Data-Centric Workflows in Exascale Weather Forecasting

ECMWF's approach in Destination Earth Programme

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ECMWF

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7th ENES HPC Workshop

ECMWF

ECMWF's Forecasting Systems

Established in 1975, Intergovernmental Organisation

- 22 Member States | 12 Cooperation States
- 350+ staff

24/7 operational service

- Operational NWP – 4x HRES+ENS forecasts / day
- Supporting NWS (coupled models) and businesses

Research institution

- Experiments to continuously improve our models
- Reforecasts and Climate Reanalysis

Operate 2 EU Copernicus Services

- Climate Change Service (C3S)
- Atmosphere Monitoring Service (CAMS)
- Support Copernicus Emergency Management Service (CEMS)

Reading, GB

Bonn, DE

Bologna, IT

EU Destination Earth Programme

Started January 2022

- ECMWF
- European Space Agency (ESA)
- EUMETSAT

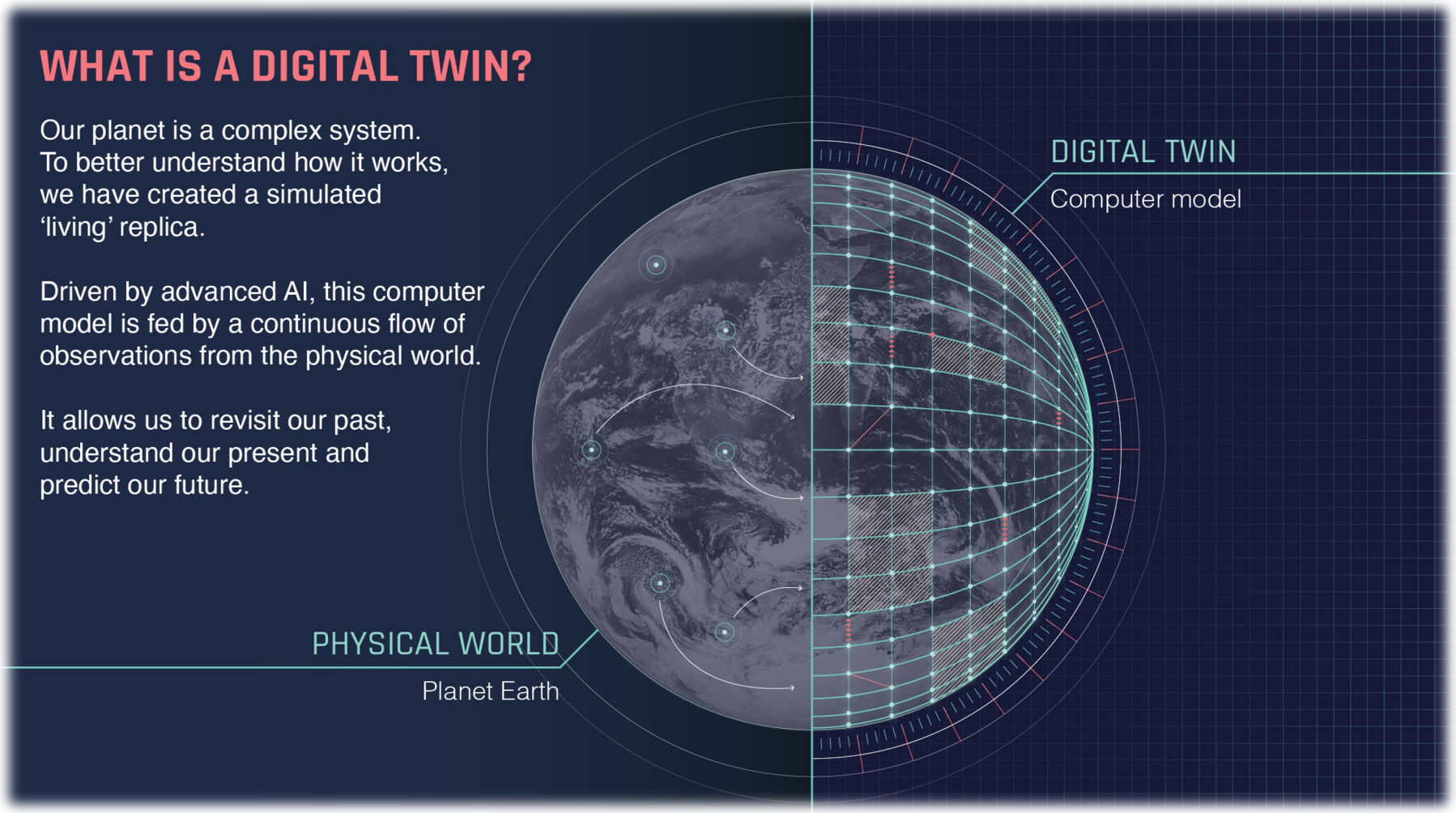
Part of EU's Green Deal and Digital Strategy

Build 2 Digital Twins:

