is placed on the object storage.

TODO: Picture. Is the image fine? Caption is missing..

5.2.1 Identifying Resources

Searching for objects In many cases, metadata of logical objects can easily be searched by specifying query. API calls will be translated to the internal metadata storage. An example query is shown in **??**.

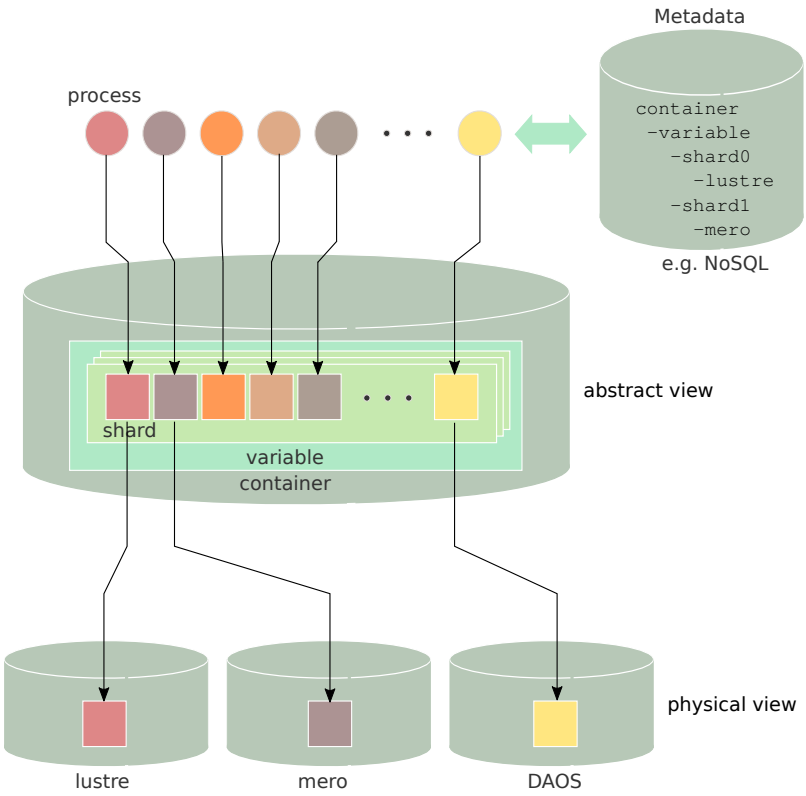


Figure 5.1
;

Listing 5.1: Advanced object search

```
{ $and : [
  { "domain.longitude": { "$gt" : -40, "$lt" : -10 } },
  { "domain.latitude" : { "$gt" : 90}},
  { "domain.time"     : { "$gt" : datetime(2001, 11, 01)} },
  { "info.model.name" : "my model" },
  { "info.environment.system" : "mistral" }
]}
```

An issue are external references, such as the longitude and latitude variables in our example, as they use an index to reference to the specific value indirectly. One solution to enable search of such variables would be for users to define metadata for a bounding box that will always be included in the metadata and searchable.

Additionally, for convenience of the model, different variables may use alternative coordinate systems or simply use the same metadata field for different meanings. Luckily in the

domain of NWP/climate, there are conventions such as CF that define the metadata.

Identifying all objects that depend on a specific document requires to query the reference field and check if the document ID is part of it.

Sealed objects Data becomes immutable, once the container is closed... Useful for referencing to the objects, checksums can then be created and persisted.

TODO: Just thoughts so far?

Deleting of objects When a logical object is about to be deleted, it has to be checked if it is referenced by any other document. Since the dependencies are stored in each document and this array is indexed, it can be quickly checked if there are any dependencies. If so, the object cannot be deleted, or the data must be embedded into all referencing documents. Since this would multiply the storage space for the objects, it is usually favorable to keep the data and the references.

I/O Modes The initial version of ESD will support only two modes of access for the data of a variable: 1) write-only append mode; 2) read-only access. It is not allowed that different independent applications write to the same logical variable.

5.3 Implications for Developers and End-Users

For exiting applications the middleware aims to be transparent, albeit not expecting optimal performance exploitation for every use case.

