Data Management and File Systems on Expanse

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Ref: HPC training presentation by Mahidhar Tatineni and Rick Wagner

Example Workflow

- Login (ssh) to the supercomputer
  - Copy (git clone) the source code to $HOME
  - Compile your application
- “Upload” input data
  - Copy (Globus transfer) files from a client to project space
  - Split the files into groups to fit into the node local NVMe
- Run batch jobs
  - Copy files from project space to node local NVMe
  - Do analysis
  - Bundle results (tar –zcf) in node local NVMe and copy back to project space
- “Download” results
  - Copy (Globus transfer) files from project space to laptop

Overview

- Example Workflow
- File Systems - Expanse
  - Pros and cons of different file systems
  - Example local scratch usage
  - Lustre File System
  - Impact of usage poor usage patterns on Lustre
- Data Management Using Globus
  - Globus basics
  - Some hard-learned recommendations
  - Resources & references
- Summary


FILE
SYSTEMS
FILES & FILE SYSTEMS

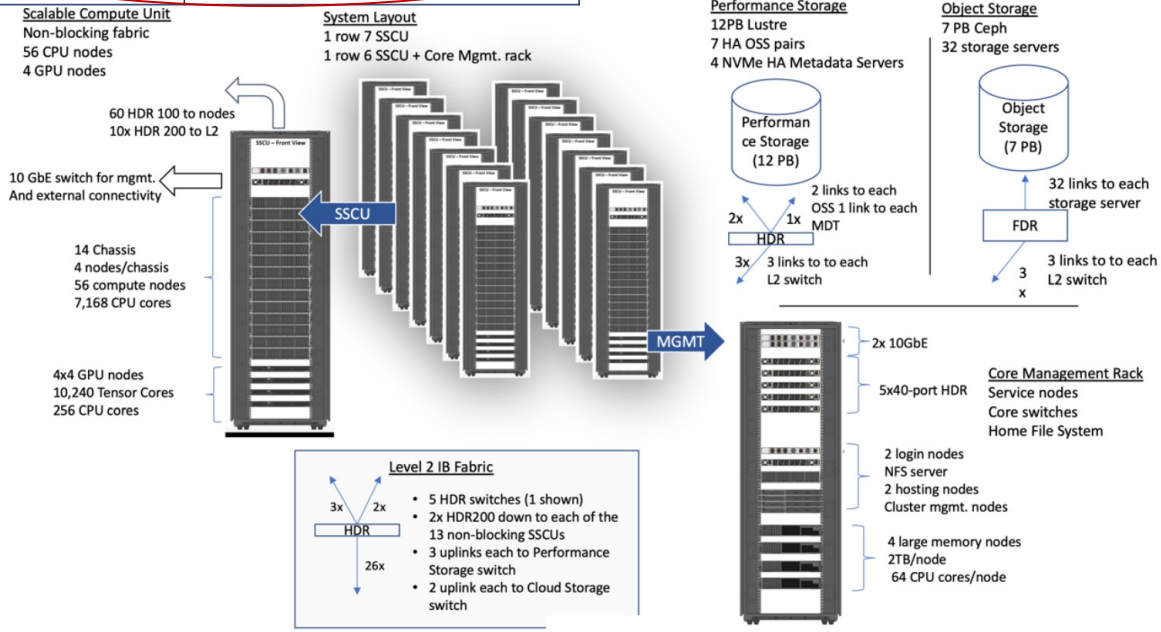
Why File Systems

- Place to store data / files – manage data
- Computations involving 1000s of files – temporary files during genome sequencing, images…
- Large shared files due to checkpointing – weather forecasting, long running machine learning jobs

Expanse System

System Component	Configuration
AMD EPYC (Rome) 7742 Compute Nodes	
Node count	728
Clock speed	2.25 GHz
Cores/node	128
Total # cores	93,184
DRAM/node	256 GB
NVMe/node	1 TB
NVIDIA V100 GPU Nodes	
Node count	52
Total # GPUs	208
GPUs/node	4
GPU Type	V100 SMX2
Memory/GPU	32 GB
CPU cores; DRAM; clock (per node)	40; 384 GB; 2.5 GHz;
CPU	6248 Xeon
NVMe/node	1.6TB
Large Memory Nodes	
Number of nodes	4
Memory per node	2 TB
CPUs	2x AMD 7742/node;

Storage	
Lustre file system	12 PB (split between scratch & allocable projects)
Ceph file system	7 PB Coming soon
Home File system	1 PB



Expanse's tiered storage

- Node local NVMe drives for workloads that don't need to share data files across nodes
- Lustre filesystem for I/O workloads that require high-bandwidth and large capacity shared storage
- Network Files System (NFS) cluster for user home directory storage
- Ceph Object Storage for short-term archival storage and staging data transfers to cloud-based storage (coming soon)

Why Various File Systems

- Performance
- Shared access across nodes
- Backup / long-term
- Quota

Applications and Performance

```
[manu1729@exp-2-09 src]$ mpirun -np 4 ./ior --posix.od
IOR-3.4.0+dev: MPI Coordinated Test of Parallel I/O
Began               : Thu Oct 21 05:47:11 2021
Command line        : ./ior --posix.odirect -F -b 5m -
Machine             : Linux exp-2-09
TestID              : 0
StartTime           : Thu Oct 21 05:47:11 2021
Path                : testFile.00000000
FS                  : 10842.9 TiB   Used FS: 14.0%   I

Options:
api                 : POSIX
apiVersion          :
test filename       : testFile
access              : file-per-process
type                : independent
segments            : 1
ordering in a file  : sequential
ordering inter file : no tasks offsets
nodes               : 1
tasks               : 4
clients per node    : 4
repetitions         : 1
xfersize            : 131072 bytes
blocksize           : 5 MiB
aggregate filesize  : 20 MiB

Results:

access    bw(MiB/s)  IOPS       Latency(s)  block(KiB)
------    ---------  ----       ----------  ----------
write     3.39       27.09      0.135989    5120
read      1249.61    10220      0.000339    5120
```

```
[manu1729@exp-2-09 job_6589251]$ mpirun -np 4 ./ior --posix.o
IOR-3.4.0+dev: MPI Coordinated Test of Parallel I/O
Began               : Thu Oct 21 05:48:56 2021
Command line        : ./ior --posix.odirect -F -b 5m -t 128k
Machine             : Linux exp-2-09
TestID              : 0
StartTime           : Thu Oct 21 05:48:56 2021
Path                : testFile.00000000
FS                  : 915.9 GiB   Used FS: 0.0%   Inodes: 58.

Options:
api                 : POSIX
apiVersion          :
test filename       : testFile
access              : file-per-process
type                : independent
segments            : 1
ordering in a file  : sequential
ordering inter file : no tasks offsets
nodes               : 1
tasks               : 4
clients per node    : 4
repetitions         : 1
xfersize            : 131072 bytes
blocksize           : 5 MiB
aggregate filesize  : 20 MiB

Results:

access    bw(MiB/s)  IOPS       Latency(s)  block(KiB) xfer(K
------    ---------  ----       ----------  ---------- ------
write     1319.96    10606      0.000367    5120       128.00
read      752.81     6024       0.000631    5120       128.00
```

Application Focus

Storage choices should be driven by application need, not just what's available.

Writing a few small files to an NFS server is fine…
writing 1000's simultaneously will wipe out the server.

But, applications need to adapt as they scale.