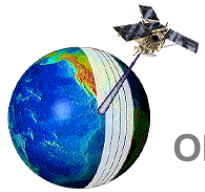
- Weather Extremes
- Climate

Weather Extreme DT

- daily run(s)
- Km-scale resolutions



ECMWF's Production Workflow



Global Observations

200M obs/day

Destination Earth Data Set

1000 TiB/day

45TiB/day

~350 world destinations

Acquisition

Earth System Model

Product Generation

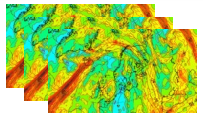
Product Dissemination

Obs

Fields

Archive

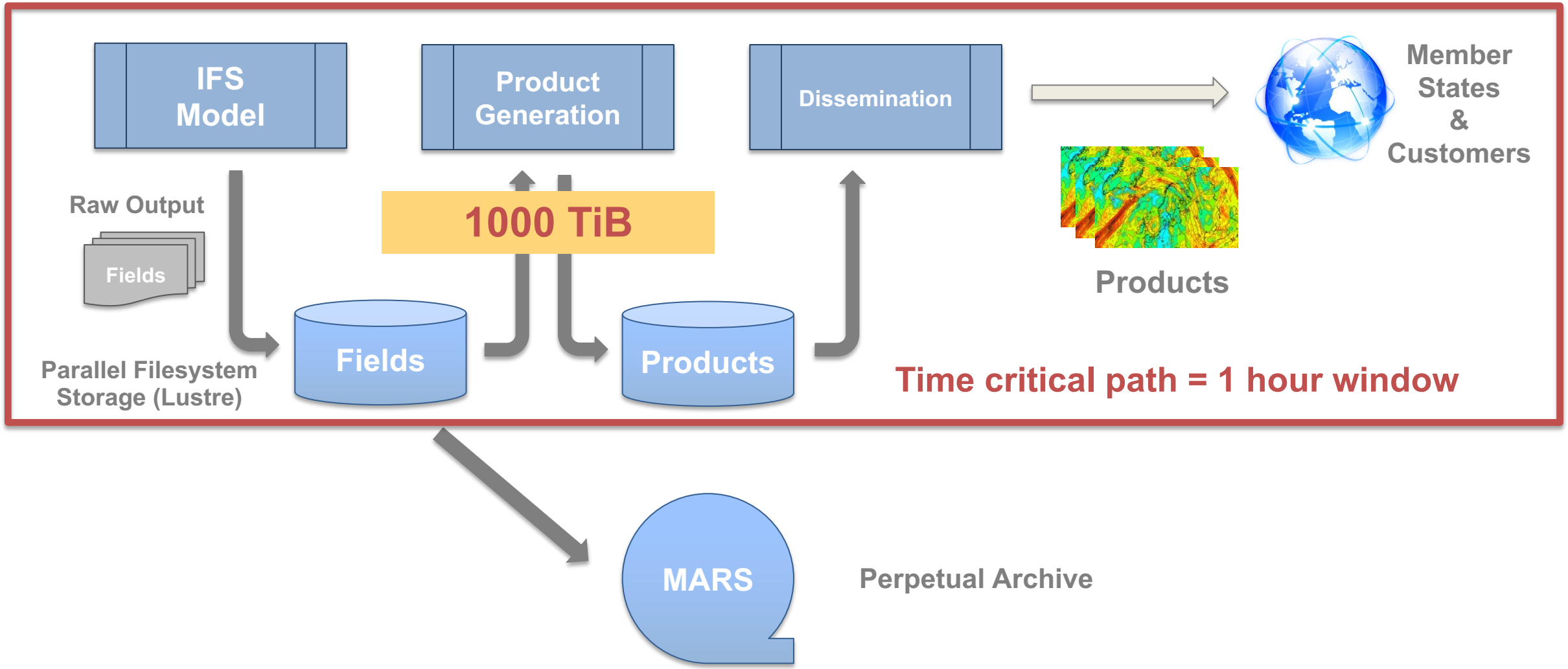
Perpetual Archive



Products

Member States & Customers

ECMWF's Production Workflow - Challenges



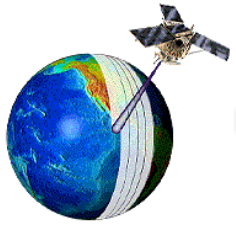
Effects of Product Generation using Parallel Filesystem

	IFS Model (No I/O)	IFS Model + I/O	IFS Model + I/O + PGen
Nodes	2440	2776	2926
Run time [s]	5765	6749	7260
Relative	-	**+ 17%**	**+ 26%**

Runtimes affected by the existence of another parallel job in the system:
Product Generation reading the data the model is writing
"Coupling" via the file system!

9Km 50 member ensemble
Broadwell nodes 2x18 cores
Cray XC40 Aries interconnect
Lustre FS IOR 90GiB/s

Storage View of Workflow



Observations

Acquisition

Product Dissemination

Member States & Customers

Acquire

Disseminate

Produce

Earth Sys Model

Storage Parallel FS

Analyse

ML + Analytics

Archive

Modify

Product Generation

Data is Central!

