Data Systems at Scale in Climate and Weather

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CENTRE OF EXCELLENCE IN SIMULATION OF WEATHER AND CLIMATE IN EUROPE

Outline

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ESiWACE: http://esiwace.eu

The Centre of Excellence in Simulation of Weather and Climate in Europe

- Prepare the European weather and climate community
  - Make use of future exascale systems
- Goals in respect to HPC environments
  - Improve efficiency and productivity
  - Supporting the end-to-end workflow of global Earth system modelling
  - Establish demonstrator simulations that run at the highest affordable resolution
- Funding via the European Union's Horizon 2020 program (ESiWACE2 2019-2022)

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The ESiWACE Community

- 20 partners from 9 countries
- 35 supporters

Figure: Group Photo during the ESiWACE2 Kick-Off Meeting (March 2019)

Climate/Weather Workflows

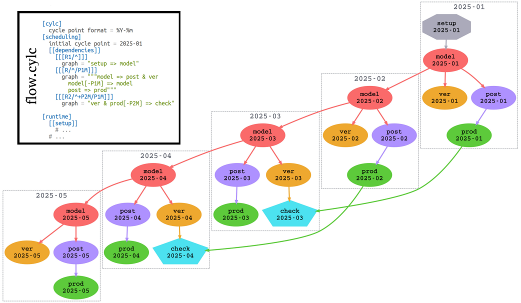
Challenges

1. Programming of efficient workflows
2. Efficient analysis of data
3. Organizing data sets
4. Ensuring reproducibility of workflows/provenance of data
5. Meeting the compute/storage needs in future complex hardware landscape

Scientists should rather focus on 1 and 2

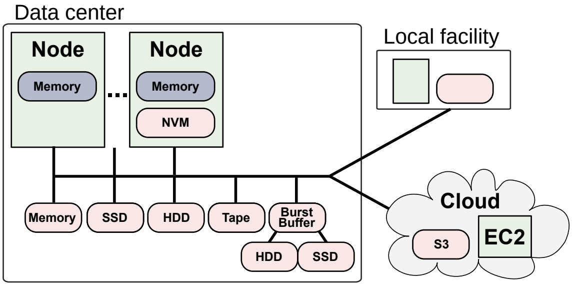
Workflows in Climate and Weather

- A workflow consists of many steps
  - Repeated for simulation time
  - E.g., weather for 14 days
- A Cyclc workflow specifies
  - Tasks with commands
  - Environment variables
  - Dependencies



- Data placement could be optimized by considering available hardware
  - Different and heterogenous storage systems available
  - Prefetching of data, using local storage, using IME hints, ...
- Goal: Explore higher-level abstraction - scientists don't need to worry where data is

The Coexistence of Storage – Impact of Local Storage



- May utilize local storage, SSDs, NVMe
  - Even without communication used in workflows
- Goal: We shall be able to use all storage technologies concurrently
  - Without explicit migration, put data where it fits
  - Administrators just add new technology (e.g., SSD pool) and users benefit from it

Outline

Long Term Vision: Full Separation of Concerns

Decisions made by users/scientists

- Scientific metadata (e.g., what is the data about)
- Declaring workflows
  - Covering data ingestion, processing, product generation, and analysis
  - Data life cycle (and archive/exchange file format)
  - Declaring value of data (logfile, data-product, observation)
  - Constraints on: accessibility (permissions), ...
  - Expectations: completion time (interactive feedback human/system)
- Flexibly adapt to needs of users/scientists
  - Modify workflows on the fly
  - Analyse interactive, e.g., Visual Analytics

Separation of Concerns

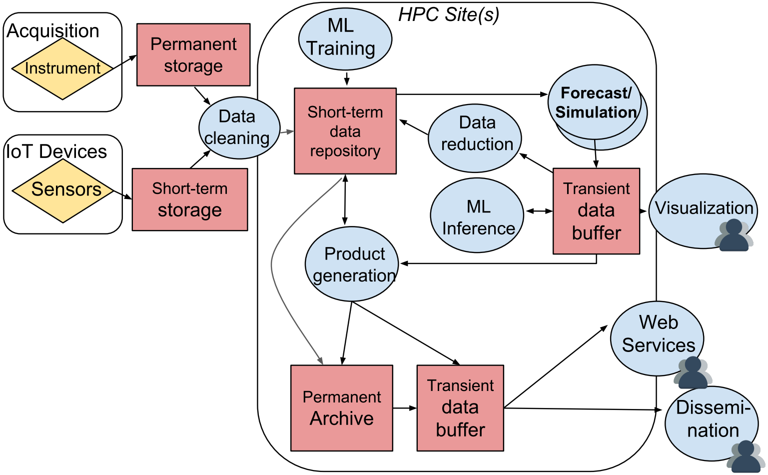
Decision made by programmers of models/tools