Expanse File Systems: $HOME

- Location of the home directory – when you login to Expanse
- Network File System (NFS) storage
  - Typically used to store source codes, important files…
  - Storage limit around 100 GB
- Limited number of snapshots (~1-2 months) available. Make offsite copies of anything critical.

Expanse File Systems: Lustre scratch

- Location: /expanse/lustre/scratch/$USER/temp_project
- Lustre File System (LFS) performance storage
  - Typically used to store input / output data, large files…
  - Allows distributed access
  - Storage limit around 1TB
  - Purged after 90 days (creation)
- No Backup

Expanse File Systems: Lustre projects

- Location: /expanse/lustre/projects/…
- Lustre File System (LFS) performance storage
  - Typically used to store input / output data, large files…
  - Project specific data
  - Allows distributed access
  - Storage limit around 2.5 PB
- No Backup

Expanse File Systems: Node Local Storage

- Location: /scratch/$USER/job_$SLURM_JOB_ID…

- Node local NVMe storage
  - Typically used to store large number of files…
  - Fast node-local access
  - Storage limits: compute, shared: 1 TB; gpu, gpu-shared: 1.6 TB; large-shared: 3.2 TB
  - Only accessible from a compute node
  - Purged after the job ends

Expanse File Systems Summary

Path	Purpose	User Access Limits	Lifetime	Globus Access
$HOME	NFS storage; Source code, important files	100 GB	Limited number of snapshots (~1-2 month)	No Git, SVN for repos scp/rsync
/expanse/lustre/scratch/$USER/temp_project	Parallel Lustre FS; temp storage for distributed access	Need-based	No backup	Yes **Collection:** SDSC Expanse Lustre
/expanse/lustre/projects/	Parallel Lustre FS; project storage	Need-based	No backup	Yes **Collection**: SDSC Expanse Lustre
/scratch/$USER/job_$SLURM_JOB_ID	Local NVMe on batch job node fast per-node access	More than 1 TB	Purged after job ends	No

File Systems Guidelines

(a) Lustre scratch space: /expanse/lustre/scratch/$USER/temp_project

- *Meant for storing data required for active simulations*
- *Not backed up and should not be used for storing data long term*
- *90-day purge policy (based on *create* date)*
- *Large block scalable IO*

(b) Compute/GPU node local NVMe storage: /scratch/$USER/job_$SLURM_JOBID

- *Meta-data intensive jobs, high IOPs*
- *File per core type I/O with continuous writes*
- *Purged at end of job*

(c) Lustre projects space: /expanse/lustre/projects/GROUP/$USER

- *Not backed up*
- *Meant for storing data needed for duration of project - an example is reference datasets*

(d) Home directory (/home/$USER): *Only for source files, libraries, binaries.* ****Do not* use for I/O intensive jobs.***

Example script showing local scratch use
/cm/shared/examples/sdsc/localscratch

Localscratch-slurm.sb

```
#!/bin/bash
#SBATCH --job-name="localscratch"
#SBATCH --output="localscratch.%j.%N.out"
#SBATCH --partition=shared
#SBATCH --account=XYZ123
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=16
#SBATCH --export=ALL
#SBATCH -t 01:30:00

#Copy binary to SSD
#Can also copy inputs there if needed
cp IOR-mpiio.exe /scratch/$USER/job_$SLURM_JOBID

#Change to local scratch (SSD) and run IOR benchmark
cd /scratch/$USER/job_$SLURM_JOBID

#Run IO benchmark
module reset
module load gcc/10.2.0
module load openmpi/4.0.4
module load sdsc
ibrun -np 16 ./IOR-mpiio.exe -F -t 1m -b 1g -v -v >
IOR.out.$SLURM_JOBID

#Copy output file back
cp IOR.out.$SLURM_JOBID $SLURM_SUBMIT_DIR
```

Sample IOR Output

```
Summary:
        api                = POSIX
        test filename      = testFile
        access             = file-per-process
        pattern            = segmented (1 segment)
        ordering in a file = sequential offsets
        ordering inter file= no tasks offsets
        clients            = 16 (16 per node)
        repetitions        = 1
        xfersize           = 1 MiB
        blocksize          = 1 GiB
        aggregate filesize = 16 GiB

Using Time Stamp 1635794780 (0x61803f5c) for Data Signature
Commencing write performance test.
Mon Nov  1 12:26:20 2021

access    bw(MiB/s)  block(KiB) xfer(KiB)  open(s)    wr/rd(s)   close(s) total(s)  iter
------    ---------  ---------- ---------  --------   --------   -------- --------   ----
write     4147       1048576    1024.00    0.002891   3.95       0.974847   3.95       0    XXCEL
[RANK 000] open for reading file testFile.00000000 XXCEL
Commencing read performance test.
Mon Nov  1 12:26:24 2021

read      3988       1048576    1024.00    0.002485   4.11       3.68       4.11       0    XXCEL
Operation  Max (MiB)  Min (MiB)  Mean (MiB)   Std Dev  Max (OPs)  Min (OPs)  Mean (OPs)   Std Dev  Mean (s)  Op grep #Tasks tPN
 reps  fPP reord reordoff reordrand seed segcnt blksiz xsize aggsize

---------  ---------  ---------  ----------   -------  ---------  ---------  ----------   -------  --------
write        4147.15    4147.15     4147.15      0.00    4147.15    4147.15     4147.15      0.00   3.95066   16 16 1 1 0 1 0 0
 1 1073741824 1048576 17179869184 -1 POSIX EXCEL
read         3988.35    3988.35     3988.35      0.00    3988.35    3988.35     3988.35      0.00   4.10796   16 16 1 1 0 1 0 0
 1 1073741824 1048576 17179869184 -1 POSIX EXCEL

Max Write: 4147.15 MiB/sec (4348.60 MB/sec)
Max Read:  3988.35 MiB/sec (4182.09 MB/sec)

Run finished: Mon Nov  1 12:26:29 2021
```