Perpetual Archive

Data is only as useful as what you do with it

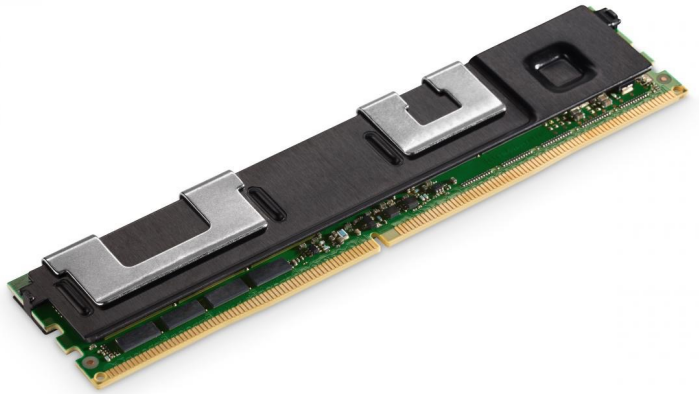
How to make data more useful?

Destination Earth Engine

- Framework for Earth System Model Workflows
- Think of a *Game Engine* but for Earth Systems…
  - It's a Framework – not model specific
  - Series of API's and services
  - Opt-in Components
- **Components:**
  - Workflow manager
  - Data structures and Parallelization library
  - Model Plugin architecture
  - **Key-Value Object Storage with Semantic Data access**
  - **IO-Server**
  - Data Notification system
  - **Data Cube API**
  - Post-Processing API

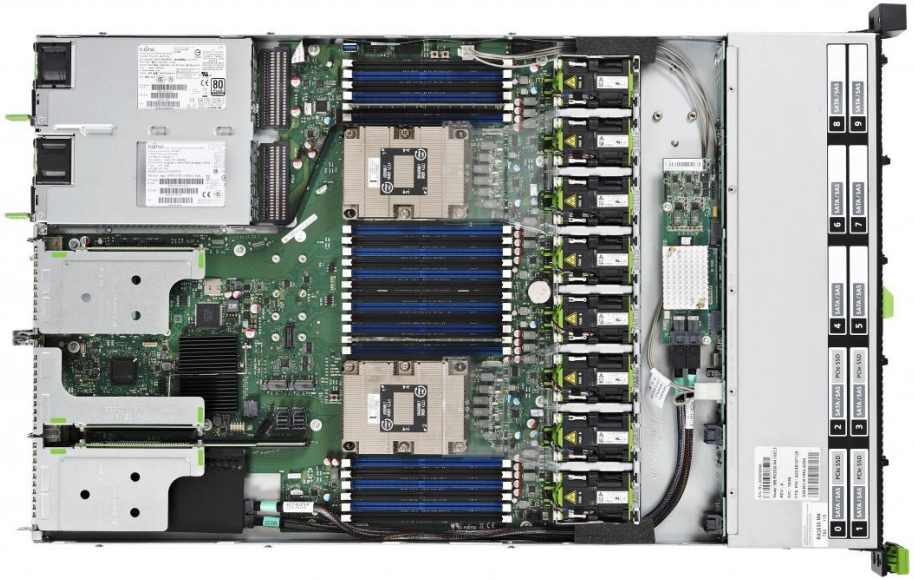
FDB – Domain Specific Object Store

- Read all @ www.nextgenio.eu (finished 2019)
- Development of an HPC node by **with Intel Optane DCPMM**
- Dual-CPU Intel® Xeon® SP nodes (48 cores)
- OmniPath network
- 192GB DRAM
- **3TiB of NVRAM DIMMs (max 6 TiB)**