5.3.1 MPI Parallel Applications

This section describes the implications on a existing parallel application that uses one of the supported interfaces such as NetCDF4/HDF5. The semantics of the API calls will change slightly but mostly in a way that is backwards compatible.

Open

Traditionally, when opening a file with NetCDF the filename specifies the location, i.e., an URI where the data resides on a storage system. We change the notion of the file name to be the descriptor for a virtual container (virtual container descriptor). The virtual container can be composed of multiple URIs to integrate different variables into one virtual environment on the fly. Thus, from the reader's perspective it does not matter if data of a model is split into one or multiple physical files; upon read, all those files can be loaded together as if they would already exist in one logical file.

The ESD does not support concurrent read and write scenarios, it is allowed to either write data or to read it (see Epoch).

TODO: extend?

Concurrency semantics

In general, the system is designed for coordinated parallel applications that access data independently of each other. That means, within one parallel (MPI) application, some kind of coordination happens to allow the shared access to containers, variables and shards.

Data sharing between independent applications is intended to happen after applications completed. It is not allowed that multiple currently running parallel applications write data to the same variable. This is considered to be sufficient for most scenarios, e.g., a model produces some output, once the model completed, the produced data is post-processed. If an application uses the write-only mode to append data to a variable, the concurrent read-only access of the same or independent applications will not immediate see the new data. Instead, ESD ensures that all changes to the data (and metadata) becomes atomically visible when the logical container is closed by the application. At this point, all the new data becomes immediately visible to the readers.

Especially in NWP applications it is useful to access intermediate results and start post-processing as soon as possible to minimize the overall delay. To support this scenario, we provide the concept of Epoch-Semantics to the developers (see below).

Writing data follows the expected semantics for writes but when multiple writers write data to the same variable coordinates, i.e., they overwrite data, the result is undefined. In fact, applications in which multiple processes write to the same region are considered to be wrong.

Reading data that is available in the container but has been written by a previously terminated application will be returned in the correct fashion. Reading data that has been written by the same application (i.e., reads after writes) should not happen, as users should use means of communication inside the application to prevent this kind of access pattern. If such a fine-grained update of data is necessary, again the Epoch-semantics must be used.

Epoch Semantics

An epoch is an instant in time chosen by the parallel application. Starting with Epoch 0, all processes of the parallel application participating in the I/O have to agree on moving to a new epoch. This will finalize the outstanding write requests, make the changes durable and publish the information about new data to other applications that registered to read this data. Writing data to a variable that existed previously will overwrite the data of previous Epochs. Similarly, if a variable is opened for read/write access, the same application may now read the data from a previous Epoch. Thus, a read request will never return the data of the current epoch but the merged perspective of all previous Epochs.

Thus, the Epoch semantics is similar to the semantics of transactions but application wide and only one transaction can be active at a given time.

If a parallel applications overwrites data stored in a previously by another application written variable, then this is handled similarly to a new Epoch.

TODO: Figure necessary

5.3.2 Implementing Workflows via Virtual Containers

This section will demonstrate how multiple post-processing applications can process data that is created from a simulation. Firstly, we consider the case in which each job in this worklow is run after the previous job completed.

Simulation large parallel application

```
Virtual container (Input)\footnote{The virtual container provides a hierarchical namespac
- input for simulation
-- grid
--- var 1
--- var 2
-- configuration.xml

Virtual container (Output)
time series
- var 3
- var 4


Post-processing
few processes

Virtual container (Input)
time series
- var 3

Output
- var 5 (time series)
- var 6: single number
```

TODO: Figure necessary

When moving to the Epoch semantics, a time step can be considered as an Epoch. Whenever one is completed, the post-processing can ingest the new data and process it.

The mapping of the variable name and the actual content is based on the scientific metadata.

An example configuration file for setting up the virtual containers is shown in:

TODO: Configuration file

5.3.3 POSIX Tools

5.3.4 Next Generation Applications

The ESD middleware could satisfy the need of future applications e.g. for in situ/in transit workflows virtualisation parallel in time?

5.3.5 Data Services

TODO: AS this is in the design chapter, there is many references to related work, but it is not immediately clear what the resulting requirements are.

