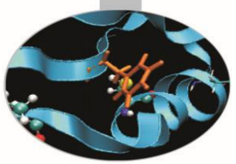
Management of large scientific data

Giovanni Morelli, Giuseppe Fiameni

{g.morelli, g.fiameni}@cineca.it

SuperComputing Applications and Innovation Department

Agenda



Bulk data transfer

Basic concepts, tools and techniques

Data post-processing

Remote visualization

Data management across the Europe

The EUDAT project overview

Agenda

Bulk data transfer

Basic concepts, tools and techniques

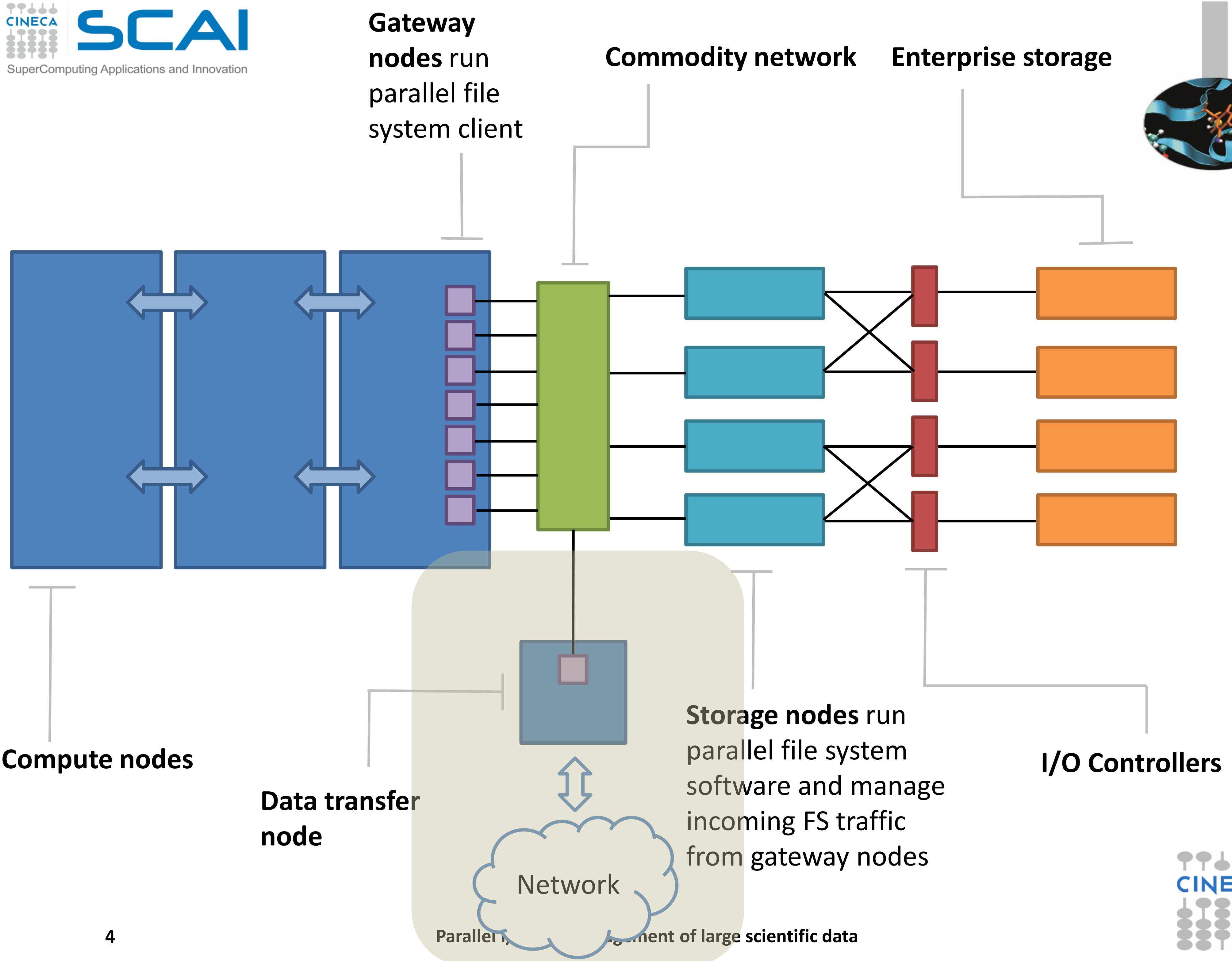
*Bulk data transfer is a software application feature that uses data **compression, data blocking and buffering** to optimize transfer rates when moving large data files*

Data post-processing

Remote visualization

Data management across the Europe

The EUDAT project overview



Gateway nodes run parallel file system client
Commodity network
Enterprise storage
Compute nodes
Data transfer node
Network
Storage nodes run parallel file system software and manage incoming FS traffic from gateway nodes
I/O Controllers