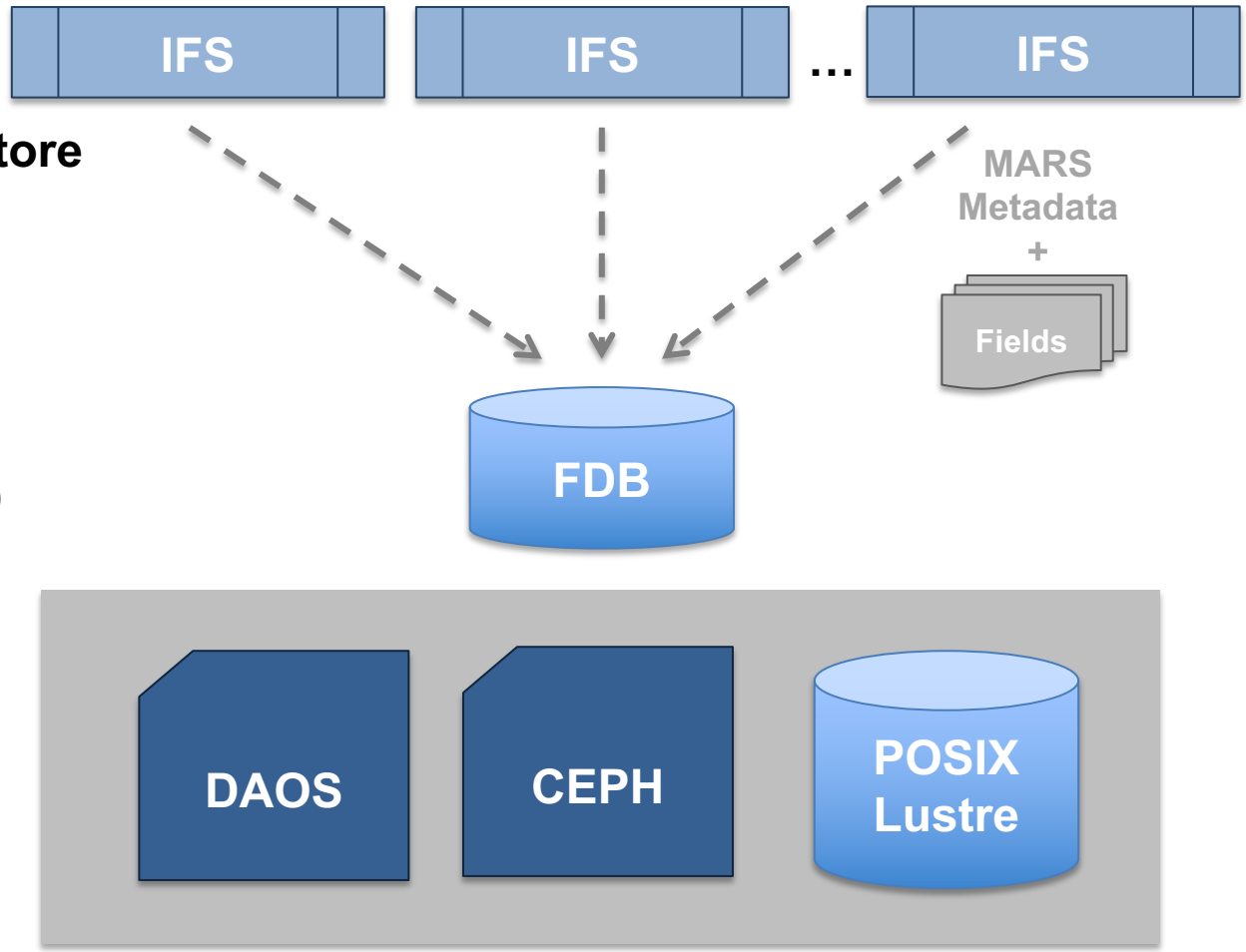
- **Prototype system**
  - **34 compute nodes**
  - **Hosted @ EPCC, Edinburgh**

FUJITSU



34 x 3 TiB Byte Addressable Storage

FDB (version 5)



- **Domain specific (NWP) Distributed object store**
- Transactional, No synchronization
- Semantic access to data
- Key-value store
  - Keys are scientific meta-data (MARS Metadata)
  - Values are byte streams (GRIB)
- Support for multiple back-ends:
  - POSIX file-system (currently on Lustre)
  - Intel DAOS (under development)
  - CEPH (Cloud suited object store)
- Supports wild card searches, ranges, data conversion
  - ***In the semantic/scientific language of the user:***

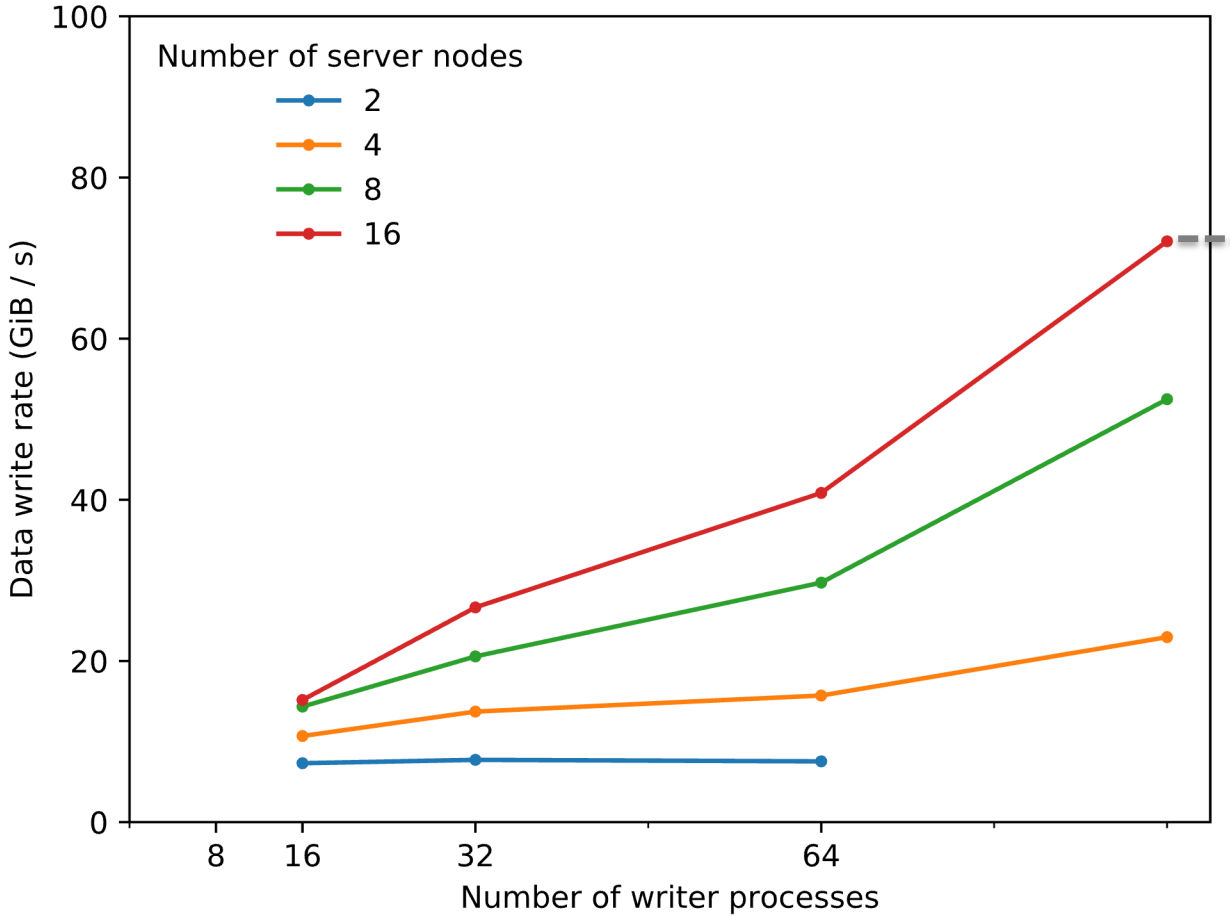
```
param=temperature/humidity,
levels=all,
steps=0/240/by/3
date=01011999/to/31122015,
```

