

10-SEA introduction, concepts, and challenges

Philippe Couvée, ATOS R&D, IO-SEA Work Package 2 leader





This project has received funding from the European High-Performance Computing Joint Undertaking (JU) under grant agreement No 955811. The JU receives support from the European Union's Horizon 2020 research and innovation programme and France, the Czech Republic, Germany, Ireland, Sweden, and the United Kingdom.

Introduction

Philippe COUVEE ATOS Distinguished Expert

Working at ATOS HPC SW R&D since 20 years, leading the « Data Management » group with 15 engineers and PhD students



IO-SEA Work Package 2 Leader : https://iosea-project.eu/

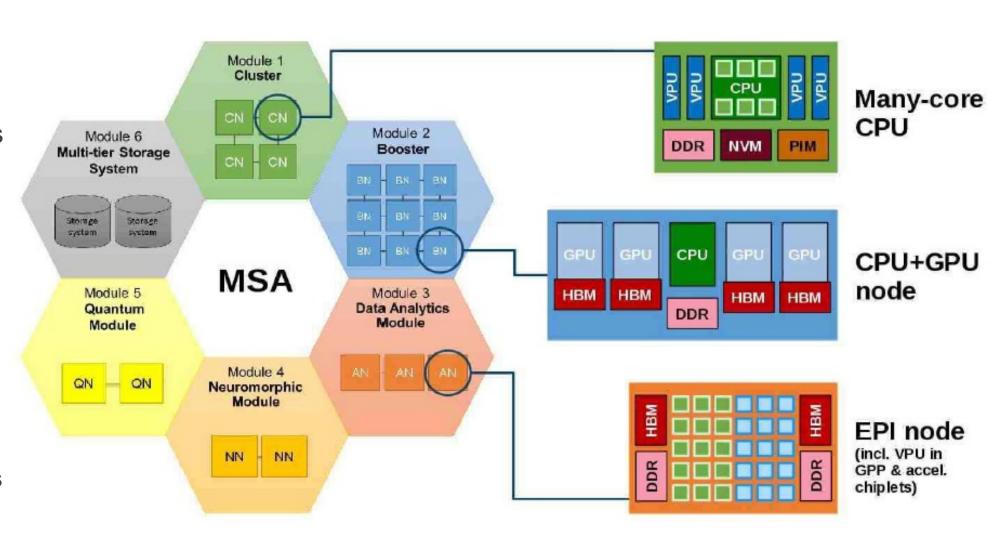


Context



Modular SuperComputer Architecture

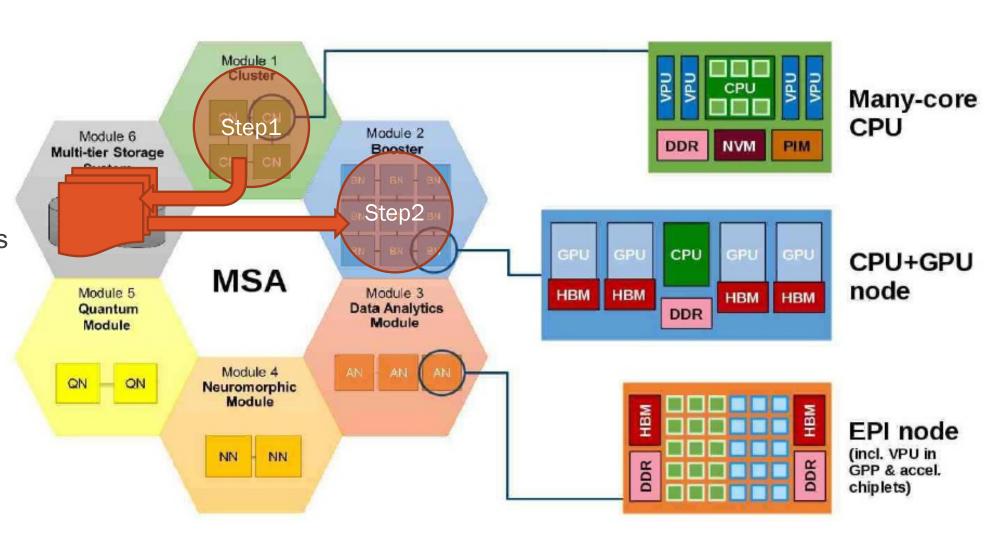
- HeterogeneousCompute modules
- « Long Term »
 Storage module
 with multiple
 technologies
- No cluster-wide interconnect
 - High speed
 Ethernet to
 connect modules