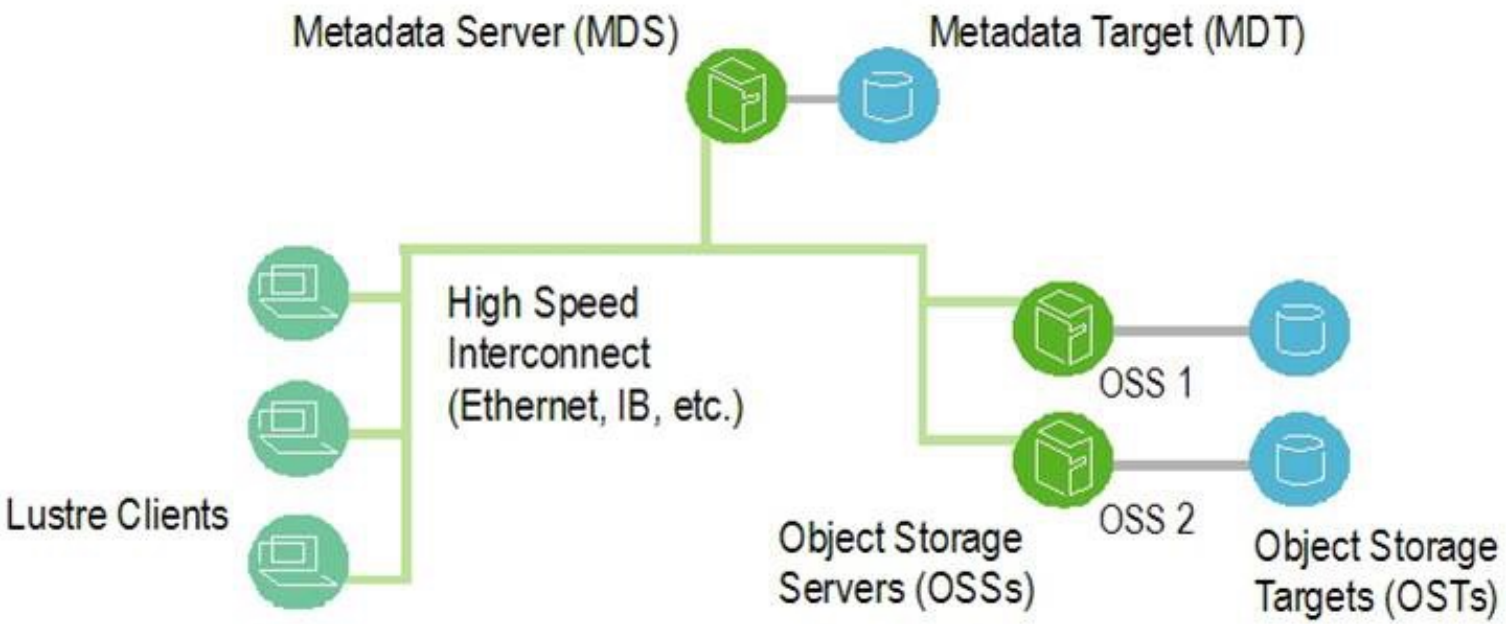
Order of Magnitude Guide

Storage	file/directory	file sizes	BW
Local HDD	1000s	GB	100 MB/s
Local NVMe	1000s	GB	1000 MB/s
RAM FS	10000s	GB	Several GB/s
NFS	100s	GB	100 MB/s
Lustre	100s	TB	100 GB/s

Local file systems are good for small and temporary files (low latency, modest bandwidth)

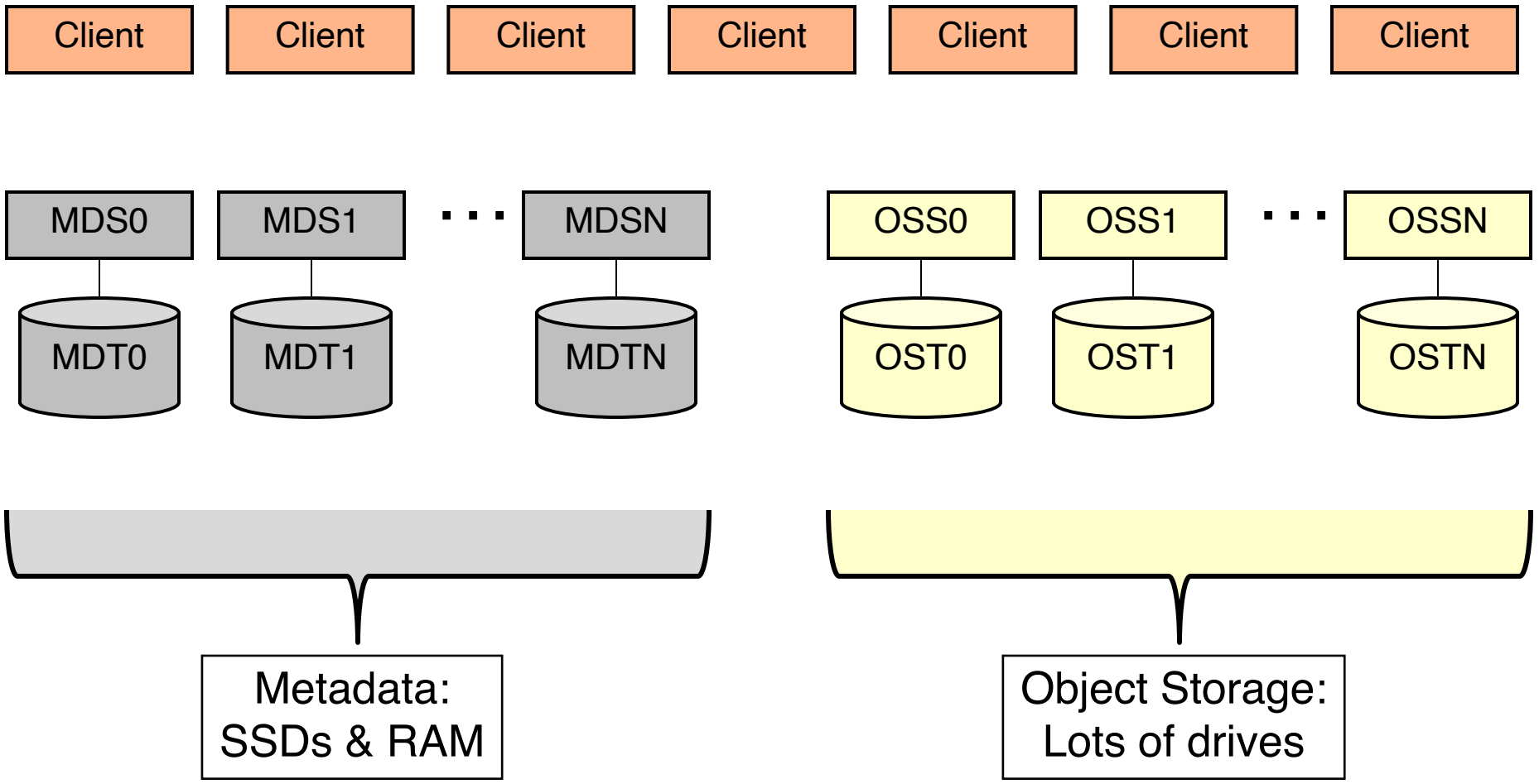
Parallel file systems very convenient for sharing data between the nodes (high latency, high bandwidth)