FDB 5 Semantics

1. ACID – ***Transactional***
2. Write blocks until data handed over – ***Asynchronous***
3. `flush()` blocks until data is visible – ***Consistent***
4. Write-once, don't overwrite - ***Immutable***
5. Data can be masked – ***Versioned***

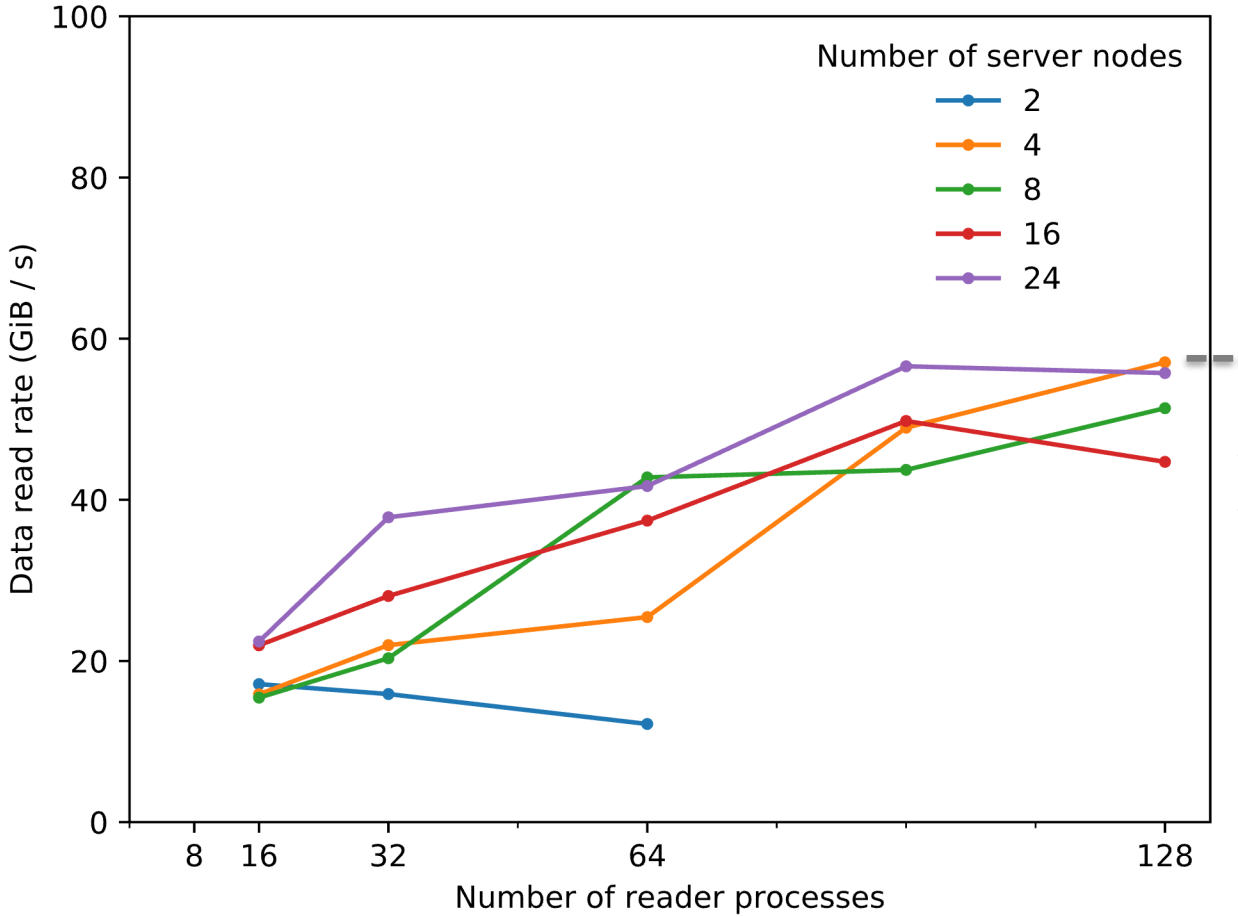
- All I/O operations are asynchronous, so computation can continue
- Distributed to all servers using a ***Rendezvous Hash***, *so no synchronisation needed*

FDB 5 Parallel Write Performance to NVRAM DIMMs



- **Application data measured**
- **Consistency semantics**
- **Includes wait for *flush()***

FDB 5 Parallel Read Performance to NVRAM DIMMs



60 GiB/s

- **Read slower than write**
- **Includes the *data lookup* in the indexes**

FDB 5 Running the forecast model

	Model + I/O	Model + I/O + PGen
Run time (Lustre) [s]	1793	1928
Run time (Distributed) [s]	1610	**1599**

Runtimes no longer affected by the Product Generation!!!