Data Processing

One of the common themes of research in storage has been to bring specific types of processing closer to the storage. Obvious first steps in storage-side processing is checking basic data integrity ("did we get all the bytes, and in the right order?" as well as updating metadata systems ("we have a new file"). The next steps were to automate metadata extraction in a file-type dependent way, so a process would recognise the file type and apply file-specific checks on its structural integrity ("is this a well-formed HDF5/PDF/Word document"). These types of checks are widely used in production infrastructures.

The next obvious extension to this was twofold: one proposed direction would bring higher level features closer to the device, to remove the load on filesystems. For example, in conventional magnetic hard drives one originally had to know the number of cylinders, sectors, and so on, but LBA vastly simplified supporting hard drives without having to reconfigure the operating system (or file system), and in a similar vein, hard drives can do their own checking and management of bad blocks.

TODO: It may be worth investigating this further, as LFTS could provide similar benefits for tape? or are those benefits irrelevant for the purposes we are discussing here?

A research extension by SNIA proposed drives that provided direct object storage with metadata, thus bringing some of the work required by the filesystem into the storage device; the flip side is that the interface would not be full POSIX but more like an object store. This particular research, however, never came to production, and we must conclude that there were not sufficient requirements for it to have a market.

The other direction was in storage management services that would implement programmable storage side workflows, such as iRODS. Generally microservices would need to be added in order to support new file types and change the rules, but the system would be customisable to provide relatively simple workflows which were used to manage metadata but could be extended to do server side processing.

Grids provide similar features but in a different way, as there is technically no difference between storage-side processing and user-side processing: they are done using the same mechanisms, but essentially in different data centres. WLCG operates a tiered model where data is generated at a Tier 0 centre, copied to Tier 1 centres whence it is copied to Tier 2s (these should not be confused with data centre tiers which are essentially the other way around.) Raw processing of data – what we would call storage side processing – is done at the Tier 0 and 1s, with no end user access at all. End user analysis of data would happen at Tier 2s and 3s, and data which need archiving would be copied back to the local T1 [diagram]

An alternative approach is to treat the storage as a basic service – like an object store, typically – and let higher level workflow engines manage the writing and processing of the data as a part of a (loosely coupled) workflow. This approach would also work well provided it can get notifications back from the store. Indeed, CASTOR2 was originally written on top of LSF, but LSF was removed (around 2010?) in favour of a bespoke "transfer manager" when it was found that original versions of CASTOR didn't scale well with the WLCG workloads10.

(A novel approach is to treat the data structure transparently within the applications, without the requirement to integrate the data management in the application; see future directions

TODO: JJ: check what is available

Staging and Caching

State of the art: ERADAT, the BNL extension of (90PB) HPSS [Yu]. The main question is whether every recall can always be automated or at which stage would it need operator intervention in order to me maximally efficient?

State of the art – NERSC CORI (2017?) [Dosanjh], NVRAM burst buffers; 28 PB secondary disk (Lustre) supporting data placement "close" to the CPU; thus a further staging process is required anyway (cf. diagram). Also JASMIN's PANASAS with 15PB (using ET for temporarily staging data in order to free up fast disk)

Note the follow-up requirement on meta-operations on data, e.g. staging, pinning.

TODO: NUMA?

Is it necessary to generate models for this? Is it useful? For example, the allocation of drives to each individual user community, and optionally prioritising recalls.

Could the same be applied for other types of file operations that are scheduled, such as replication and integrity checking. It would be useful to do opportunistic operations: if a tape (resp. collection) is mounted (resp. fetched/unpacked), take the opportunity to act on other collections (files/objects), instead of waiting for their scheduled operation.

Chapter 6

Architecture Description

We use the 4+1 view model of architecture according to Philippe Kruchten.

To meet the aforementioned challenges, we have designed the Earth System Data (ESD) middleware, which:

1. *can understand application data structures and scientific metadata, letting us expose the same data via different APIs;*
2. *can map data structures to different storage backends with different performance characteristics based on site specific performance model configuration;*
3. *can yield best write performance via optimized data layout schemes that utilize elements from log-structured file systems;*
4. *can provide relaxed access semantics, tailored to scientific data generation for independent writes, and;*
5. *includes a FUSE module which will provide backwards compatibility through existing file formats with a configurable namespace based on scientific metadata.*

Together these allow storing small and frequently accessed data on node-local storage, while serializing multi-dimensional data onto multiple storage backends – providing fault-tolerance and performance benefits for various access patterns at the same time. Compact-on-read instead of garbage collection will additionally optimize and replicate the data layout during reads via a background service. Additional tools allow data import/export for exchange between sites and tape archives.