Bulk data movement

- **The problem**
- Involved components
  - Network architecture
  - Dedicated hosts
  - Software tools

PHOTO: DAVIES & STARR

Bulk Data Movement

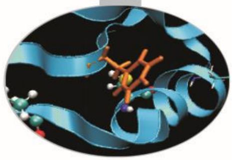
- Common task at all data scales
- Driven by collaboration, distributed resources
  - Computing centers
  - Facilities
  - Major instruments (e.g. LHC)
- Fundamental to the conduct of science (scientific productivity follows data locality)
- Data sets of 200GB to 5TB are now common
- Often a difficult task for various reasons
- Storage capacity grows faster with respect to Public Network bandwidth

Time to copy 1TB

- **10 Mb/s network:** 300 hrs (12.5 days)
- **100 Mb/s network:** 30 hrs
- **1 Gb/s network:** 3 hrs (are your disks fast enough?)
- **10 Gb/s network:** 20 minutes (need *really fast disks and* file system)
- **Compare these speeds to:**
  - USB 2.0 portable disk
    - 60 MB/sec (480 Mbps) peak
    - 20 MB/sec (160 Mbps) reported on line
    - 15-40 hours to load 1 Terabyte

SuperComputing Applications and Innovation

Data Throughput – Transfer Times



Bandwidth Requrements to move Y Bytes of data in Time X

Bits per Second Requirements

	1H	8H	24H	7Days	30Days
10PB	25,020.0 Gbps	3,127.5 Gbps	1,042.5 Gbps	148.9 Gbps	34.7 Gbps
1PB	2,502.0 Gbps	312.7 Gbps	104.2 Gbps	14.9 Gbps	3.5 Gbps
100TB	244.3 Gbps	30.5 Gbps	10.2 Gbps	1.5 Gbps	339.4 Mbps
10TB	24.4 Gbps	3.1 Gbps	1.0 Gbps	145.4 Mbps	33.9 Mbps
1TB	2.4 Gbps	305.4 Mbps	101.8 Mbps	14.5 Mbps	3.4 Mbps
100GB	238.6 Mbps	29.8 Mbps	9.9 Mbps	1.4 Mbps	331.4 Kbps
10GB	23.9 Mbps	3.0 Mbps	994.2 Kbps	142.0 Kbps	33.1 Kbps
1GB	2.4 Mbps	298.3 Kbps	99.4 Kbps	14.2 Kbps	3.3 Kbps
100MB	233.0 Kbps	29.1 Kbps	9.7 Kbps	1.4 Kbps	0.3 Kbps

This table available at **http://fasterdata.es.net**

Bulk data movement

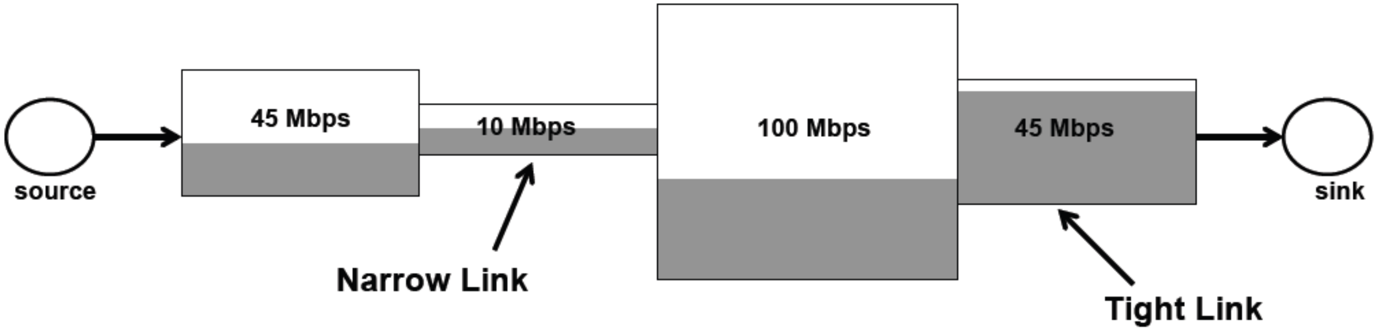
- The problem
- Involved components
  - **Network architecture**
  - Dedicated hosts
  - Software tools

PHOTO: DAVIES & STARR

Terminology

The term "Network Throughput" is vague and should be avoided

- **Capacity**: link speed
  - **Narrow Link**: link with the lowest capacity along a path
  - Capacity of the end-to-end path = capacity of the narrow link
- **Utilized bandwidth**: current traffic load
- **Available bandwidth**: capacity – utilized bandwidth
  - **Tight Link**: link with the least available bandwidth in a path
- **Achievable bandwidth**: includes protocol and host issues