Modular SuperComputer Architecture

- Complex workflows running simultaneously and/or sequentially on multiple modules
 - Exchanging data through files





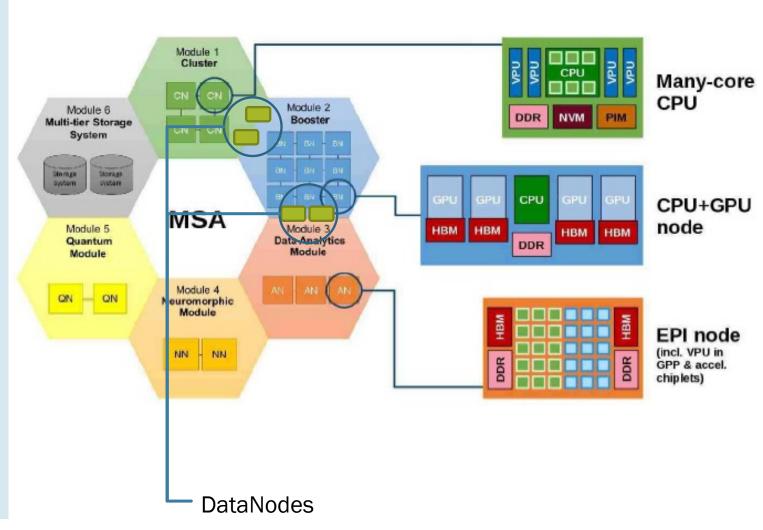
The IO-SEA Solution



IO-SEA Main Concepts 1: Data Nodes

Add **Data Nodes** between compute nodes and Long Term Storage Module

- connected to Compute Modules on their High Speed interconnects, and to the Long Term Storage Module
- Equipped with high speed storage devices
 - NVMe disks
 - NVRAM

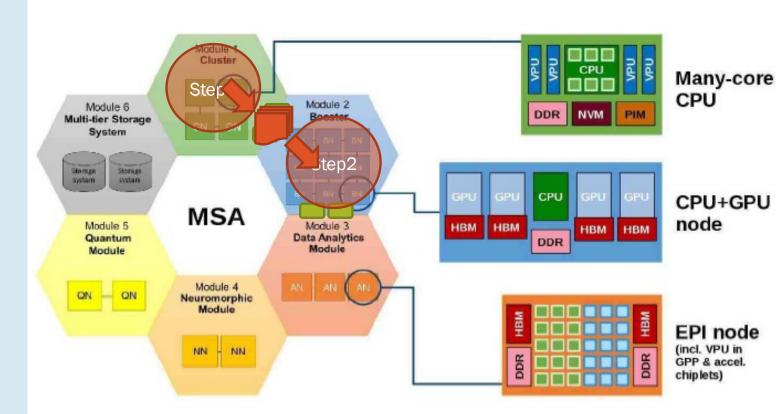




IO-SEA Main Concepts 2: Workflows Scheduling

Consider **Workflows** rather than individual applications for scheduling

- Workflows composed of many applications (steps) running on different Modules
- Allocate data nodes resources in addition to Compute nodes

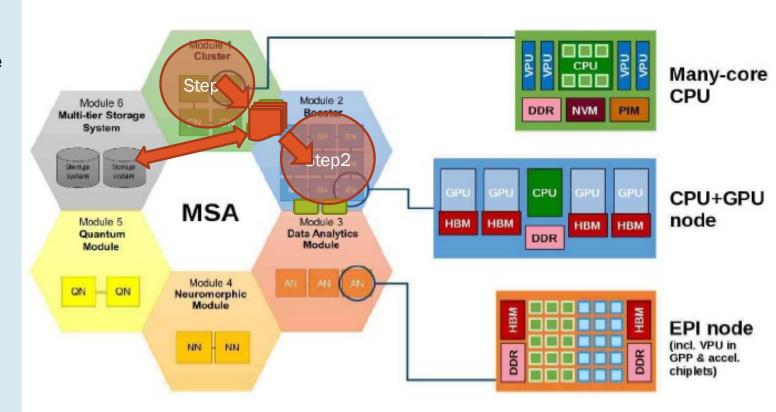




IO-SEA Main Concepts 3: Datasets & Ephemeral Services

Store Workflow data in **Datasets**

 Datasets are « data containers » stored in the long term storage as « objects », exposed to compute nodes by Ephemeral Services running on Data Nodes