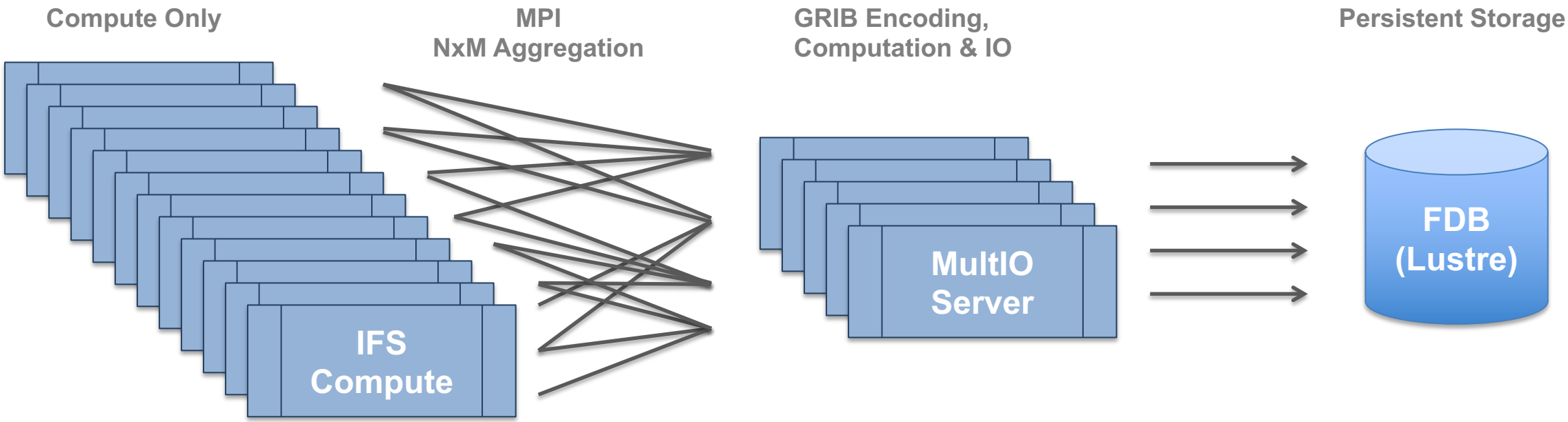
NextGenIO prototype. 32 nodes
Intel OmniPath2 interconnect
6 ensemble members

- Currently operational @ ECMWF
- Open sourced: github.com/ecmwf/fdb
- Read about it:

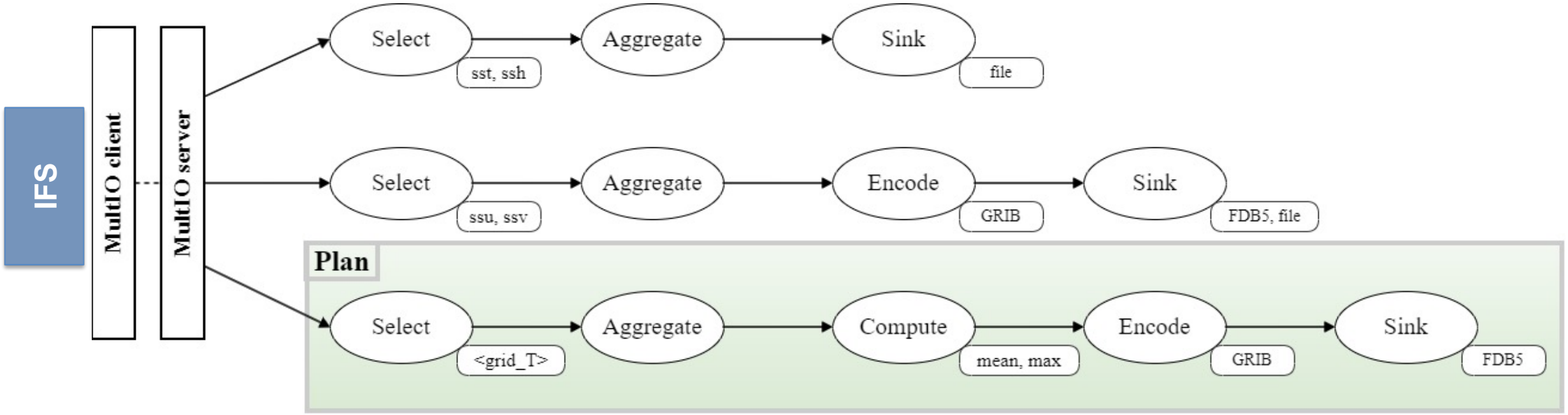
A High-Performance Distributed Object-Store for Exascale Numerical Weather Prediction and Climate
https://doi.org/10.1145/3324989.3325726