Lustre File System



Ref: Cornell Virtual Workshop

A Typical LFS

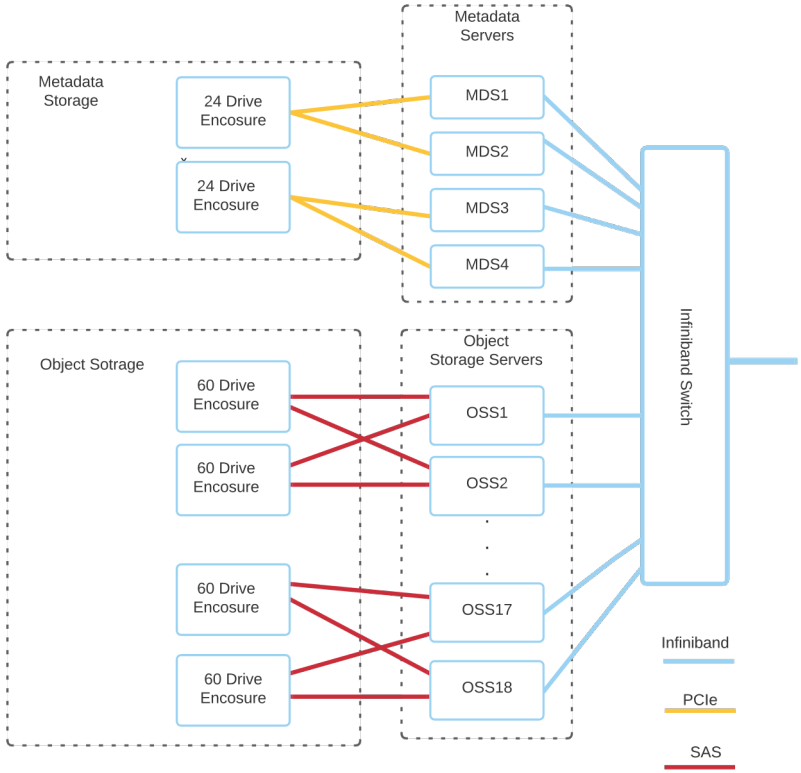


Expanse Lustre File System Architecture

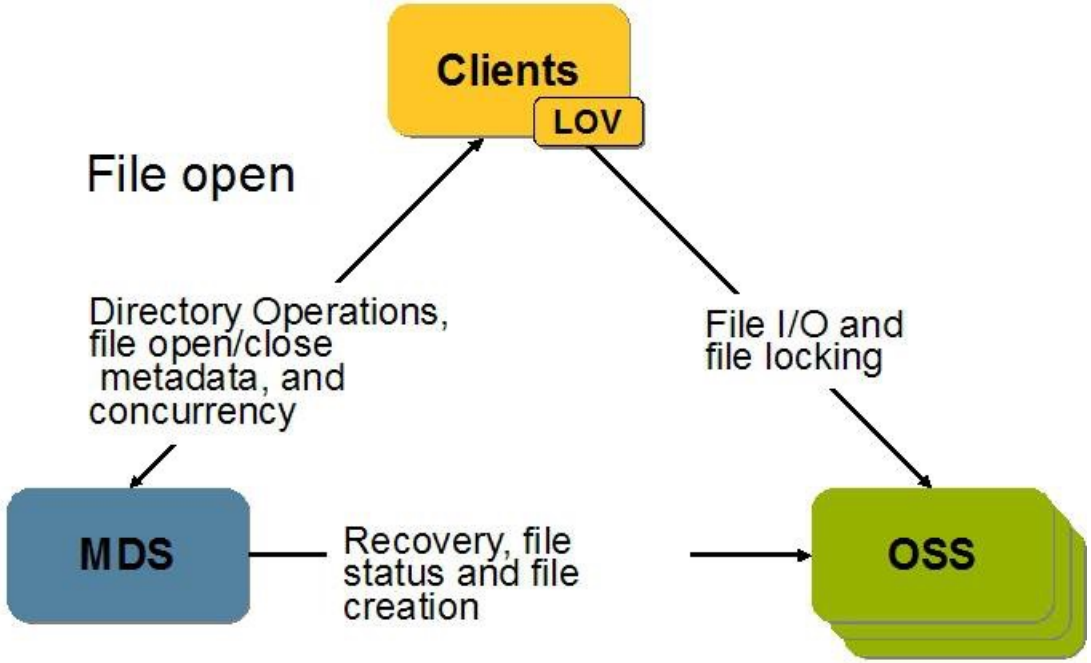
- 12 Peta Bytes of RAW capacity, approx. 11 PB formatted
- File Capacity of approx. 3 billion files.
- 140 GB/s Filesystem Bandwidth
- 200K IOPS
- Data on MDT (DoM) for small file performance

4 Lustre MDS	
Processor	2 X AMD Epyc 7302 (16 Cores)
Memory	512 GB (16 X 32GB DDR4 3200)
MDT Drives	24 X 3.8 TB NVMe per pair
Interconnect	InfiniBand HDR 200
System Drives	2 X 240 GB Intel SSDs

18 Lustre OSS	
Processor	1 AMD Epyc 7402 (24 Cores)
Memory	512 GB (16 X 32 GB DDR4 3200)
JBODS	2 Cross Connected 60 Bay JBODS
OSS Drives	120 X 14 TB 7200 SAS Drives
Interconnect	InfiniBand HDR 200
System Drives	2 X 240 GB Intel SSDs



LFS Interactions



Ref: Cornell Virtual Workshop

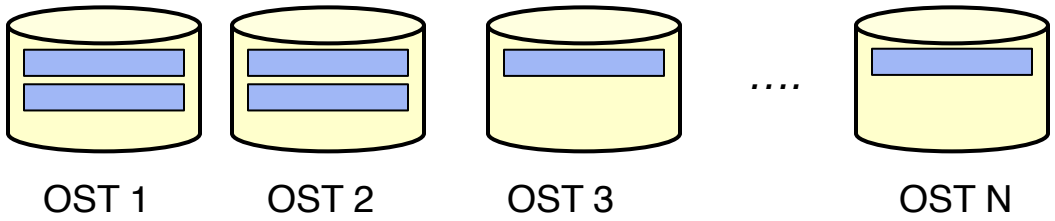
File View

Logical view of a file with N+2 segments

Stripe count = N

Stripe size = sz

Physical view of the file across OSTs



Why is striping useful?

- a way to store a large file
- file can be accessed in parallel, increasing the bandwidth

LFS Commands

lfs help – lists all options

lfs osts – lists all the OSTs

lfs mdts – lists all the MDTs

lfs getstripe – retrieves the striping information of a file / directory

lfs setstripe – sets striping information of a file / directory

LFS Commands: getstripe

```
-bash-4.1$ lfs getstripe testout
testout
lmm_stripe_count:   1
lmm_stripe_size:    1048576
lmm_pattern:        1
lmm_layout_gen:     0
lmm_stripe_offset:  43
              obdidx                 objid                 objid                 group
                  43               8979631               0x8904af                     0

-bash-4.1$ lfs getstripe --stripe-count testout
1
-bash-4.1$ lfs getstripe --stripe-size testout
1048576
```

LFS Commands: setstripe

lfs setstripe -c 16 testout

-bash-4.1$ lfs getstripe testout
testout
lmm_stripe_count: 16
lmm_stripe_size: 1048576
lmm_pattern: 1
lmm_layout_gen: 0
lmm_stripe_offset: 89

obdidx	objid	objid	group
89	9202813	0x8c6c7d	0
45	9819070	0x95d3be	0

.....

LFS Commands: setstripe

```
bash-4.1$ lfs setstripe -c -1 test1
bash-4.1$ lfs getstripe test1
test1
lmm_stripe_count:   96
lmm_stripe_size:    1048576
lmm_pattern:        1
lmm_layout_gen:     0
lmm_stripe_offset:  65
              obdidx                objid                objid                group
                  65              9738084              0x949764                    0
                  41              9153699              0x8baca3                    0
                                  ..............................
```