6.1 Logical View

The general architecture of the ESD middleware is shown in **??**.

TODO: extend?, small guide to the chapter?

6.1.1 Interface

This represents the API exposed to other libraries and users. The API will be independent from the specific I/O backend used to store the data and will support structured queries to perform complex data selections in the variables. The API will be able to support the complex workflows of future applications, while backward compatibility with legacy codes will be provided through a FUSE module. The definition of the ESD interface is out of the scope of this document.

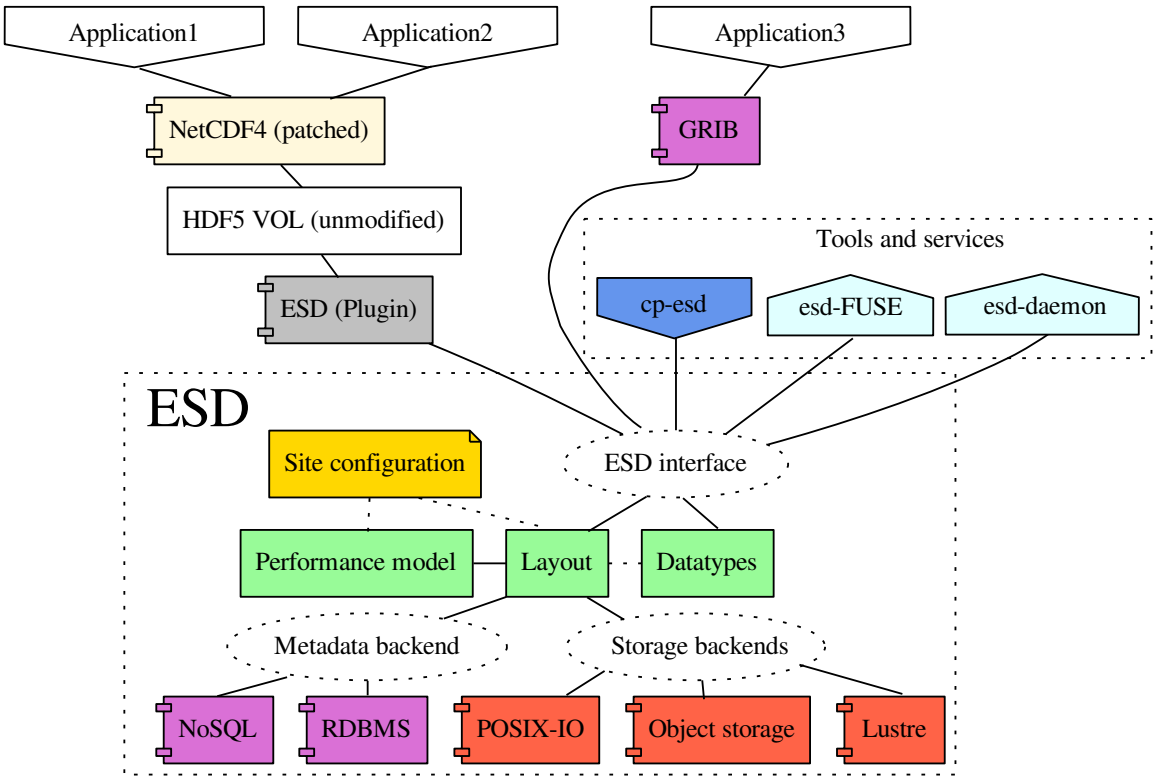


Figure 6.1: Architecture overview

6.1.2 Datatype Component

The datatype component will provide native ESD middleware datatypes that can be used by users or other libraries to describe data points inside variables. We follow the approach pursued by the HDF5 library, that is, we provide a set of native datatypes and a basic set of datatype constructors that can be used to build custom derived datatypes.

TODO: What type of datatypes are supported? In principle the ESD can support NetCDF and HDF5 by providing the same datatypes as for HDF5. Are these enough? Need to be extended to support some other type?

.