Courtesy of the Berkley Lab

Network architecture

- Most LANs are not purpose-built for science traffic they carry many types of traffic
  - Desktop machines, laptops, wireless
  - VOIP
  - HVAC control systems
  - Financial systems, HR
  - *Some science data coming from someplace*
- Bulk data transfer traffic is typically very different than enterprise traffic

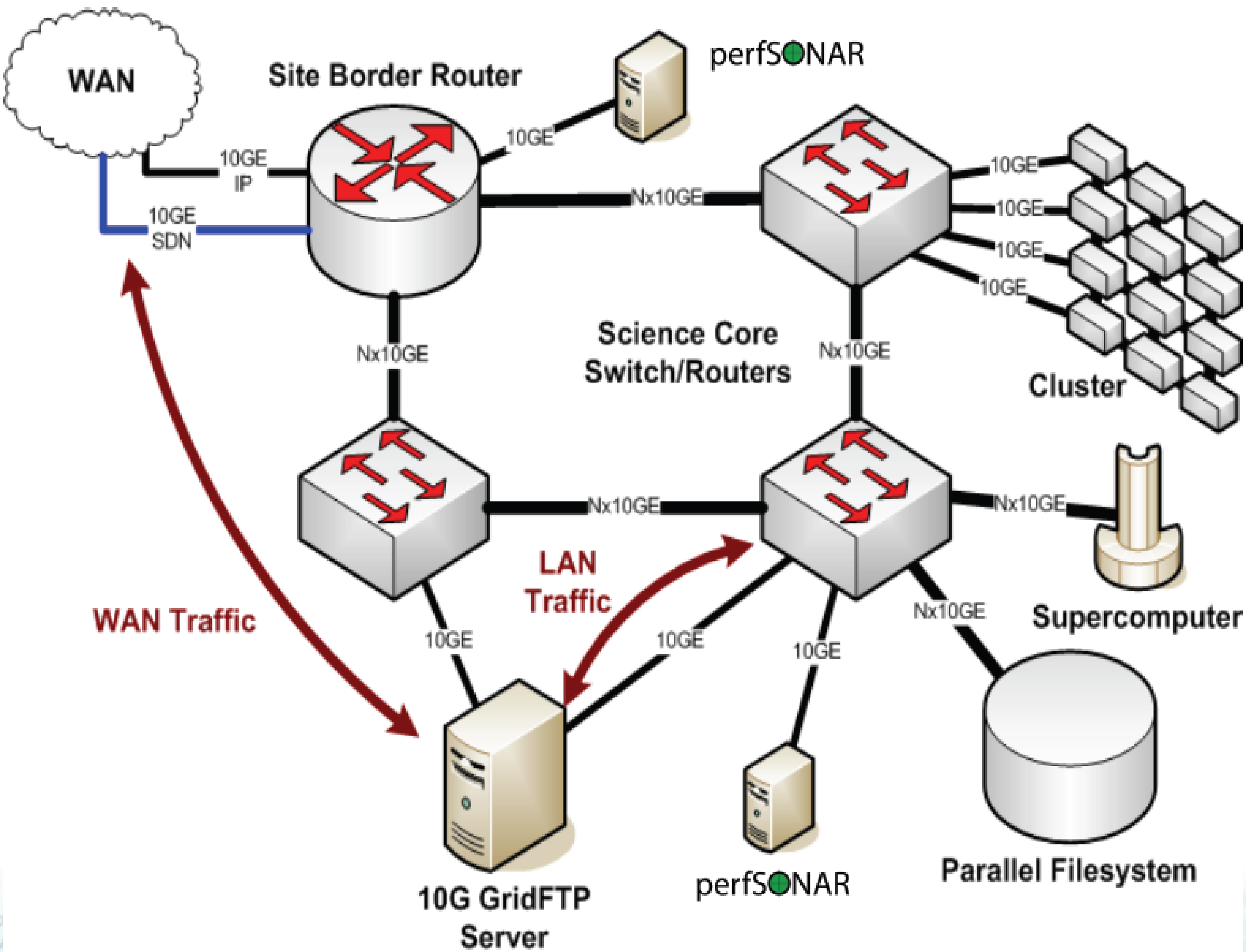
Bulk data movement

- The problem
- Involved components
  - Network architecture
  - **Dedicated hosts**
  - Software tools

Data transfer nodes

- **Reasons for dedicated hosts**
  - One thing to test and tune
  - One place for large WAN flows to go (it's easier to give one host a special configuration than to do this for all workstations)
  - One set of firewall exceptions