- Decide about the most appropriate API to use (e.g., NetCDF + X)
- Register compute snippets (analytics) to API
- Do not care **where** and **how** compute/store

Decisions made by the (compute/storage) system

- Where and how to store data, including file format
- Complete management of available storage space
- Performed data transformations, replication factors, storage to use
- Including scheduling of compute/storage/analysis jobs (using, e.g., ML)
- Where to run certain data-driven computations (**Liquid-computing**)
  - Client, server, in-network, cloud, your connected laptop

Smarter Climate/Weather Workflows in 2020+



- IoT (and mobile devices)
  - Additional data provider
  - Improves short-term weather prediction
- Machine learning support
  - Localize known patterns
  - Interactive use Visual analytics
- Data reduction
  - Output is triggered by events (ML)
  - Compress data of ensembles

Outline

Earth-System Data Middleware

A transitional approach towards a vision for I/O addressing

- Scalable data management practice
- The inhomogeneous storage stack
- Suboptimal performance and performance portability
- Data conversion/merging

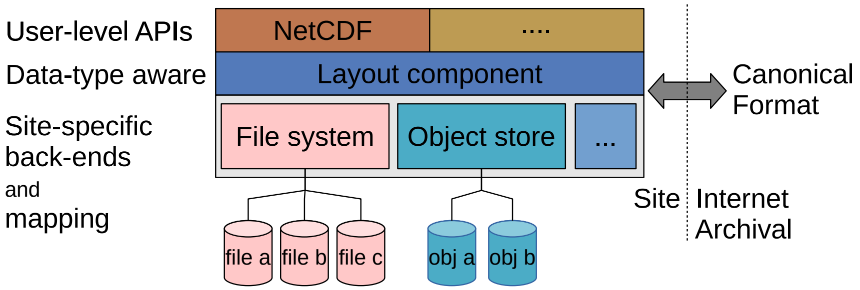
Design goals of the Earth-System Data Middleware

1. Relaxed access semantics, tailored to scientific data generation
2. Site-specific (optimized) data layout schemes
3. Ease of use and deploy a particular configuration
4. Enable a configurable namespace based on scientific metadata

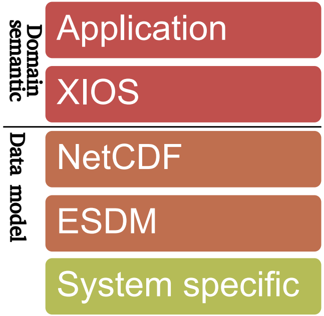
Architecture

Key concepts

- Middleware utilizes layout component to make placement decisions
- Applications work through existing API
- Data is then written/read efficiently; potential for optimization inside library

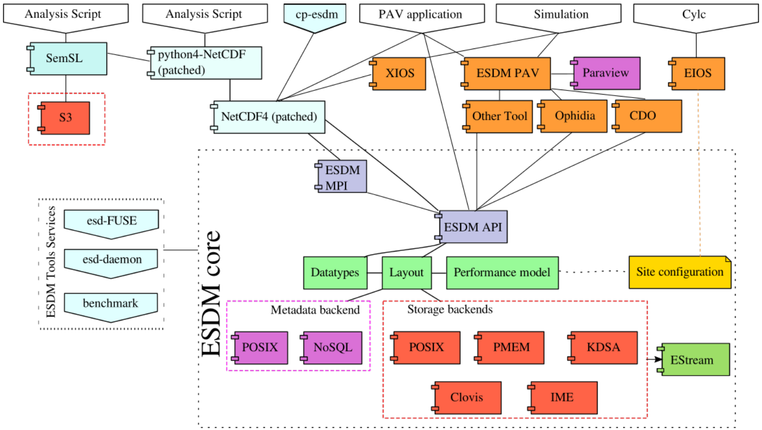


A Transitional Storage Stack for Large-Scale Ensembles



- Users run ensemble (e.g., 10x simulation with slightly different parameters)
- XIOS (climate/weather domain-specific) servers run on subset of nodes
  - Receive data from all 10 simulations
  - Reduces data, e.g., computing mean/variance
  - Store interesting data (reduced data and maximum)
- ESDM performs IO efficiently
  - Using underlying (heterogenous) storage systems efficiently

Architecture: Detailed View of the Software Landscape in ESiWACE



Backends

Storage backends

- POSIX: Backwards compatible for any shared storage
- CLOVIS: Seagate-specific interface, will be open sourced soon
- WOS: DDN-specific interface for object storage
- KDSA: Specific interface for the Kove cluster-wide memory
- PMEM: Non-volatile storage interface (`http://pmem.io`)