6.1.3 Layout Component

The layout component allows the middleware to store pieces of data on different backends depending on specific site configuration contained in the performance model. The layout component in this case takes responsibility for generating additional technical metadata describing data placement and for storing it in the appropriate metadata backend (i.e. MongoDB). A more detailed description of what technical metadata is, is given in the rest of this section.

Adaptive Data Mappings

The typical storage mapping for scientific data format libraries is the file (linear sequence of bytes organized following the POSIX file system representation, i.e. inodes and blocks). Information is translated into a linear array of bytes in the file system using appropriate schemas. Since the data model defined by the data format library can contain complex hierarchies and attributes besides raw data, the final file will contain additional scientific metadata that needs to be accessed using the POSIX-IO data interface (e.g. `read()` and

`write()`) instead of the file metadata interface (e.g. `stat()`, `lookup()`). This makes the storage model adopted by data format libraries incompatible with the typical parallel file system organization, in which metadata and data are splitted apart and assigned to different services for optimal performance. Additionally, new storage system paradigms have emerged in the last years in which files are organized in a flat namespace (e.g. object storage), removing the restrictions imposed by metadata operations like namespace traversal of POSIX file systems. Hierarchical organization can be still achieved using other dedicated storage representations like key-value stores, at the expense of reduced POSIX semantic.

There is therefore a necessity for more flexible data mappings that can take advantage of an increasing number of storage and backend alternatives, improving access efficiency at the same time. There are two different approaches to this problem: the first is to develop a new data mapping schema for every storage backend. This is the solution adopted by the HDF5 library (through the virtual file and the virtual object layers) in which multiple storage backends can be employed by developing a corresponding plugin that contains the right mapping schema. The obvious limitation of this solution is that once the user has selected a certain backend for a file, this cannot be changed without migrating the whole file to another backend. The second approach is more flexible and consists in making the storage backend selection adaptive. This has the advantage of enabling backend storage selection on the fly depending upon the type of data being stored or a set of user/system defined parameters (e.g. list of data placement policies satisfying certain requirements of quality of service).

Our proposed solution is to integrate the adaptive data mappings capabilities just discussed in the layout component of the ESD middleware. The middleware will understand the scientific metadata of other relevant data format libraries and will be able to use multiple storage backends at the same time to store and retrieve different pieces of data. To support multiple formats the datatype component in the ESD middleware will expose a datatype interface similar to the one available in HDF5 (described in Section **??**). Additionally, the middleware will add significant metadata to be used in the life cycle management and sharing of data. This can include semantic metadata describing which data is needed and how it is going to be used, the required level of resilience, etc. In this context, some metadata can be automatically generated by the middleware or defined by the user and passed to the middleware through an apposite interface (that will be part of the ESD exposed interface).

Legacy codes will have access to data using a familiar POSIX interface exported through an ESD FUSE module. The FUSE module will communicate with the ESD middleware to access data and export it to users using a namespace representation. The mapping schema definition for mapping data between the storage representation and the namespace will be done later in the project.

Another important aspect to consider when talking about adaptive data mappings is the storage tiering, that is, how many levels of storage there are in the system. Historically, HPC applications have relied on parallel file systems as first tier to store and retrieve their data. Besides the parallel file system, most high-end clusters have a second level of archival storage to which data is migrated from the parallel file system using a hierarchical storage manager. Nowadays compute nodes have access to local storage (typically a block device formatted with a local file system) and with the emergence of new storage technologies, such as non-volatile memories, permanent byte addressable memory. The ESD middleware should be able to exploit these local storage resources to implement prefetching strategies (read patterns) and burst buffers (write patterns).

