Progress of WP4: Data at Scale

WP4 Team

ESiWACE GA

September 2021

Reminder: WP4: Data Systems at Scale

Objectives

To mitigate the effects of the data deluge from high-resolution simulations (project objective d) by

1. Supporting **data reduction in ensembles** by providing tools to carry out ensemble statistics "in-flight" and compress ensemble members
2. **Hiding complexity** of multiple-storage tiers (middleware between NetCDF and storage) with industrial prototype backends
3. Delivering **portable workflow support** for manual migration of semantically important content between disk, tape, and object stores

$\Rightarrow$ *Ensemble tools, storage middleware, storage workflow*

Outline

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T2: Ensemble Services (Lister, Cole, Wilson)

Reminder: Goals

- Run ensemble members in parallel and do diagnostics "on-the-fly" using XIOS.
  - e.g., store mean and variance of ensemble results (instead of all members)

Three Key Activities

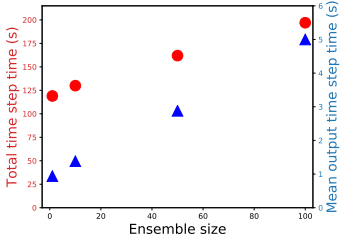
- Implement XIOS ensembles (In the Unified Model Atmosphere) on one MPI communicator.
- Proceed to real science demonstrator (with Met Office in WP1).
- Handle the risk of an ensemble member failure.

Future work: EXCALIBUR

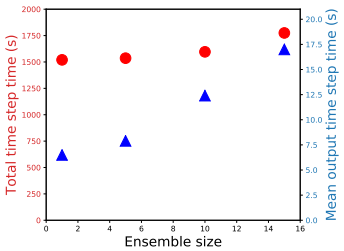
- Do this for coupled models including NEMO.

Ensemble Services: Improved Scaling

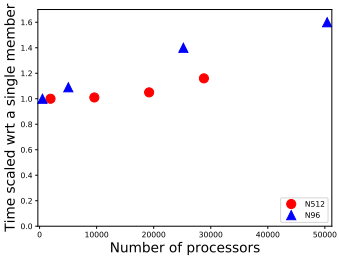
N96 (192x144x85)



N512 (1024x768x85)



Scaling



Experiments with one ensemble diagnostic and no normal output

- Relatively poor scaling for CMIP type resolutions
- Much better scaling at higher resolution.
- Ensemble calculations will be lost in noise with (some) normal I/O.

Ensemble Services: Next Steps

Further Modifications to the UM

Happening now

- Moving to all output via XIOS into NetCDF (many edge cases)
- Configuring required output.
  - Internal model pipework to route to XIOS
  - XMLApp so user can configure outputs.
- Compression via Gaussian Grids (optional, done)
- Upgrading XIOS versions.
- Performance profiling and tuning.

Further Modifications to Suite Control

- Managing an ensemble.
- Managing error handling (next slide)
- Managing data migration (JDMA and JASMIN, later slides)

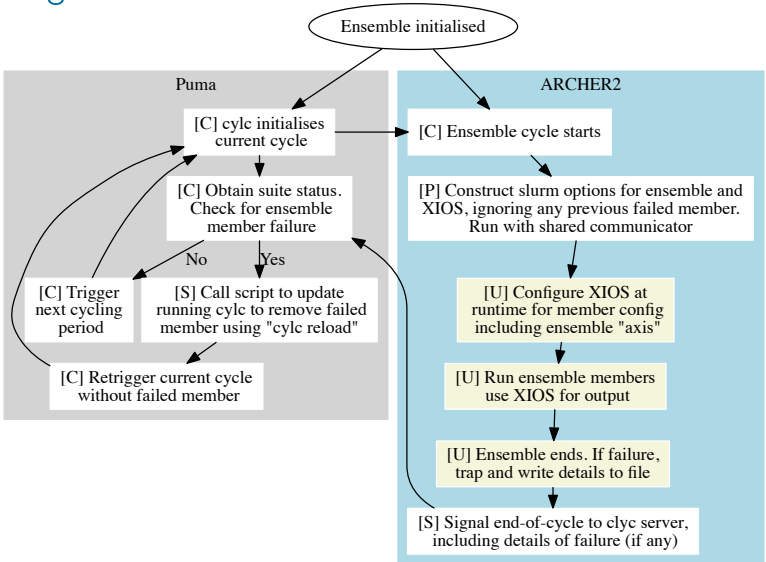
Towards Science runs for WP1

- What experiments & resolutions?
- Developing appropriate ensemble diagnostics.
- What output do we need from ensemble members?

Ensemble Services: Handling a dead ensemble member

MPI Failure?

- Original Goal: Trap MPI error from failing member.
- Better solution: Handle it in cylc.
- Algorithm and example of usage in D4.1



Outline

T4: Semantic Storage (Massey); the story thus far (early 2021)

Joint Data Migration App

- Aim: To manage large migrations between disk and tape or disk and object-store (and vice-versa).
- Status: In production on JASMIN. o(1PB) of data held by users.
- Issues: Users positive about functionality but not performance, particularly to tape. Probably too much (repeated) verification. No real semantics, still need to retrieve a file to know what as in it.