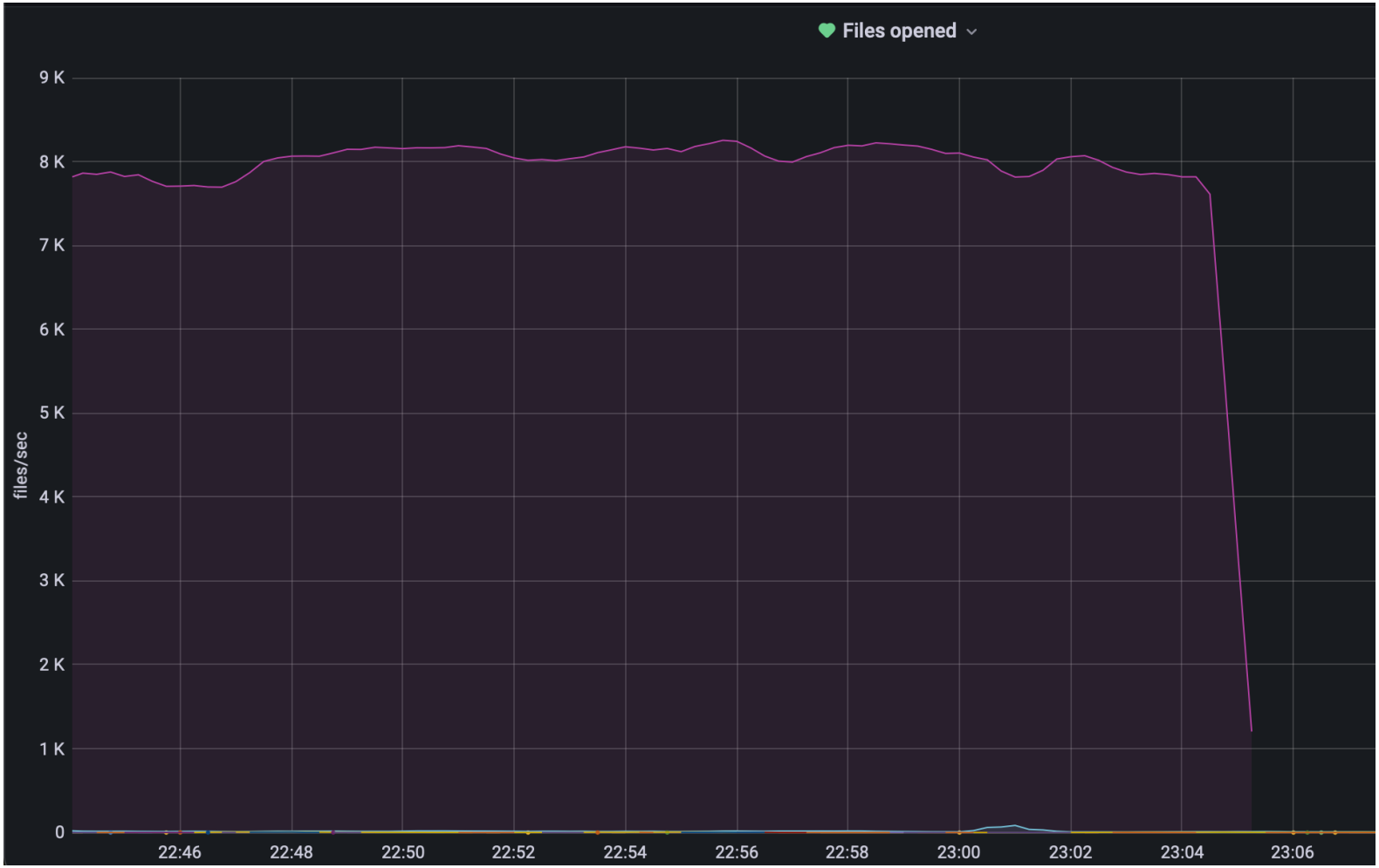
LFS Commands: setstripe

```
-bash-4.1$ mkdir dir
-bash-4.1$ lfs setstripe -c 4 dir
-bash-4.1$ vi dir/test
-bash-4.1$ lfs getstripe dir/test
dir/test
lmm_stripe_count:   4
lmm_stripe_size:    1048576
lmm_pattern:        1
lmm_layout_gen:     0
lmm_stripe_offset:  43
              obdidx                objid                objid                group
                  43              8979901           0x8905bd                    0
                  25             10609192           0xa1e228                    0
```

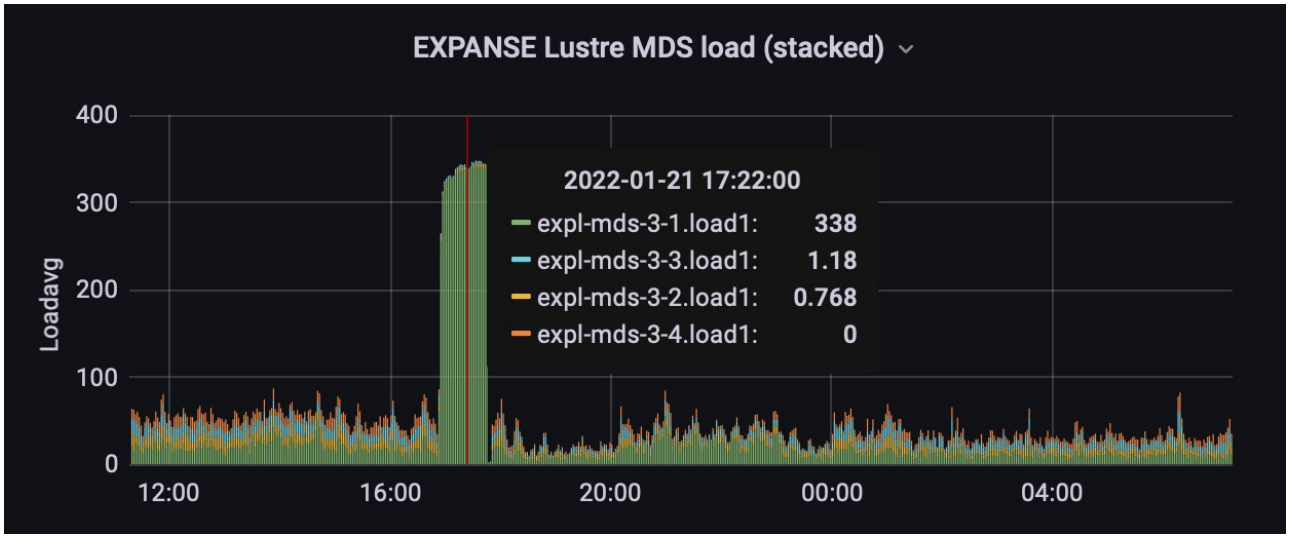
LFS Usage Guidelines

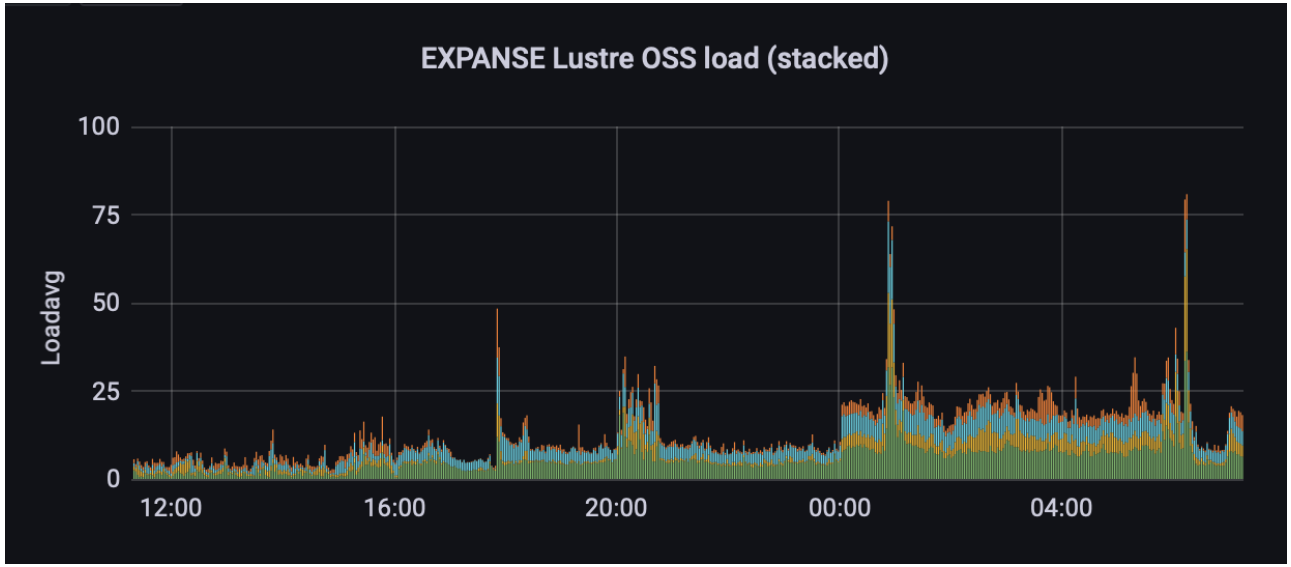
- Avoid certain operations
  - ls -l, ls with color, frequent file opens/closes
  - find, du, wildcards (ls *.out)
  - Why??
  - Try /bin/ls -U instead of ls -l
- Select appropriate stripe count / size
  - Best case selection is complicated
- Do not store too many files in one directory