MultIO Server

- Currently under development: github.com/ecmwf/multio
- Completed adaptation of NEMO v4 model

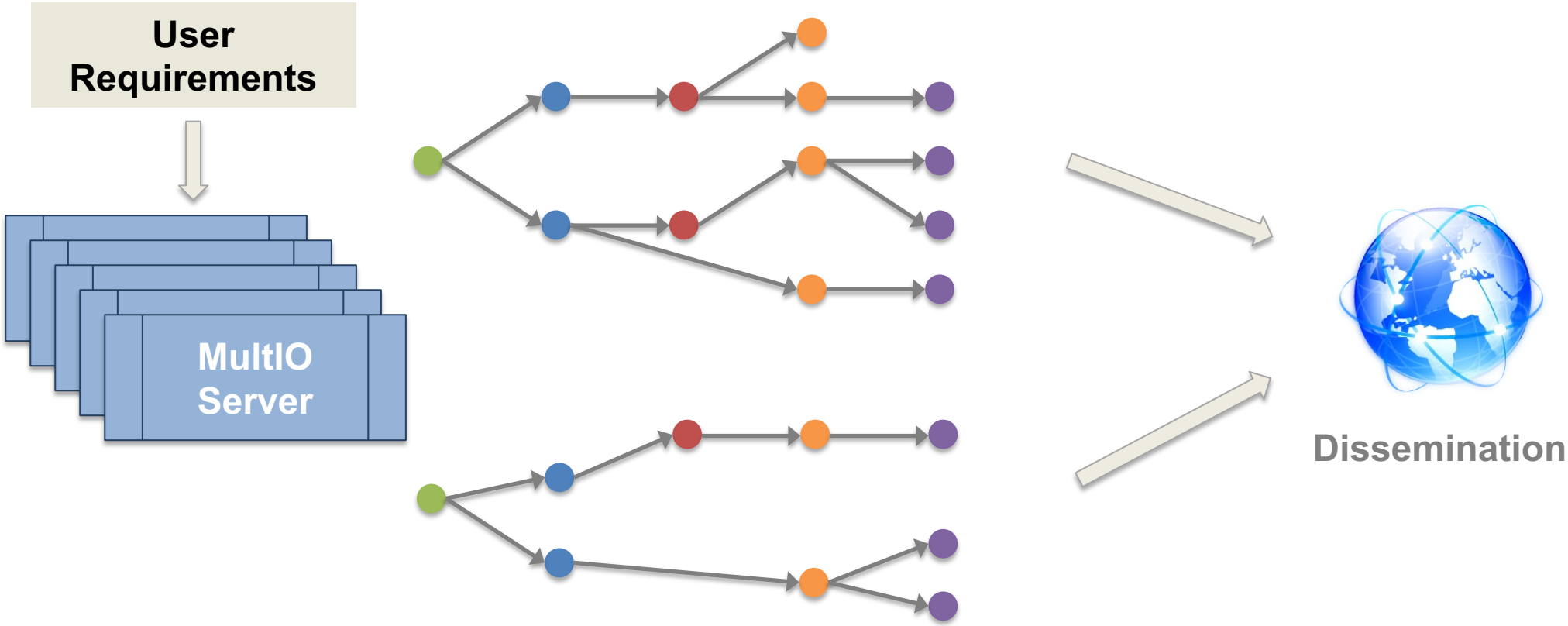


MultIO Server - Programmable Pipeline



- A generic I/O-server, user-programmable pipeline of actions
- Messages that contain **Fields** are passed to the **Plans**
- Messages are ***routed*** along multiple pipelines
- Easily extendable to new domains & grids & models

MultIO Server – On-the-fly Product Generation



All this in-memory, where the data is located

Accessing Data as Hypercubes

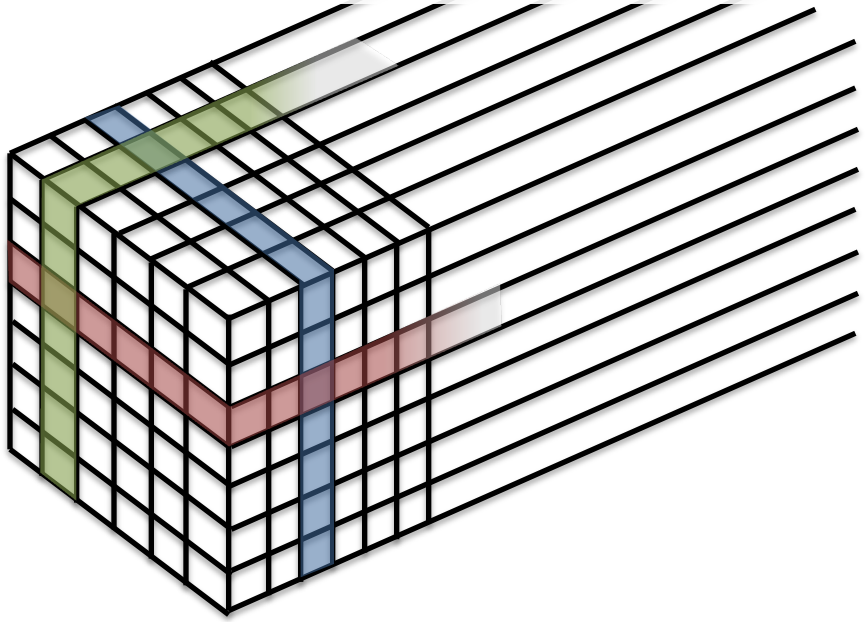
Hypercubes (6D)