Internal/external traffic

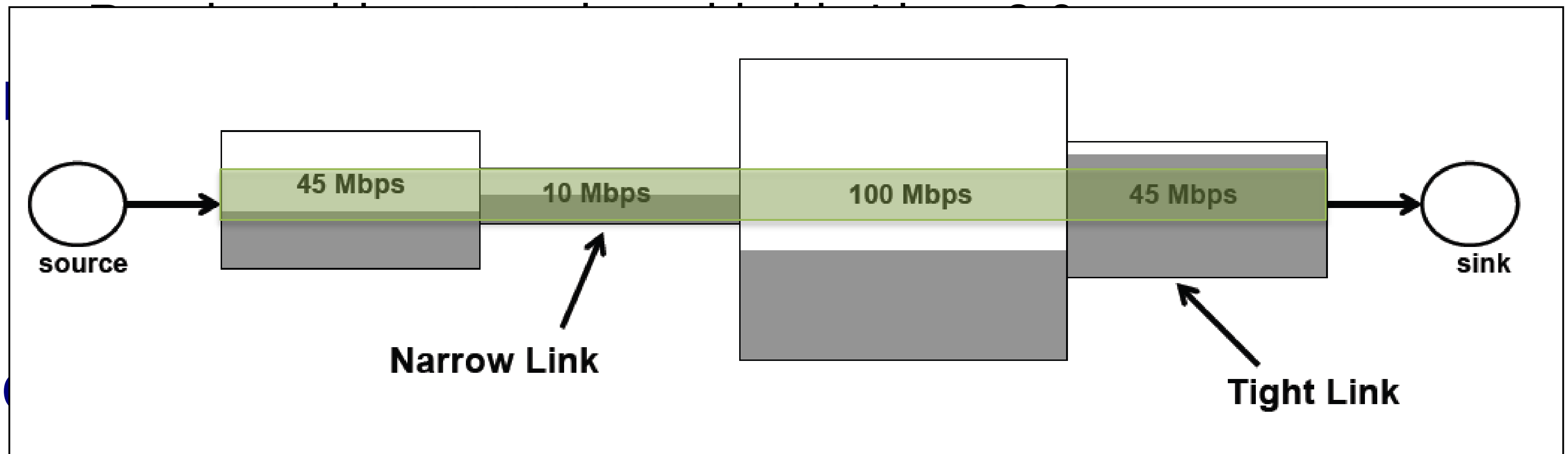


Host tuning - TCP

- TCP tuning commonly refers to the proper configuration of buffers that correspond to TCP windowing
- Historically TCP tuning parameters were host-global, with exceptions configured per-socket by applications
  - Applications had to understand the network in detail, and know how far away clients were
  - Some applications did this – most did not
- Solution: auto-tune TCP connections within preconfigured limits

Buffer autotuning

- To solve the buffer tuning problem, Linux OS added TCP Buffer autotuning
  - Sender-side TCP buffer autotuning introduced in Linux 2.4



  - Linux 2.6: 256K to 4MB, depending on distribution
  - FreeBSD 7: 256K
  - Windows 7: 16M
  - Mac OSX 10.5: 8M
- Some defaults are still wrong!

Autotuning settings (Max 16MB)

- **Linux 2.6**

```
net.core.rmem_max = 16777216
net.core.wmem_max = 16777216
# autotuning min, default, and max number of bytes to
  use
net.ipv4.tcp_rmem = 4096 87380 16777216
net.ipv4.tcp_wmem = 4096 65536 16777216
```

- **FreeBSD 7.0**

```
net.inet.tcp.sendbuf_auto=1
net.inet.tcp.recvbuf_auto=1
net.inet.tcp.sendbuf_max=16777216
net.inet.tcp.recvbuf_max=16777216
```

- **OSX 10.5 (“Self-Tuning TCP”)**

```
kern.ipc.maxsockbuf=16777216
```

Congestion control

- TCP senses network congestion by detecting packet loss
- Historically (TCP Reno) TCP used AIMD (Additive Increase, Mutiplicative Decrease) for window sizing in response to loss
- After loss, window opens back up very slowly
  - causes very poor performance
- Newer algorithms, available in Linux, offer higher performance than Reno
  - Cubic (now the default in several Linux distributions)
  - HTCP (Hamilton)