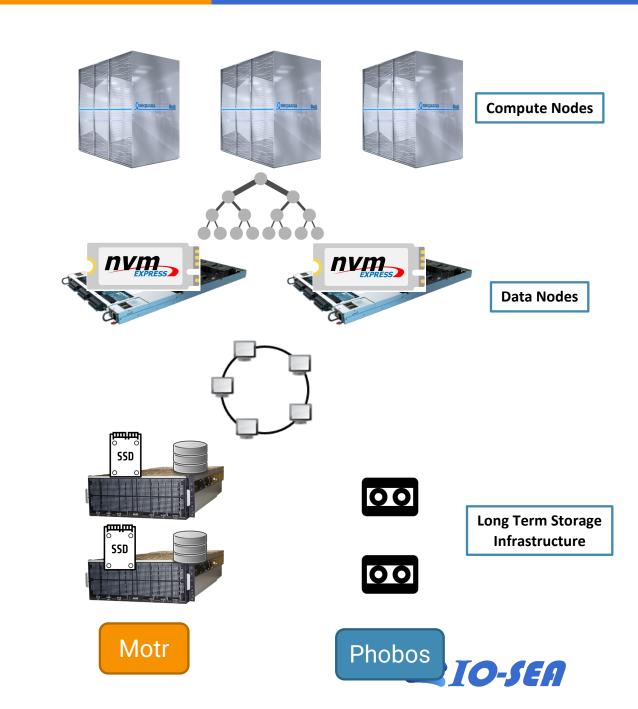


 Data nodes equipped with high-speed storage devices (NVMe, NVRAM)

 Long Term Storage composed of different tiers unified by an HSM software solution

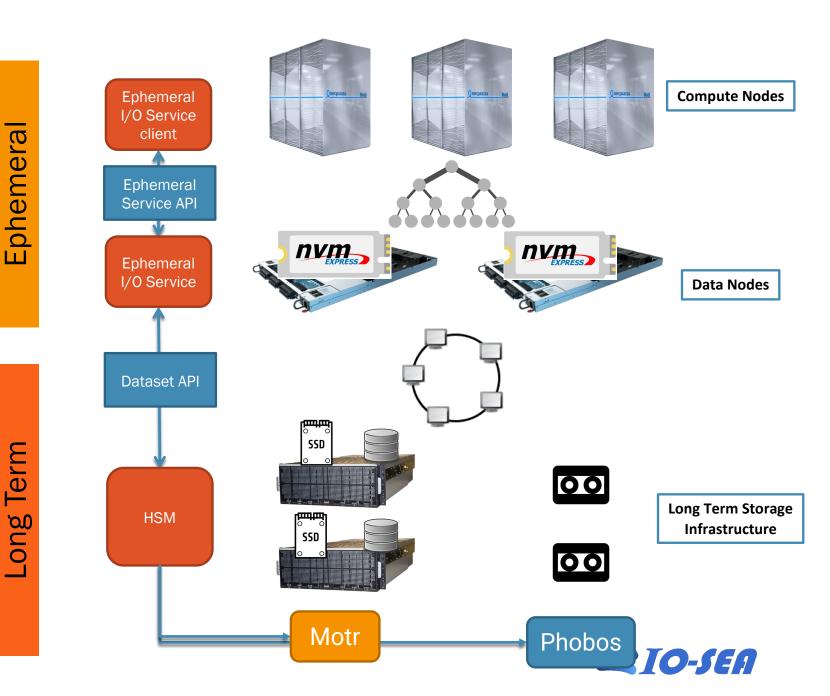
Long Term

phemeral



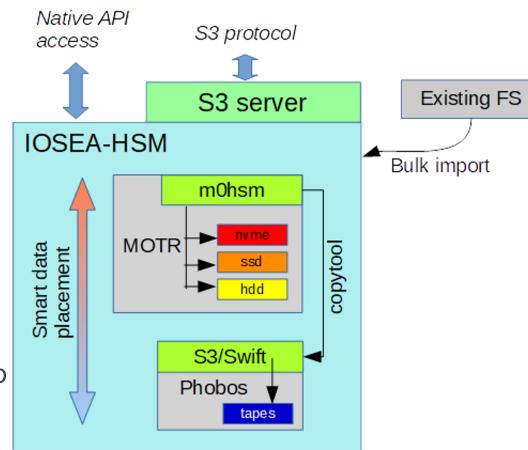
■ POSIX, S3, DASI protocols

- Long Term Storage composed of different tiers unified by an HSM software solution
 - Object Storage based, no POSIX limitations



IO-SEA Long Term Storage : Hierarchical Storage

- Leverage a wide variety of **storage technologies** in a single system
- -from NVMe to tapes
- Implement **transparent** data migration between many storage tiers
- Smart data placement / movements:
- > Place data according to application needs
- ➤ Gather needs from all running applications and develop a global data placement strategy
- >Prevent tiers from being fullfilled
- ➤ Arbitrate conflicting requests / resource usage 12





DataSets & Namespaces

- Datasets are data containers hosting objects
 - Could be seen as private file systems or object stores
 - No data organization, just collections of objects...