Performance Model

The performance model characteristics are not clear at this point in time. Nevertheless, we have defined this component in the ESD middleware so we can use performance parameters

Metadata	Field	Creation	Description
Domain	M	Auto	The subdomain this data covers from the variable
Type	M	Auto	The (potentially derived) datatype of this shard
Variable	M	Auto	The ID of the variable this data belongs to
Storage	M	Auto	The storage backend used and its options
References	M	Auto	A list of objects that are referenced by this data
Sealed	M	Auto	A sealed shard is read-only

(a) For a shard

Metadata	Field	Creation	Description
Domain	M	Manual	Describes the overall domain
Type	M	Manual	The (potentially derived) datatype
Info	M	Manual	The scientific metadata of this document
References	M	Auto	A list of objects that are referenced by this data
Permissions	M	Auto/Manual	The owner and permissions
Shards	M	Auto	The list of shard objects for this variable
Sealed	M	Auto	A sealed variable is read-only

(b) For a variable

Metadata	Field	Creation	Description
Owner	O	Manual	The owner of this file view (see the permission model)
Info	O	Manual	Additional scientific metadata for this view
Directory	O	Manual	Contains a mapping from names to variables
Environment	O	Automatic	Information about the application run
Permissions	M	Auto/Manual	The owner and permissions
References	M	Auto	A list of objects that are referenced by this data.

(c) For a container

Table 6.1: Excerpt of additional technical metadata

to drive data placement in the appropriate storage backend.

Technical Metadata

Besides scientific metadata, the dynamic mapping of data to storage backends requires further metadata that must be managed. To distinguish technical metadata from scientific metadata, an internal namespace is created. Relevant metadata is shown in **??** for shards, variables and containers, respectively.

Metadata can be optional (O) or mandatory (M), and either is created automatically or must be set manually via the APIs. Automatic fields cannot be changed. Some of the data can be automatically inferred if not set manually, but manual setting may allow further optimizations.

Some of the metadata is used on several places, for example, information about the data lineage might be used to create several output variables. In our initial implementation, the metadata is stored redundantly as this: 1) simplifies search; 2) enables us to restore data on corrupted storage systems by reading the metadata; 3) reduces contention and potentially false sharing of metadata. An implementation might decide to reduce this by utilizing a normalized schema.

References is the list of objects that are directly used by this object, e.g., other variables that are used to define the data further.

Example This example illustrates data of a predictive model could be stored on the system and the resulting metadata. The dimensionality of the underlying grid is fixed.

The application uses the following information to drive the simulation:

- Timerange: the simulated model time (from a starting datetime to the specified end)
- Longitude/Latitude: 1D data field with the coordinates [float]
- Temperature: Initial 2D field defined on (lon, lat)

A real model would use further parameters to estimate the temperature but these are sufficient to demonstrate the concepts. This information is either given as parameter to the simulation or read from an input (container). A mixture of both settings is possible.

The application produces the following output:

- Longitude/Latitude: 1D data field with the coordinates [float]
- Model time: the current datatime for the simulation
- Temperature: 2D field defined on (lon, lat, time) [float], containing the precise temperature on the coordinates defined by lon and lat for the given timestep
- AvgTemp: 1D field defined on (time) [float]; contains the mean temperature for the given time

Upon application startup, we create a new virtual container that provide links to the already existing input. In **??**, the metadata for the container is shown, after the application is started. We assume it has used the APIs to provide the information (input, output, scientific metadata). In this example, we explicitly define the objects used as input; it is possible to also define the input as an already existing container. It is also possible to define the input a-priori if the objectIDs are known / looked up prior application run. The intended output variables could be given with their rough sizes. This would allow the scheduler to pre-stage the input and ensure that there is enough storage space available for the output. The environment information is inferred to the info object but can be changed from the user.

TODO: How does this align with the use case chapter?

TODO: Do the examples deserve a clear seperation.. so that general abstractions and vague requirements hidden in a example are clearer?

Listing 6.1: JSON document describing the container

```
"_id" : ObjectId(".."),
"directory" : {
  "input" : {
    "longitude" : ObjectId(".."),
    "latitude" : ObjectId(".."),
    "temperature" : ObjectId("..")
   },
  "output" {
     "temperature" : ObjectId(".."),
     "avgTemp" : ObjectId("..")
   }
},
"info" : {
  "model" : { "name" : "my model", "version" : "git ...4711" },
  "experiment" : {
    "tags"        : ["simulation", "poisson", "temperature"]
    "description" : "Trivial simulation of temperature using a poisson
    ↪ process"
  },
},
"environment" : {
  "date"   : datetime(2016, 12, 1),
  "system" : "mistral",
  "nodes" : ["m[1-1000]"]
},
"permissions" : {
  "UID"   : 1012,
  "GID"   : 400,
  "group" : "w", # allows read also
  "other" : "r"
},
"references" : {
  [ all links to used object IDs from input / output ]
}
```

The metadata for a single variable is build based on the information available in the container and additional data provided by the user. An example for the temperature variable is shown in **??**. When describing the domain that is covered by the variable, there are two alternatives: 1) a reference to an existing variable is embedded and the minimum / maximum value is provided. This allows to reuse descriptive information as data has to be stored only once. Min and max describe the multidimensional index of the subdomain in the variable that is actually referenced; 2) data becomes embedded into the file. This option is used when the size of the variable is small.