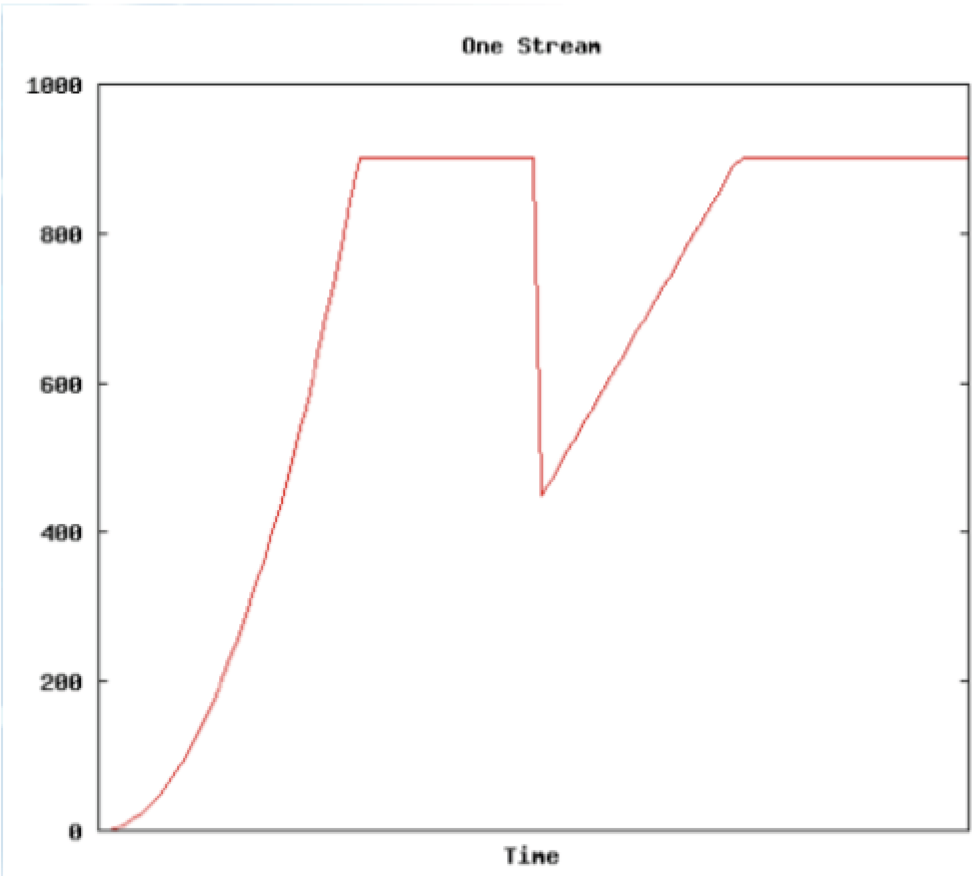
Bulk data movement

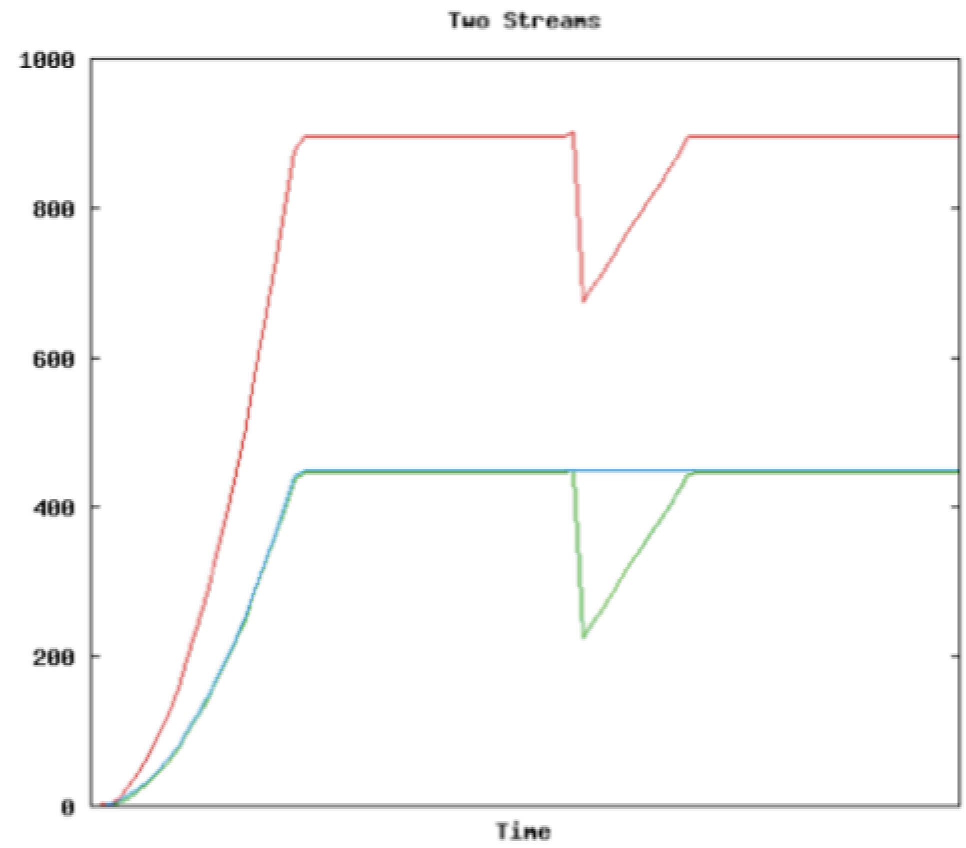
- The problem
- Involved components
  - Network architecture
  - Dedicated hosts
  - **Software tools**