Metadata backends

- POSIX: Backwards compatible for any shared storage
- Investigated performance of ElasticSearch, MongoDB as potential NoSQL solutions

ESDM as NetCDF Drop-In is Easy to Use

- Create a ESDM configuration with storage locations
- Run esdm-mkfs to prepare storage systems (e.g., mkdir on POSIX)
- Change file names when running NetCDF applications
  - The namespace of ESDM is separated from the file system (hierarchical too)
  - NetCDF can use ESDM by just utilizing the **esdm://** prefix
- Examples:
  - Import/Inspection/Export of data using NetCDF
    $ nccopy test_echam_spectral.nc esdm://user/test_echam_spectral
    $ ncdump -h esdm://user/test_echam_spectral
    $ nccopy -4 esdm://user/test_echam_spectral out.nc
  - Usage in XIOS, change iodef. Example:
    `<file id="output" name="esdm://output" enabled=".TRUE.">`
    `prec=8` in axis_definition, domain_definition and field_definition

Converting an Existing Code: Shallow Water Model

Facts about the model

- Stores data column-wise in memory
- Separates compute phase and IO phase[1]

Existing NetCDF code for IO phase

```
size_t start[] = {0, 0};
size_t count[] = {nY, 1};
for(unsigned int col = 0; col < nX; col++) {
  start[1] = col; //select col (dim "x")
  nc_put_vara_float(dataFile, i_ncVariable, start, count,
    &i_matrix[col+boundarySize[0]][boundarySize[2]]);
}
```

[1] DSLs will help to separate those phases

ESDM Code for the Application

```
int64_t offset[] = {(int64_t) timeStep, offsetY, offsetX};
int64_t size[] = {1, (int64_t) nY, (int64_t) nX};

esdm_wstream_float_t stream;
esdm_wstream_start(&stream, dset, 3, offset, size);
for(int y = 0; y < nY; y++) {
 for(int x = 0; x < nX; x++) {
   esdm_wstream_pack(stream,
       i_matrix[x + boundarySize[0]][boundarySize[2] + y])
   // this may trigger actual IO and postprocessing!
 }
}
esdm_wstream_commit(stream);
```

- Ultimately, using DSLs an IO phase could mix in compute and "stream output" to minimize memory pressure (and trigger initial post-processing)

Outline

Evaluation

System

- Test system: DKRZ Mistral supercomputer
- Nodes: 100, 200, 500

Benchmark

- Uses ESDM interface directly; metadata on Lustre
- Write/read a timeseries of a 2D variable; 3x repeated
- Grid size: 200k $\times$ 200k $\times$ 8 Bytes $\times$ 10 iterations
- Data volume: size = 2980 GiB; compared to IOR performance

ESDM configurations

- Splitting data into fragments of 100 MiB
- Use /dev/shm (TMPFS) or /tmp directory (Local SSD)

Performance Growth of ESDM on Lustre (PPN = 1)

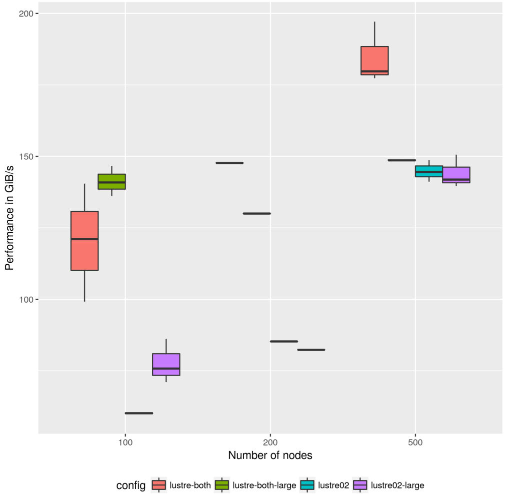


Figure: Write

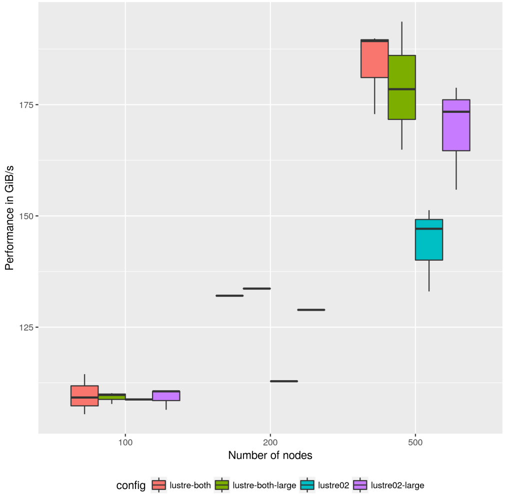


Figure: Read

Discussion

- Benefit when accessing multiple global file systems
- Write performance benefits from using both file systems
  - Most benefit when using 200 nodes (2x)
  - 500 nodes: 180 GiB/s vs. 140 GiB/s (single fs)
- Read performance shows some benefit for larger configurations
- ESDM achieves similar performance regardless of PPN (not shown)
- What is the performance when we use node-local storage?