Example of IOPs load from ill-designed IO workflow

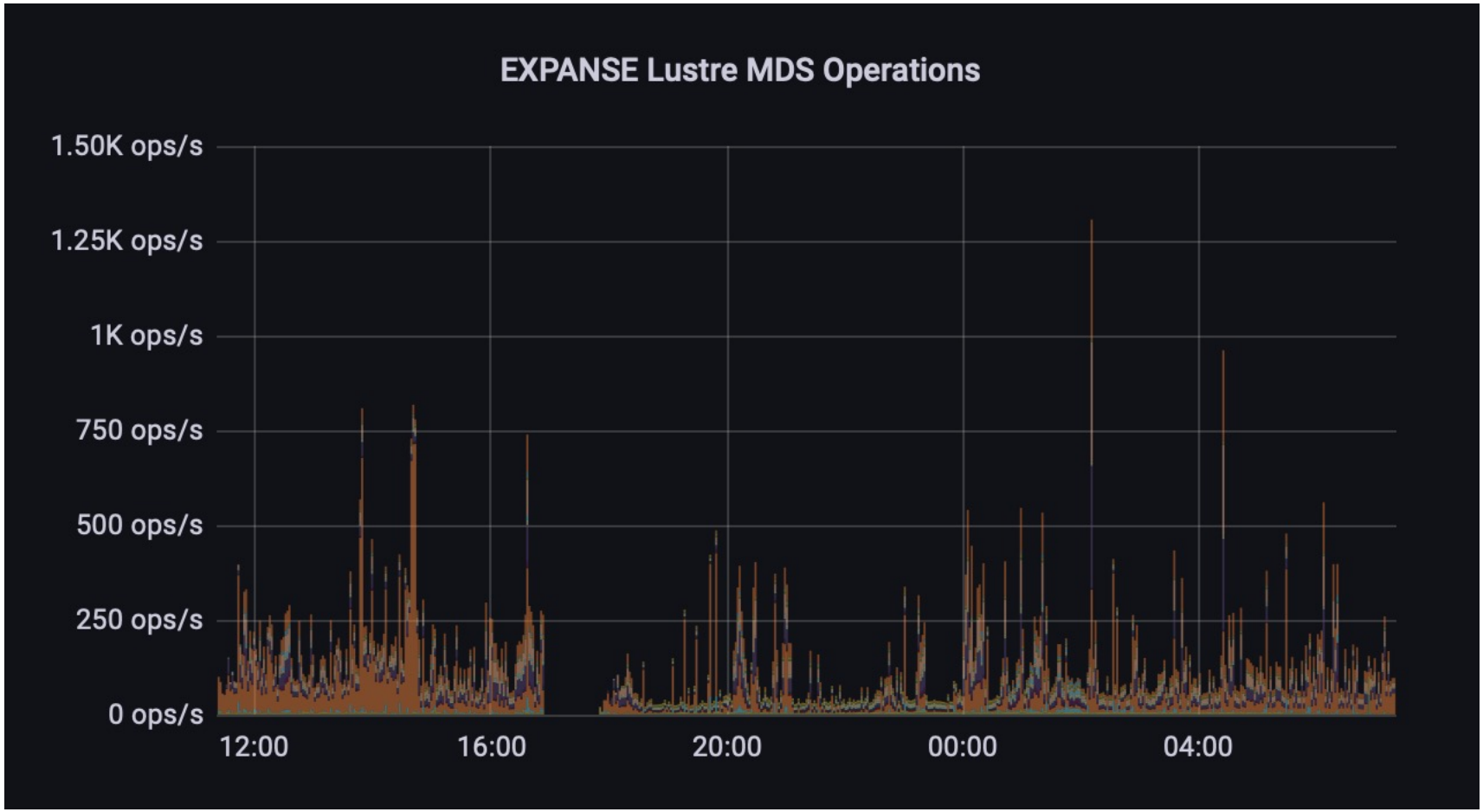


Impact on Filesystem Servers





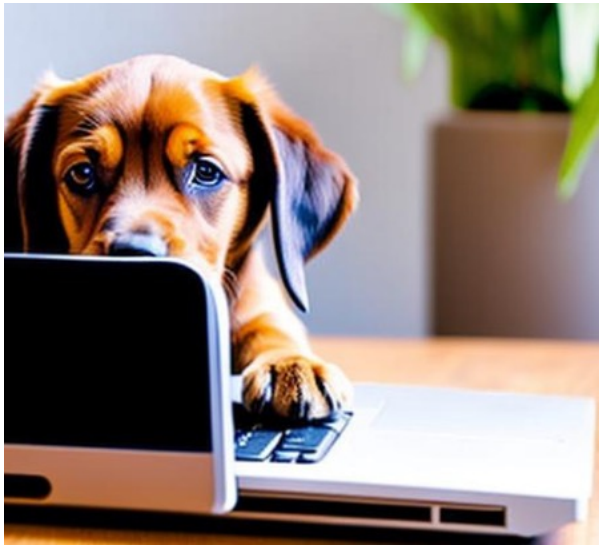
Impact on Filesystem Servers



Data Management Using Globus

(puppies optional)

globus



What is Data Management?