Data transfer tools

- **Parallelism is key**
  - It is much easier to achieve a given performance level with four parallel connections than one connection
  - Several tools offer parallel transfers
- **Latency interaction is critical**
  - Wide area data transfers have much higher latency than LAN transfers
  - Many tools and protocols assume a LAN
  - Examples: SCP/SFTP, HPSS mover protocol

Parallel Streams Help With TCP Congestion Control Recovery Time





Sample data transfer rate

Using the right tool is very important

- **SCP/SFTP: 10 Mb/s**
  - standard Unix file copy tools
  - fixed 1 MB TCP window in OpenSSH
    - only 64 KB in OpenSSH versions < 4.7
- **FTP: 400-500 Mb/s**
  - assumes TCP buffer autotuning
  - Parallel stream FTP: 800-900 Mbps

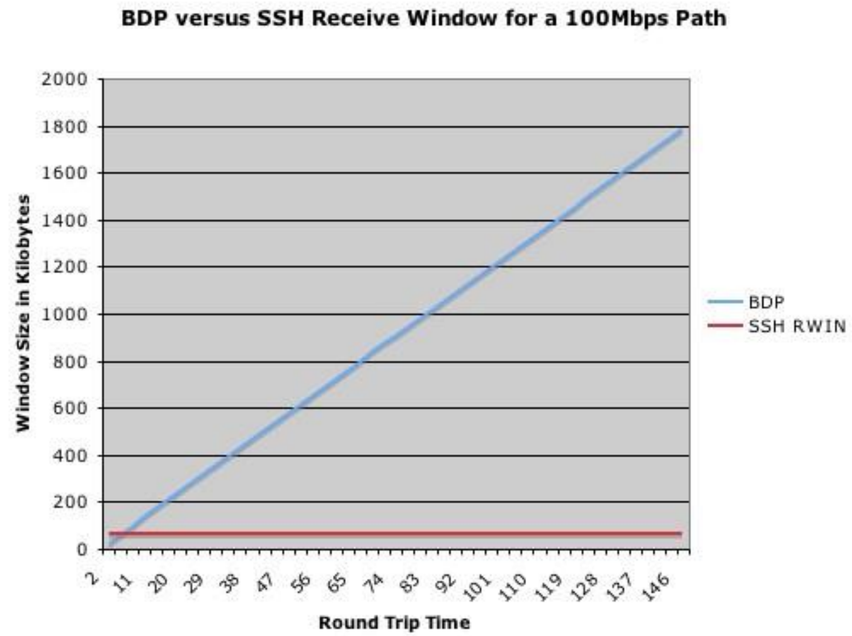
Why Not Use SCP or SFTP?

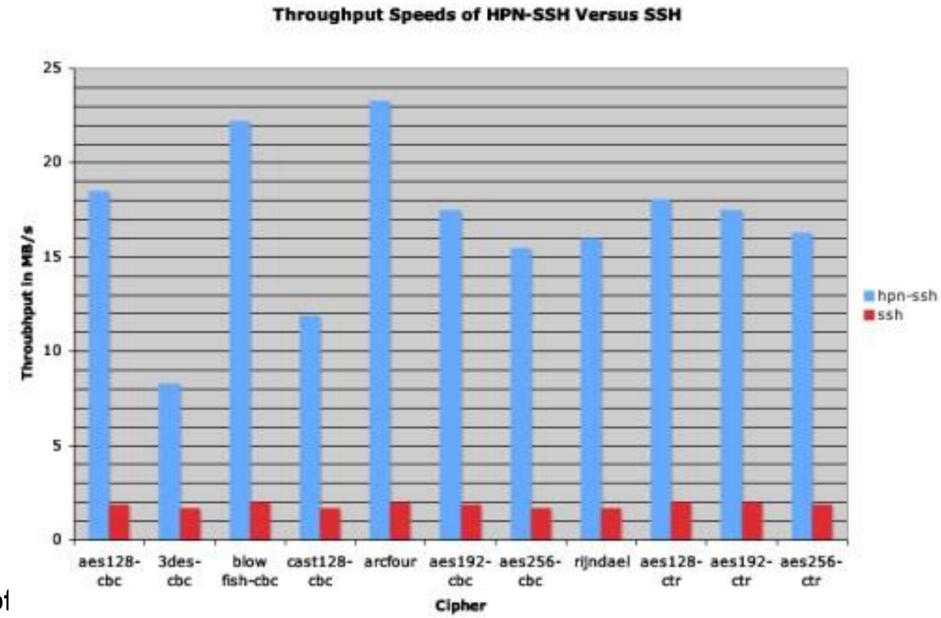
- **Pros:**
  - Most scientific systems are accessed via OpenSSH
  - SCP/SFTP are therefore installed by default
  - Modern CPUs encrypt and decrypt well enough for small to medium scale transfers
  - Credentials for system access and credentials for data transfer are the same
- **Cons:**
  - The protocol used by SCP/SFTP has a fundamental flaw that limits WAN performance
  - CPU speed doesn't matter – latency matters
  - Fixed-size buffers reduce performance as latency increases
  - It doesn't matter how easy it is to use SCP and SFTP – they simply do not perform
- **Verdict: Do Not Use Without Performance Patches**

CINECA SCAI SuperComputing Applications and Innovation

Why Not Use SCP or SFTP?