Performance on TMPFS vs. IOR (nodes = 500, varied PPN)

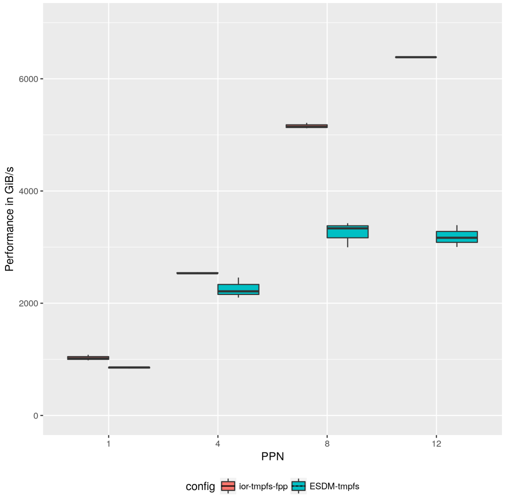


Figure: Write

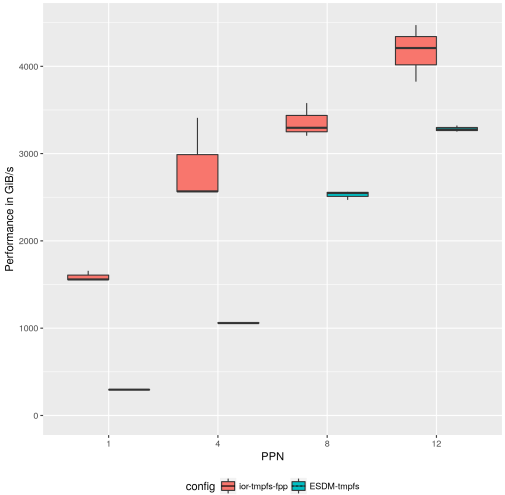


Figure: Read

Discussion

- Node-local storage is much faster than global storage
  - TMP achieves 750-1,000 GB/s for write (500 SSDs, some caching)
  - TMP reads are actually cached (6 GB data per node)
  - TMPFS achieves up to 3,000 GB/s
- TMP write is invariant to PPN
  - ESDM configured to use at least four threads per node
- TMPFS write depends on PPN
  - ESDM configured to not use threads, could use them to improve performance!
- IOR is faster; potential to improve ESDM path further
  - Localization of fragments using r-tree

Performance on NVDIMMs

- ESDM on the NextGenIO Prototype with a first naive approach (with PMEM)
- Test run on four dual-socket nodes with 80 GByte of data
- Theoretic HW performance per node (12 NVDIMMs) W: 96 GB/s, R: 36 GB/s
- Max test: explore best case performance (single file)

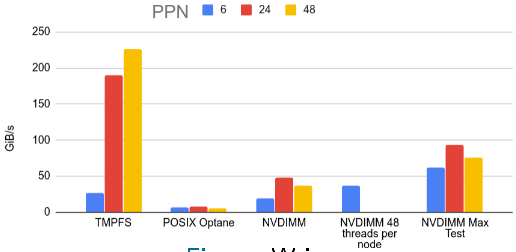


Figure: Write

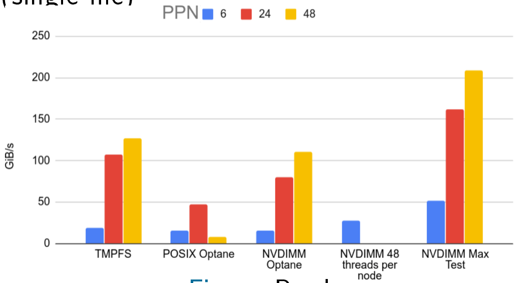


Figure: Read

Outline

Summary

ESDM: Performance-portable I/O utilizing heterogeneous storage

1. The data model is mostly backwards compatible to NetCDF
2. NetCDF/Python workflows supported
3. Working toward workflow and active storage support
4. Next activities:
   - Comparison of flexible (ESDM) vs. fixed chunking (NetCDF)
   - Data re-mapping on read (transform-on-read) to optimize data access

Various other IO-related activities in ESiWACE

...

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