S3NetCDF (Python Module)

- Aim: S3 aware replacement for netcdf4-python.
- Status: At V2 utilising notions of an "aggregation file" and "fragments". The former on POSIX disk, the latter anywhere (but in particular, behind and S3 interface).
- Issues: Some use cases overtaken by zarr and netcdf c-lib. Performance issues. Aggregation rules & syntax not widely known & supported.

Decision Time

- Choices: New Excalibur Funding Available, so there was a clear route to continued funding, but when and how should we take-on the lessons learned. Now, or between projects? But projects overlapped?

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- Decisions:
  - Take the planned JDMA refactor, but build into a bigger activity.
  - Take the best ideas of S3NetCDF (smart aggregation) and "socialise" them.
  - Take the existing software of both and refactor into even further modularity so wider chance of re-use of both end-to-end functionality and components.

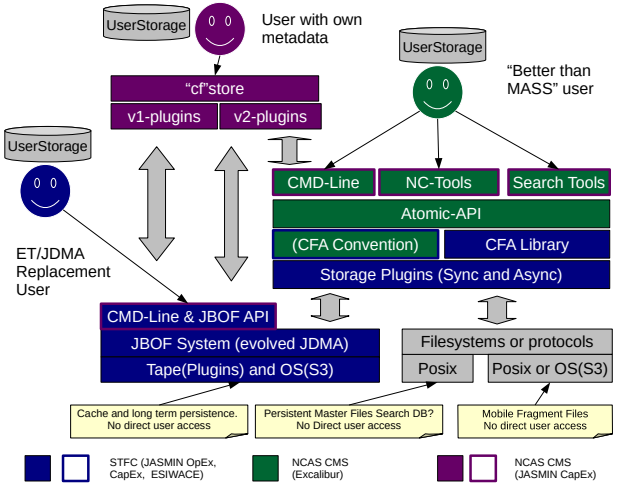
Three distinct tape and object store use cases

Use Cases

Multiple funding sources:

1. Managing "Just a bunch of files" (evolution of JDMA).
2. Adding semantic information.
3. Portable "MASS" for NetCDF functionality.

(Not including Object-Store only use case, e.g. pangeo)



Tape: Developments and Progress

- New name: NLDS (Near Line Data Store)
- Key idea: move to using object store as a cache for a "lightweight" HSM.
- Open Policy Agent for “HSM” policies.
- Using RabbitMQ to manage work queue.
- OAuth2 for authorisation.
- CERN’s FT3 to manage transfers.
  - S3, CTA, and maybe StrongBox (?) plugins?
- New staff member (Jack Leland) joined Neil Massey at STFC to work on it.

Meanwhile:

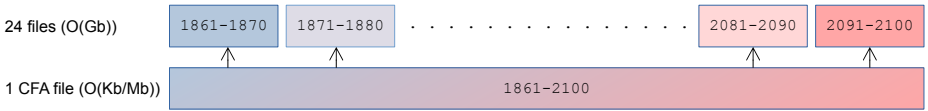
- Three member ten-year high-resolution N1280 (10km) ensemble begun on ARCHER2, is using JDMA in Cylc suite running on ARCHER2 to write to JASMIN.
- (So backwards compatible with JDMA is necessary.)

Aggregation File Syntax

https://github.com/NCAS-CMS/cfa-conventions

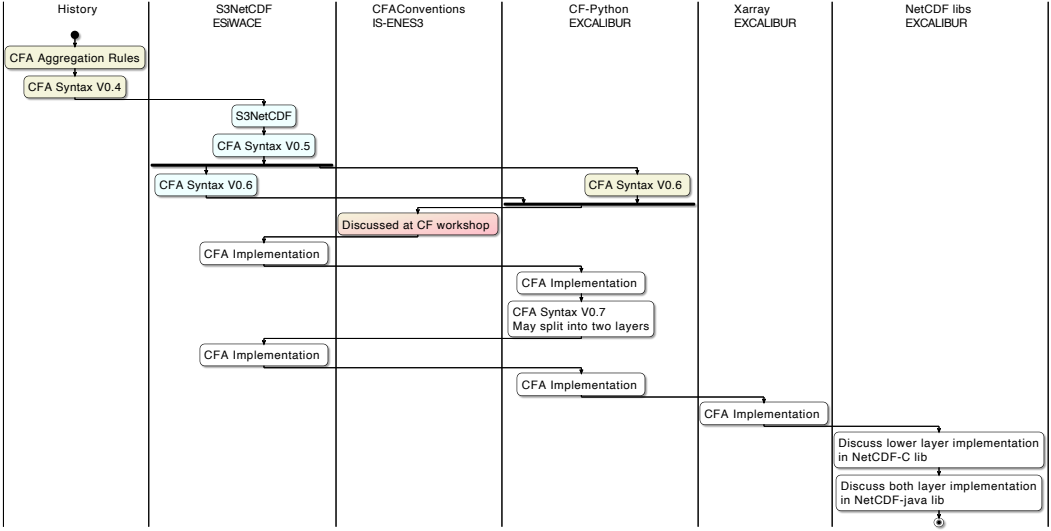
- Storing aggregations of existing datasets is useful
  - Data analysis
  - Archive curation

- **Example:** For a timeseries of surface air temperature from 1861 to 2100 that is stored in 24 files each spanning 10 years, it is useful to view this as if it were a single dataset spanning 240 years.