An advantage of option 2) is that searches for data with a certain property do not require to lookup information in additional metadata.

Similarly, information about the data lineage (history) can originally be inferred from the objects linked in the directory mapping. The metadata of the referenced object must be copied, if the original object is removed.

Listing 6.2: JSON document for temperature

```
"_id" : ObjectId("<TEMPID>"),
"sealed" : true,
"domain" : [
    "longitude" : [ "min" : 0, "max" : 359999, "reference" : ObjectId("..") ],
    "latitude" : [ "min" : 0, "max" : 179999, "reference" : ObjectId("..") ],
    "time" : [ datetime(...), datetime(...), ... ]
  ],
"type" : "float",
"info" : {
  "convention" : "CF-1.0",
  "name" : "temperature",
  "unit" : "K",
  "long description" : "This is the temperature",
  "experiment" : {
    "tags"        : ["simulation", "poisson", "temperature"]
    "description" : "Trivial simulation of temperature using a poisson process"
  },
  "model" : { "name" : "my model", "version" : "git ...4711" },
  "directory" : {
  "input" : {
    "longitude" : ObjectId("<LONID>"),
    "latitude" : ObjectId("<LATID>"),
    "temperature" : ObjectId("<TEMPID>")
  }
  },
  "environment" : {
    "date"    : datetime(2016, 12, 1),
    "system" : "mistral",
    "nodes"  : ["m[1-1000]"]
  },
  "history" : [
    #The history for the inputs, if the data lineage must be embedded
    ObjectId(<LONID>) : [
      # Assume LONID does not exist any more
    ],
  ]
},
"permissions" : {
  "UID"  : 1012,
  "GID"  : 400,
  "group" : "w", # allows read also
  "other" : "r"
},
"references" : {
  [ all links to used object IDs ]
},
"shards" : [
  ObjectId(<SHARD1 ID>),
  # For a sealed object, the domains of its shards can optionally be embedded:
  { "reference" : ObjectId(<SHARD2 ID>), "storage" : ... , "domain" },
  ObjectId(<SHARD3 ID>),
  ObjectId(<SHARD4 ID>)
]
```

The variable is split into multiple shards; metadata for one of them is shown in **??**. Since we assume domain decomposition in the application, the longitude and latitude variables are now only partially stored in a shard. In the example, we assume two processes create one shard each and the surface of the earth is partitioned into four non-overlapping rectangles.

Listing 6.3: JSON document for a shard of the temperature variable

```
"_id" : ObjectId("<SHARD1 ID>"),
"sealed" : true,
"variable" : ObjectId("<TEMPID>"),
"type" : "float",
"domain" : {
    "longitude" : [ "min" : 0, "max" : 179999, "reference" : ObjectId("..") ],
    "latitude" : [ "min" : 0, "max" : 89999, "reference" : ObjectId("..") ],
    "time" : [ datetime(...), datetime(...), ... ]
  },
"storage" : {
    "plugin" : "pfs",
    "options" : {
      "path" : "/mnt/lustre/testdir/file1",
    },
    "serialization" : "row-major"
  },
"references : [
  ObjectId("<TEMPID>"),
  ObjectId(".."),
  ObjectId("..")
]
```

6.1.4 Data/Metadata Backend Drivers

A prototypical metadata backend will be realized using MongoDB. Advantages of using MongoDB are that it scales horizontally with the number of servers, provides fault-tolerance and that the document model supports arbitrary schemas.