- PSC has a patch set that fixes problems with SSH
  - http://www.psc.edu/networking/projects/hpnssh/
- Significant performance Increase
- Advantage – this helps rsync too





What's about SFTP?

- Uses same code as SCP, so don't use SFTP for WAN transfers unless you have installed the HPN patch from PSC
- But even with the patch, SFTP has yet another flow control mechanism
  - By default, SFTP limits the total number of outstanding messages to 16 (32KB) messages
  - Since each datagram is a distinct message you end up with a 512KB outstanding data limit
  - You can increase both the number of outstanding messages ('-R') and the size of the message ('-B') from the command line though
- Sample command:
  - sftp -R 512 -B 262144 user@host:/path/to/file outfile

GridFTP

Open Grid Forum
Community of users and vendors

GridFTP Working group

GridFTP Protocol

Globus Toolkit
A specific implementation of GridFTP Protocol

GridFTP

- **GridFTP from ANL has everything needed to fill the network pipe**
  - Buffer Tuning
  - Parallel Streams
- **Supports multiple authentication options**
  - Anonymous
  - X.509 (Personal certificates)
- **Ability to define a range of data ports**
  - helpful to get through firewalls
- **Sample Use:**
  - globus-url-copy -p 4 sshftp://data.lbl.gov/home/mydata/myfile file://home/mydir/myfile
- Available from: http://www.globus.org/toolkit/downloads/

GridFTP new features

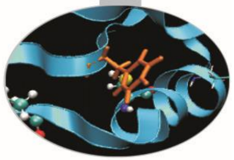
- ssh authentication option
  - Not all users need or want to deal with X.509 certificates
  - Solution: Use SSH for Control Channel
    - Data channel remains as is, so performance is the same
- Optimizations for small files
  - Concurrency option (-cc)
    - establishes multiple control channel connections and transfer multiple files simultaneously
    - Pipelining option:
      - Client sends next request before the current completes
  - Cached Data channel connections
    - Reuse established data channels (Mode E)
    - No additional TCP or GSI connect overhead
- Support for UDT protocol

GridFTP

The Globus Toolkit provides a GridFTP client called `globus-url-copy`, a command line interface, suitable for scripting.

For example, the following command:

```
globus-url-copy
gsiftp://remote.host.edu/path/to/file
file:///path/on/local/host
```



GridFTP
Basic command

```
globus-url-copy -vb -p 4 source_url
destination_url
```

where:

-vb

specifies verbose mode and displays:

- number of bytes transferred,
- performance since the last update (currently every 5 seconds), and
- average performance for the whole transfer.

-p

Specifies the number of parallel data connections that should be used. This is one of the most commonly used options.

GridFTP
More options…

```
globus-url-copy -vb -p 4 -r -cd - cc 4 source_url
destination_url
```

where:

-cc Specifies the number of concurrent FTP connections to use for multiple transfers.

-cd Creates destination directories, **if needed**.

-r Copies files in subdirectories.