- **CFA-netCDF** is a(nother) proposed standard for recording an aggregation without copying the data so that it doesn't need to be remade on-the-fly (expensive), and is available as an archive index

Aggregation Files: where next?



Outline

Reminder: Earth-System Data Middleware (ESDM)

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

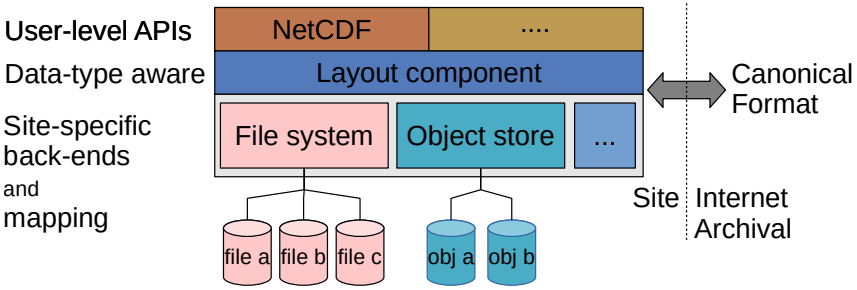
Design goals of the Earth-System Data Middleware

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)

Reminder: Architecture

Key concept: Decouple data localization decisions from science

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



Reminder: 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

Selected Activities: Status Overview

- Submission of WP4 deliverable
- Integrated ESDM with Paraview, patch for CDO support
- ESDM NetCDF supported version updated to current NetCDF Git
- Benchmarking efforts at CMCC and NCAS
- S3 backend implemented
- Prototype for transparent data transformation/replication upon reads
- Ophidia integration / evaluation (details next slide)

Integration of Ophidia with ESDM and Evaluation

- Different integration strategies implemented
  - Linking Ophidia with the ESDM-NetCDF library
    - Code rebuilding and minor modifications required
  - Direct integration of the ESDM API in Ophidia
    - New Ophidia operators for data loading and storing developed (OPH_IMPORTESDM, OPH_EXPORTESDM)
- Preliminary testing of the two integrations performed
  - Initial (small scale) results show no clear difference in the two approaches (direct integration slightly faster in some cases)
  - More extensive benchmarking is needed (planned for Y4)
- Discussion between WP4 and WP5 for Ophidia extensions for in-flight analytics based on ESDM
  - Use/testing of active-storage solutions to be evaluated

ESiWACE2 TODOs for ESDM

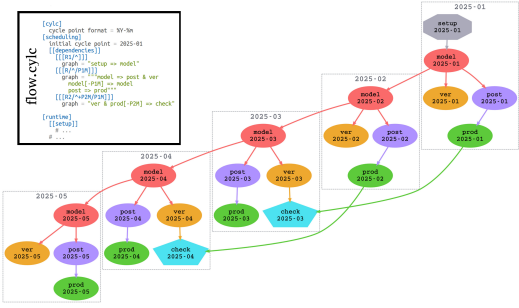
- Evaluation of ESiWACE-relevant scenarios
  - Pending activity to explore OpenIFS or NEMO at the GWDG
- Industry proof of concepts for EDSM, i.e., shipping of HW with software
- WP5: Supporting post-processing, analytics and (in-situ) visualization
- Optional
  - Hardening and optimization of ESDM
    - Integrate improved performance model
    - Further backend optimization
  - Features
    - Complete replicate data upon read (adaptive fragments) - publication was pending
    - Evaluation of structured (chunked) vs. flexible (ESDM) fragments - pub was pending
    - NoSQL metadata backend

Outline

Reminder: T5: Workflows

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

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



Activities

- Performed first analysis of integration between Cylc and ESDM
- Plan is not to pursue this research task further
  - Not a problem for our demonstrator
  - Could harvest some low-hanging fruits if there would be high interest in ESiWACE
- Action: DDN (Konstantionos) will document IME SLURM integration

Outline

T7: Industry PoC

- Goal: Usage of ESDM in a data center storage environment, using either Vendor storage appliance or Vendor deployment of storage software on COTS hardware
  - DDN to focus on providing a prototype appliance package
  - Seagate to focus on deploying Motr/Mero environment in weather/climate center
  - Motr is now fully open source and should work with COTS hardware
    - DKRZ identified as potential site for Motr deployment
    - Plan to explore aspects such as performance and function shipping