- Objects in Datasets are organized with Namespaces
 - Different Namespaces can be created for each Dataset
 - Namespaces can expose the same dataset through different protocols
 - POSIX, S3



Datasets/Namespaces

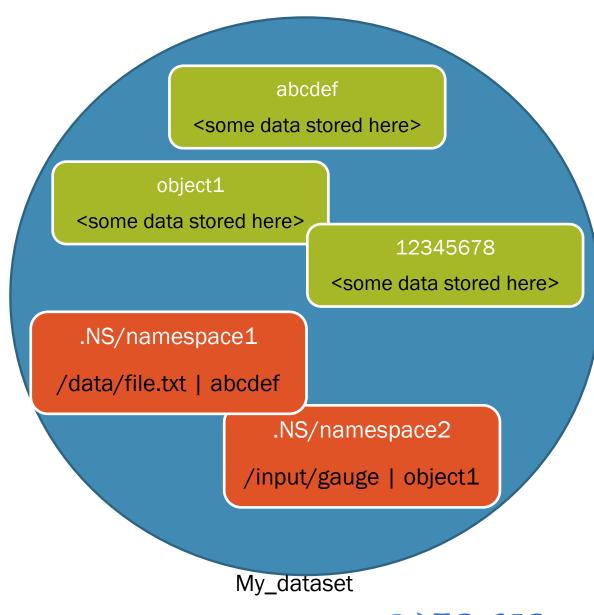
A Dataset is stored as 1 S3 Bucket Files stored as S3 object