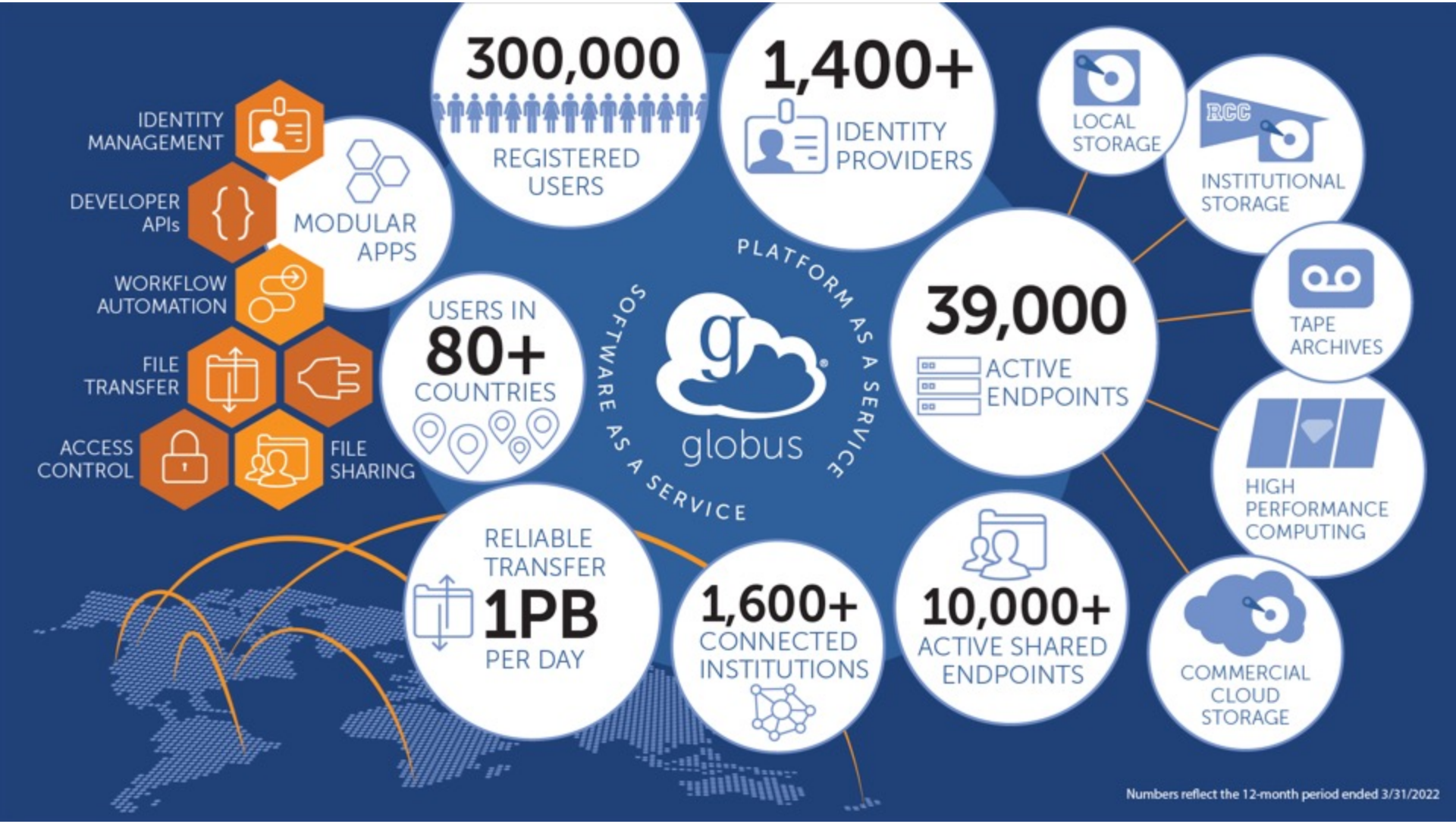
- Managing data before / after computation
  - data collection, copy, sync
- Managing data during computation
  - staging, generation
- Data provenance and integrity
- Enabling data discovery and reuse
- Answering the questions:
  - Can you find the files you need?
  - Do you know what data you have?
  - Can you access data where you need to?

About Globus

- Globus is a non-profit service developed and operated by the University of Chicago
- Free for academic & research use
- Supported by subscriptions from universities, major labs, etc.
- Has a lot of capabilities
- Today we're focusing on the basics
  - Transferring (copying) data between collections

https://www.globus.org

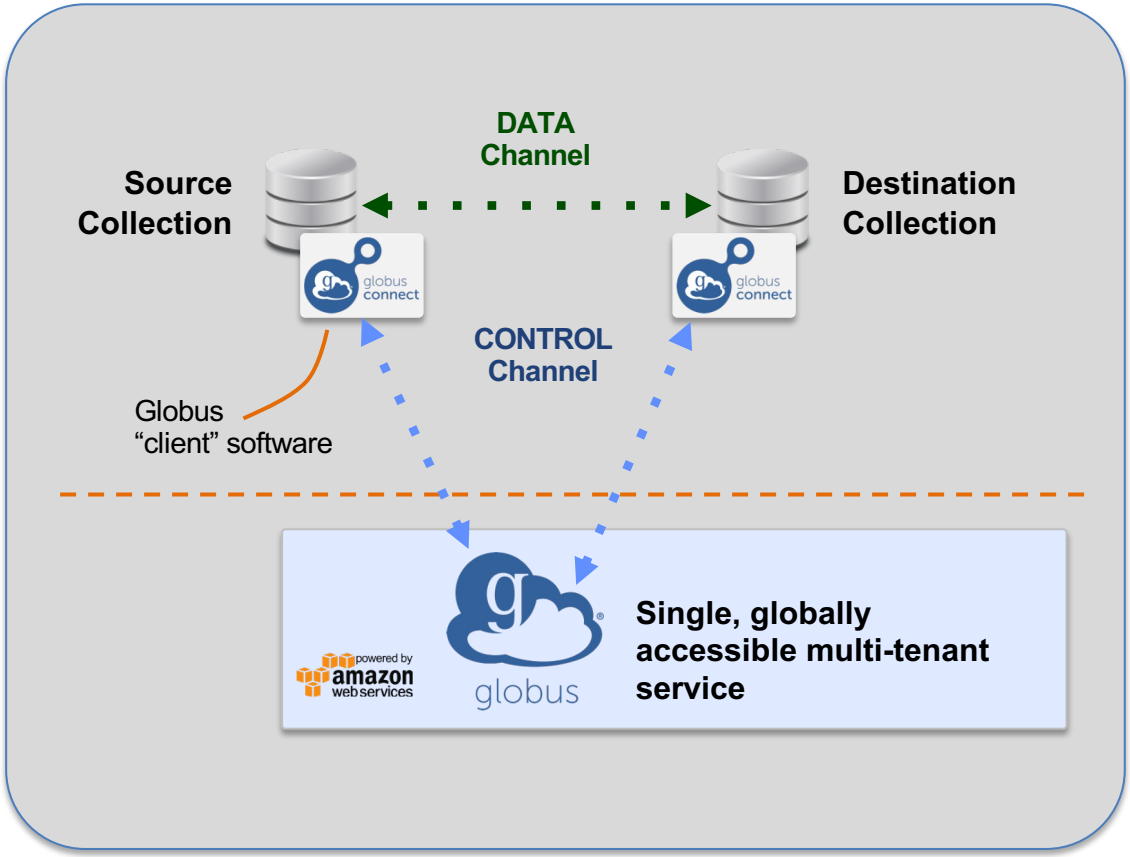
Globus Adoption Mid-2022



Globus Bread & Butter: Reliably Copying Files

Reliability:

- Get the same data from source to destination
- Deal with storage & network failures
- Retry until copied
- Verify the data after transfer



Globus Connect

…makes a storage system a Globus endpoint

Globus Connect Personal

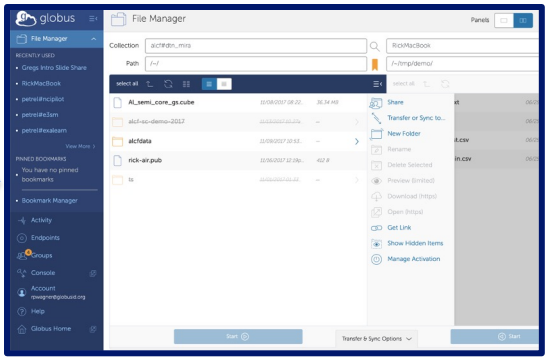
- Installers do not require admin access
- Zero configuration; auto updating
- Handles NATs
- Installs in seconds – easy to delete
- Runs on Linux, OS X, Windows
- This is probably what you want