TODO: stub

To illustrate the applied mapping, we use a subset of our NetCDF metadata described in **??**. The excerpt is given in **??**. The mapping of a single logical variable is examplarily described in

Listing 6.4: NetCDF metadata for one variable

```
dimensions:
  longitude = 480 ;
  latitude = 241 ;
  time = UNLIMITED ; // (1096 currently)
variables:
  float longitude(longitude) ;
    longitude:units = "degrees_east" ;
    longitude:long_name = "longitude" ;
  float latitude(latitude) ;
    latitude:units = "degrees_north" ;
    latitude:long_name = "latitude" ;
  int time(time) ;
    time:units = "hours since 1900-01-01 00:00:0.0" ;
    time:long_name = "time" ;
    time:calendar = "gregorian" ;
  short sund(time, latitude, longitude) ;
    sund:scale_factor = 0.659209863732776 ;
    sund:add_offset = 21599.6703950681 ;
    sund:_FillValue = -32767s ;
    sund:missing_value = -32767s ;
    sund:units = "s" ;
    sund:long_name = "Sunshine duration" ;

// global attributes:
    :Conventions = "CF-1.0" ;
    :history = "2015-06-03 08:02:17 GMT by grib_to_netcdf-1.13.1:
    ↪ grib_to_netcdf /data/data04/scratch/netcdf-atls14-
    ↪ a562cefde8a29a7288fa0b8b7f9413f7-lFD4z9.target -o /data/data04/
    ↪ scratch/netcdf-atls14-a562cefde8a29a7288fa0b8b7f9413f7-CyGl1B.nc -
    ↪ utime" ;
}
```

TODO: citations: WDCC, CERA

To simplify search and identify data clearly, data services such as the WDCC[TODO] and CERA[TODO], that offer data to the community, request scientists to provide additional metadata. Normally, such data is provided when the results of an experiment is ingested into such a database. Example metadata is listed in **??**. In existing databases, the listed metadata is split into several fields, e.g. an address and email for persons, for simplicity only a rough overview is given. Instead of encoding the history as a simple text field, it could indicate detailed steps including the arguments for the commands and versions and transformations to reproduce the data. This should include for each step, where and the time when it is performed, and the versions of software used.

It is easily imaginable that most of this information could be useful already when the data is created as it simplifies the search and data management on the online storage. Some of the data fields become only available after the initial data creation, e.g., the DOI. Potentially the data must be updated / curated after the data is created.

Mapping with MongoDB

Each object in the data model (container, variable, shard) becomes a collection with indices on certain fields. Multikey indices allow to index array fields such as the references.

Mapping with Mero

Metadata	Description
Project	The scientific project during which the data is created
Institute	The institution which conducted the experiment
Person	A natural person; could be a contact, running the experiment
Contact	Reference to person or consortium
DOI	A document object identifier; useful for identifying a data publication
Topic	Some information about the topic of the data / experiment
Experiment	Description of this particular experiment
History	A list with the history and transformations conducted with the data

Table 6.2: Excerpt of additional scientific metadata

TODO: add mero mapping description

Mero is an Exascale ready Object Store system developed by Seagate and built from the ground up to remove the performance limitations typically found in other designs. Unlike similar storage systems (e.g. Ceph and DAOS) Mero does not rely on any other file system or raid software to work. Instead, Mero can directly access raw block storage devices and provide consistency, durability and availability of data through dedicated core components. Like Ceph Mero provides a key-value store component for small data and metadata and an object storage for raw data.

The key-value store component in Mero can be used to keep track of containers, corresponding variables and shard inside them. For example, each container will be represented as index in Mero. Every index will have references to all the contained variables. Variable are also represented as indices and will contain variable metatada as well as references to shards. Shards in this case can be stored as different Mero objects or files in other storage backends.

6.1.5 Services

TODO:

6.1.6 Import/Export of Data

TODO:

6.2 Process View

TODO:

6.2.1 Services

TODO:

6.3 Physical View

TODO:

6.3.1 Deployment on DKRZ

TODO:

6.3.2 Deployment on STFC

TODO:

6.3.3 Deployment on CMCC

TODO:

6.4 Development View

TODO:

Chapter 7

Summary and Conclusions

The ESD aids the interests of stakeholders: developers have less burden to provide system specific optimizations and can access their data in various ways. Data centers can utilize storage of different characteristics. We expect a working prototype with the core functionality within the next year. Following work will implement and fine-tune the cost model and layout component and provide additional backends.

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