All namespaces stored in « metadata » objects

Think of it as a set of directories and symbolic links to objects in dataset

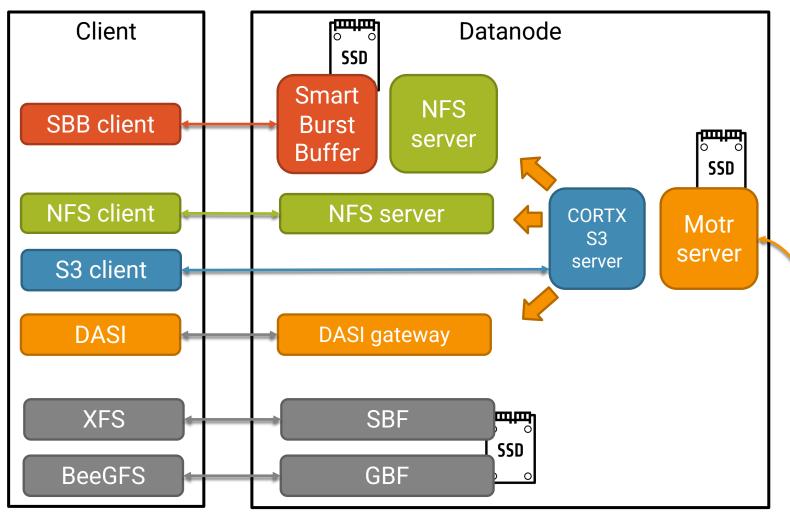
.NS/namespace1

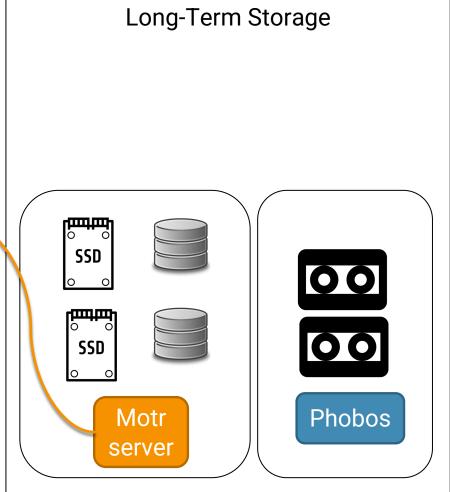
.NS/namespace2



6 Ephemeral I/O Services

NFS, BB-NFS, S3, DASI, SBF, GBF





10/13/22

Example: NAMD

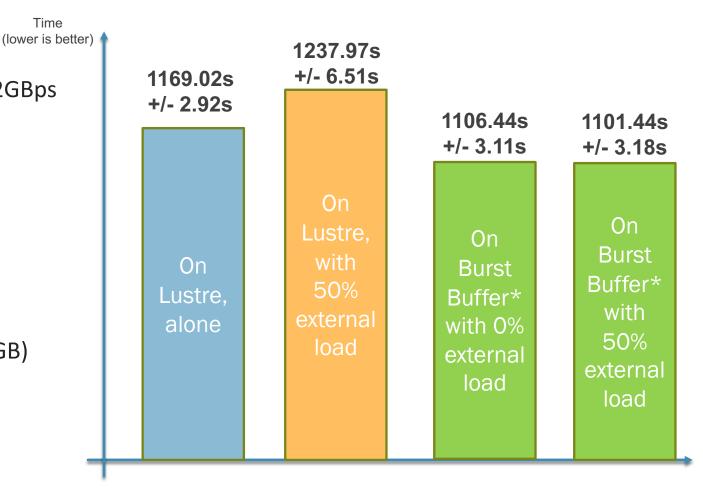
Filesystem: Lustre, max measured bandwidth ~ 2GBps

Time

2 Datanodes, each 50GB RAM, 1.5T Flash 200Gbps network, 16 allocated CPU cores

NAMD:

12 computes nodes (2x 16c/32t@3GHz) 200Gbps network interconnect MPI mpich 3.4.2 1 checkpoint each ~ 3 min (checkpoint size ~ 12GB) input: STMV_210M, size ~ 17GB uncompressed, source https://repository.prace- ri.eu/ueabs/NAMD/2.2/NAMD TestCaseC.tar.gz



^{* :} prefetch of input data into SBB not included in application runtime measurement



End User Interfaces & APIs

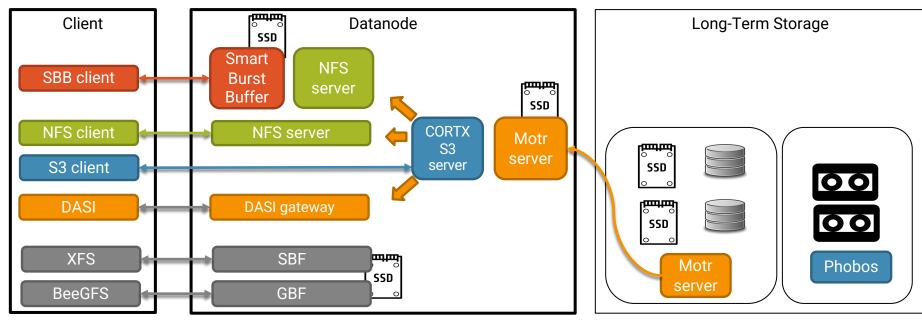


User Interfaces

- Workflows are described in a « Workflow Description File » . yaml, and managed through command line tools
- Datasets/Namespaces are created with command line tools

Workflow Manager

Dataset/Namespace





Workflow Sessions

- The steps processing the same data are run within a « session »
 - Access tokens protect against dataset access by multiple sessions in parallel
- Sessions have a user provided name
 - (UID, Session_Name) as identifier

```
# start a session for my workflow described in the WDF.yaml file
iosea-wf start WORKFLOW=WDF.yaml SESSION=My_Session

#run the workflow steps
iosea-wf run SESSION=My_Session STEP=step1
iosea-wf run SESSION=My_Session STEP=step2
iosea-wf run SESSION=My_Session STEP=step3

#stop the session and release the datanode
iosea-wf stop SESSION=My_Session
```



Workflow Session Management

- status & list commands to report information
- access command to launch an interactive access environment
 - Slurm salloc to launch a shell in which Ephemeral Services clients will be configured
 - Will be « shareable » with team members

```
# display info about jobs & ephemeral services
iosea-wf status SESSION=My_Session

# list all active sessions of the user (report the session-names)
iosea-wf list

# Start an interactive access environment for all or limited to [<service>]
iosea-wf access SESSION=My_Session [NS=service]
```