Globus Connect Server

- Multi-user setup
- Linux (RedHat, Ubuntu, etc.)
- SDSC runs this
- May be deployed at your institution

Globus Interfaces

globus



Web

```
(globus-cli) jupiter:~ vas$ globus
Usage: globus [OPTIONS] COMMAND [ARGS]...

Options:
  -v, --verbose              Control level of output
  -h, --help                 Show this message and exit.
  -F, --format [json|text]   Output format for stdout. Defaults to text
  --map-http-status TEXT     Map HTTP statuses to any of these exit codes:
                             0,1,50-99. e.g. "404=50,403=51"

Commands:
  bookmark        Manage Endpoint Bookmarks
  config          Modify, view, and manage your Globus CLI config.
```

CLI

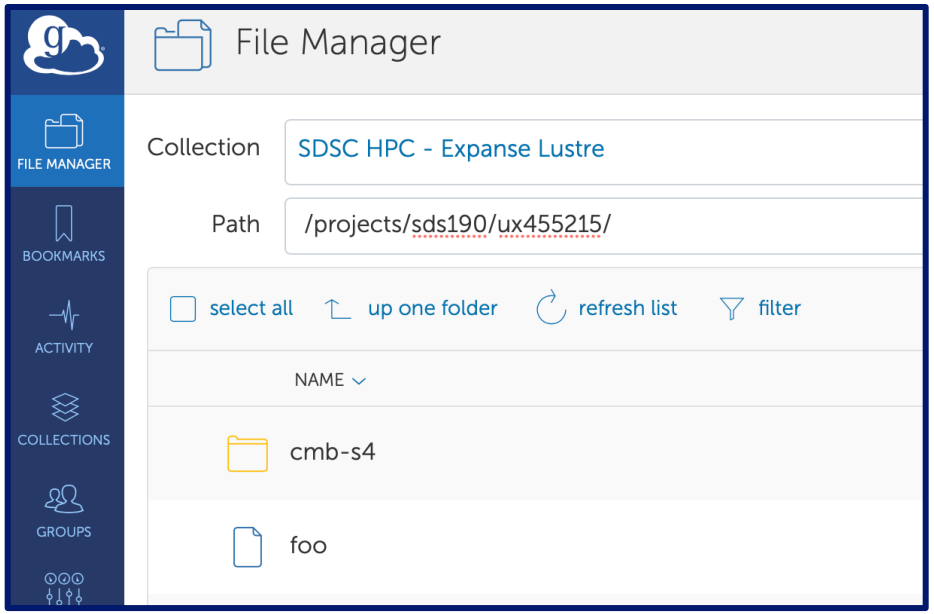
```
GET /endpoint/go%23ep1
PUT /endpoint/vas#my_endpt
200 OK
X-Transfer-API-Version: 0.10
Content-Type: application/json
…
```

Rest API

Complexity scales with your needs.

Using Globus at SDSC
(Very similar at other HPC centers)

- Log in to Globus using ACCESS CI
  - Create an account
  - Or link to existing one
- Search for ”SDSC HPC” collections
- Navigate to your folders and transfer data



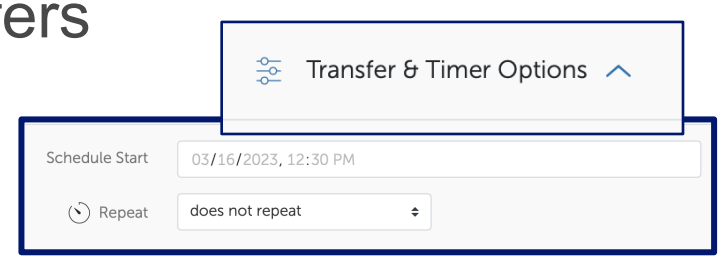
SDSC HPC Globus Collections

Collection	System	Path
SDSC HPC - Expanse Lustre	Expanse	`/expanse/lustre`
SDSC HPC - Projects	Expanse	`/expanse/projects`
SDSC HPC - TSCC Scratch	TSCC	`/oasis/tscc/scratch`

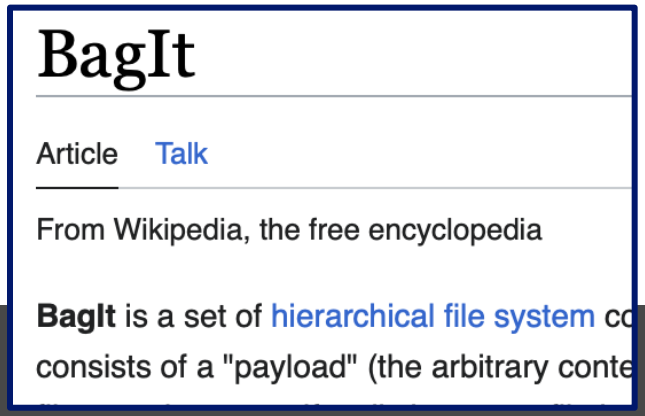
- **Several other collections at SDSC and UCSD**
- **Search for collections where you're trying to get data to and from**
  - Remember that adoption slide!

Recommendations

- You can schedule recurring transfers
  - Get results as the job progresses!



- Bundle your data
  - Lots of files make life challenging
  - Use manifests (checksums) and archives (tar & zip)
  - Helps you to define datasets
  - Checkout `bdbag`
    https://github.com/fair-research/bdbag
  - Extends BagIt, simple format used by libraries & data repositories



https://docs.globus.org

globus docs

APIs How To Guides Support

Harness the power of the Globus research data management cloud.

Manage Your Data

MOVE AND SHARE YOUR DATA
Get started by transferring and sharing your data using the Globus Web app

ACCESS DATA ON YOUR COMPUTER
Move data to or from any modern Windows, macOS or Linux machine using Globus

COMMAND LINE INTERFACE
Use the Globus CLI to transfer and share data and much more

VIDEO TUTORIALS
Watch tutorials on everything from transferring data to automating tasks

SECURE YOUR DATA

Integrate Your App

TRANSFER & SHARING
Integrate transfer and data sharing in your app

AUTH
Leverage a standards-based identity broker that facilitates authentication and authorization from over 1,000 identity providers

GROUPS
Create and manage groups and their members

SEARCH
Store data, set visibility policies, and retrieve data through search queries

AUTOMATE TASKS

Make Your Data Accessible

GLOBUS CONNECT SERVER
Create a Globus endpoint on multi-user systems such as lab servers, campus research computing clusters, and other high-performance computing or storage resources.

GLOBUS CONNECT PERSONAL
Move data to or from any modern Windows, macOS or Linux machine using Globus

PREMIUM CONNECTORS
Enable a uniform interface for accessing, moving, and sharing across a diverse set of storage systems

Summary

- Data Management is important in all stages of your computational workflow - before, during, and after simulations are done.

- Important for performance and scalability of your computations and workflow. ***Poor IO choices can lead to systemwide issues impacting *all* other users.***

- Data provenance and integrity are important considerations.

- Several filesystem options available on Expanse, ranging from node local NVMe that can handle high IOPs workloads to the large Lustre parallel filesystem that can handle large scale large block IO. ***Choose the right filesystem for your workload depending on IOPs (metadata load) and performance considerations.***

- Always have offsite (multiple) backups of anything critical. Expanse Lustre scratch is on a 90-day purge policy => ***backup anything important.***

Thank You!

Questions?