- Longitude (3600)
- Latitude (1800)
- Variables (~1000)
  - Atmospheric levels (~ 8 x 100)
  - Physical parameters (~200)
- Time steps (~100)
- Probabilistic perturbations (50)

@ double precision

- 16km **80 TiB**
- 9km **235 TiB**
- 5km **690 TiB**

Clients want to do **different** analytics across **multiple** axis



ECMWF Novel Data-Centric Workflows

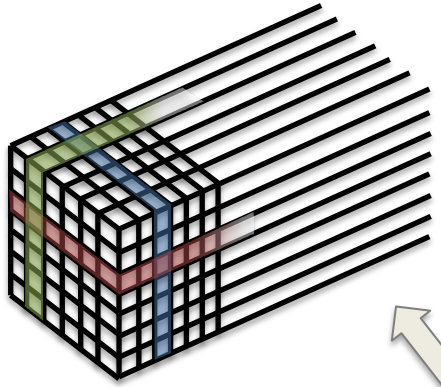
Data Analytics / Machine Learning

HPC Model Producer

Data Consumer

Cloud

- Bring **users** to the data
- Use data while it is **hot**



Object Store
Data Hypercube

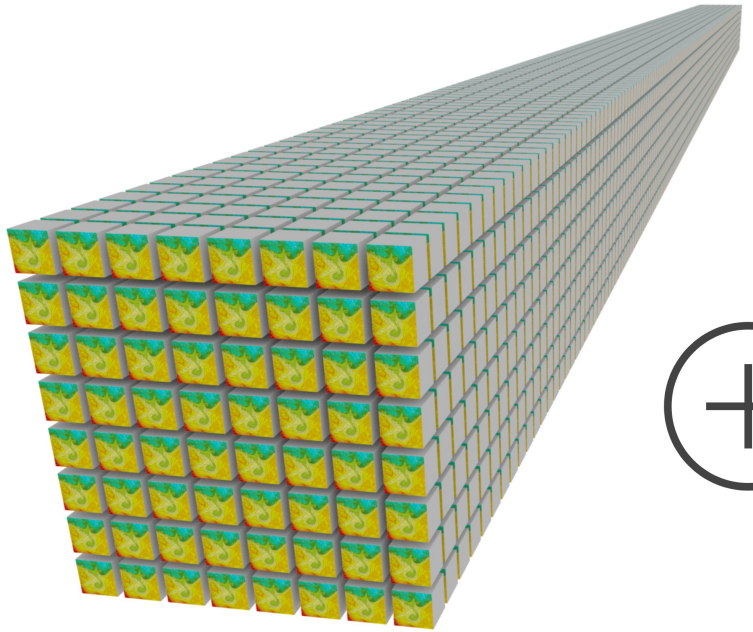
Parallel FS

Data Archive

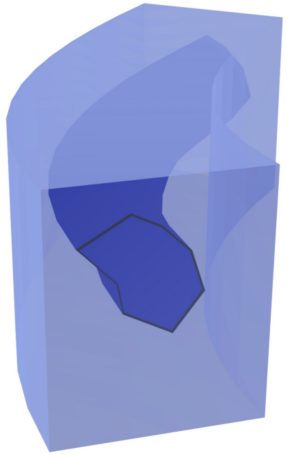
HDD

Tape

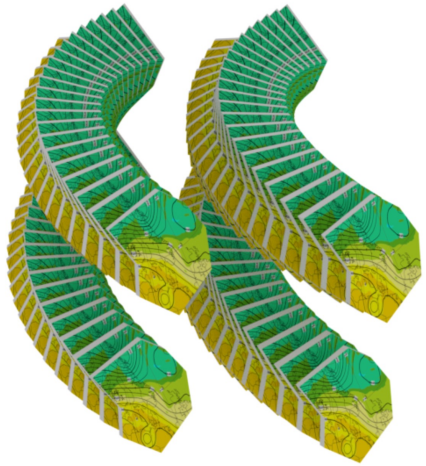
Hypercube Feature Extraction at Scale (~1 PiB)



Real-time Model Output
(Datacube on FDB)



Polytope Query



Resultant Data
Extraction

Polytope (under development)

Messages To Take Home

Ensemble data sets are growing quadratically to cubically in size. A challenge for time critical applications

*ECMWF is engaged in building **Km-scale Digital Twin** for Weather Extremes*

*ECMWF is adapting to **data centric workflows** for Exascale weather forecasting, exploring **in-situ data analysis** and **hypercube feature extraction***

ECMWF is refactoring software stack end-to-end to enable Exascale datasets in Weather Forecasting

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