Workflow Description File (WDF)

 services describe the ephemeral services needed to run the workflow

steps describe how to configure the run time environment to run the steps

```
workflow:
 name: My Workflow
services:
  - name: ephemeral service 1
    type: NFS
    attributes:
      namespace: dataset.My namespace
      mountpoint: /mnt/USER/My Workflow
      flavor: medium
steps:
  - name: step A
    location:
      - gpu module
    command: "srun My_Step_A"
    services:
      - name: ephemeral service 1
```

Parametric Workflow Description File (WDF)

- To run multiple sessions in parallel, or to make the WDF more generic, variables can be used for most fields
- Variables must be defined « before use »

```
services:
   - name: ephemeral_service_1
   type: NFS
   attributes:
     namespace: {{ NS1 }}
   mountpoint: /mnt/USER/{{ SESSION }} My_Workflow
   flavor: medium
```

```
# start a session for my workflow
iosea-wf start WORKFLOW=WDF.yaml SESSION=My_Session NS1=My_namespace
#run the workflow steps
iosea-wf run SESSION=My_Session STEP=step1 NS1=My_other_namespace
```

Status command

to monitor steps progress

```
> iosea-wf status SESSION=My session
Workflow Name
                : My Workflow
Workflow SessionID : My session <timestamp>
Pending Steps
Step Name Slurm ID Tag Command
step B 2767 last srun My_Step_B
SaveResults ----
                            srun My Copy Script
Active Steps
Step Name Slurm ID
                           Command
                     Tag
step B 2763
                            srun My Step B
Terminated Steps
Step Name Slurm ID
                     Tag Command
step A 2760
                     init srun My_Step_A
Ephemeral Services....
```

Location in the WDF

```
steps:
  - name: step_A
    location:
      - gpu module
    command: "sbatch My Step A"
    services:
      - name: ephemeral service 1
 - name: step B
    location:
      - gpu module
      - cpu module
    command: "sbatch My_Step_B"
    services:
      - name: ephemeral service 2
 - name: step C
    location:
      - datanodes
    command: "sbatch My Step C"
    services:
      - name: ephemeral service 2
```

- Steps indicate the « location » of their compute nodes
- Multiple locations are possible for complex jobs (MSA architecture)
- Location can be also « datanodes » for « on the fly » processing



Data Movers in the WDF

```
services:
  - name: ephemeral service 1
    type: NFS
    attributes:
      namespace: {{ NS1 }}
      mountpoint: /mnt/USER/{{ SESSION }}
      flavor: medium
    datamovers:
      - name: datamover1
        trigger: step start
        target: flash
        operation: copy
        elements:
          - "gauges/*.hdf5"
          - "input/*"
```

- To ensure the elements of a namespace are located in the proper storage tier, a data_mover can be activated before (step_start) and after (step_stop) a step
- Operations are either move or copy
- Data Movers are defined at the service level, but activated per step

```
steps:
    - name: step_A
    location:
        - gpu_module
    command: "sbatch My_Step_A"
    services:
        - name: ephemeral_service_1
        datamovers:
        - datamover1
```



Hints

"Hints" are optional information given by users about their future use of data, when the workflow is terminated

```
-intended access: Intended access in the short term (will access, won't change...)
    e.g. intended access="wont change"
-estimated lifetime: Estimated time until the object will be deleted (in seconds)
    e.g. estimated lifetime=2592000 (1 month)
-estimated atime: Estimated time the object will be used (in seconds)
-access period: How often the object will be accessed (in seconds)
    e.g. access period=60 (every minute)
-predefined_policy: Name of a pre-configured policy
   e.g. predefined policy="temporary data"
```



Setting hints

- User Control: CLI
- >iosea-ns {locate|move|copy|release}
- >iosea-ns hints DATASET=My_dataset hint1=value1 hint2=value2 ...

- User Control: through POSIX Ephemeral Services
- >Set_attr on files and directories



Datasets/Namespaces: Command line tools

```
# create namespaces
iosea-ns create my_dataset.my_namespace
iosea-ns create DATASET=my_dataset my_2nd_namespace
# fill my_namespace with a file
io-sea-ns put DATASET=my_dataset NAMESPACE=my_namespace ./gauge.cfg
```

Enables leveraging standard POSIX tools and scripting ls, find, ...



Challenges



Challenges

- Need an enhanced Batch & Resource Manager
 - Workflow Aware
 - Allocating Datanode resources as part of the workflow
 - Sheduling workflows steps rather than isolated jobs
 - To minimize data nodes resources allocation time
- Find the balance between compute nodes, data nodes and back end storage resources
 - New « dimensioning rules » to be invented