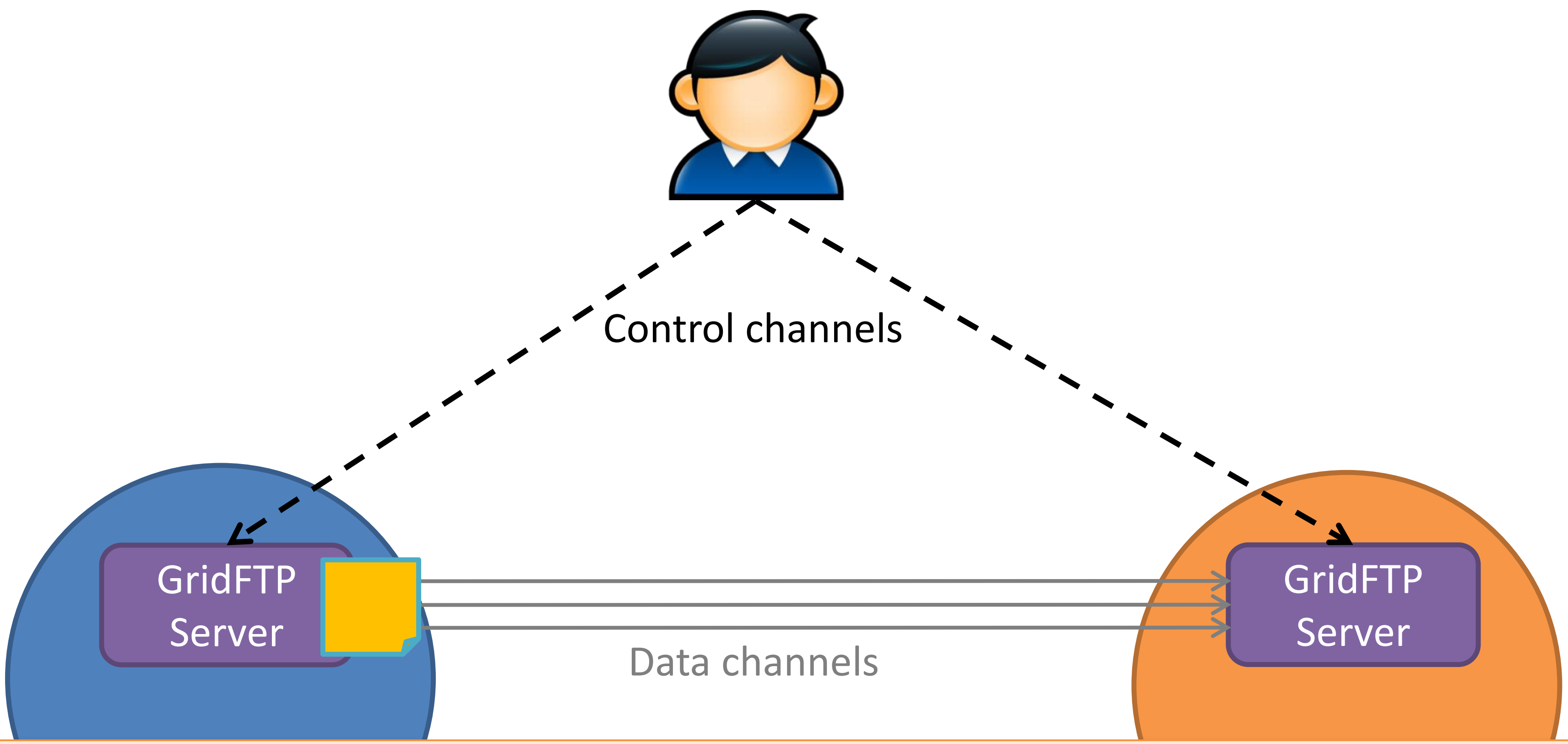
The source/destination URLs will normally be one of the following:

- `file:///path/to/my/file`

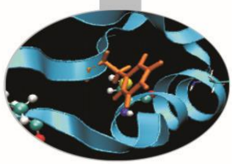
if you are accessing a file on a file system accessible by the host on which you are running your client.

- `gsiftp://hostname/path/to/remote/file` if you are accessing a file from a GridFTP server

GridFTP: third Party Transfer




```
globus-url-copy -vb -p 4
gsiftp://other.machine.my.edu/tmp/foo
gsiftp://remote.machine.my.edu/tmp/bar
```



GridFTP
Failures and retries

```
#!/bin/sh
STATEFILE=/path/to/statefile;
while [ ! -e $STATEFILE -o -s $STATEFILE ];
do
globus-url-copy -rst -p 4 -cc 4 -cd -vb -r -df
$STATEFILE gsiftp://srchost/srcdirpath/
gsiftp://dsthost/dstdirpath/;
sleep 10;
done;
```

GridFTP
Load Balancing

```
globus-url-copy -cc 4 -af /tmp/alias-file -f
/tmp/xfer-file
```

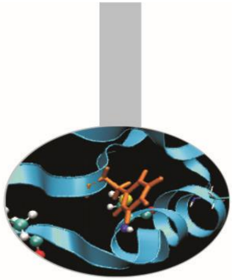
Contents of /tmp/alias-file look something like this:

```
@source
gridftp1.source-cluster.org
gridftp2.source-cluster.org
@destination
gridftp1.destination-cluster.org
gridftp2.destination-cluster.org
gridftp3.destination-cluster.org
gridftp4.destination-cluster.org
```

Contents of /tmp/xfer-file look something like this:

```
gsiftp:///tmp/x1 gsiftp:///tmp/x1
gsiftp:///tmp/x2 gsiftp:///tmp/x2
gsiftp:///tmp/x3 gsiftp:///tmp/x3
gsiftp:///tmp/x4 gsiftp:///tmp/x4
```

GridFTP
Load Balancing

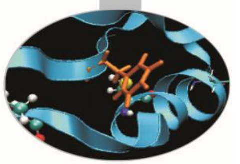


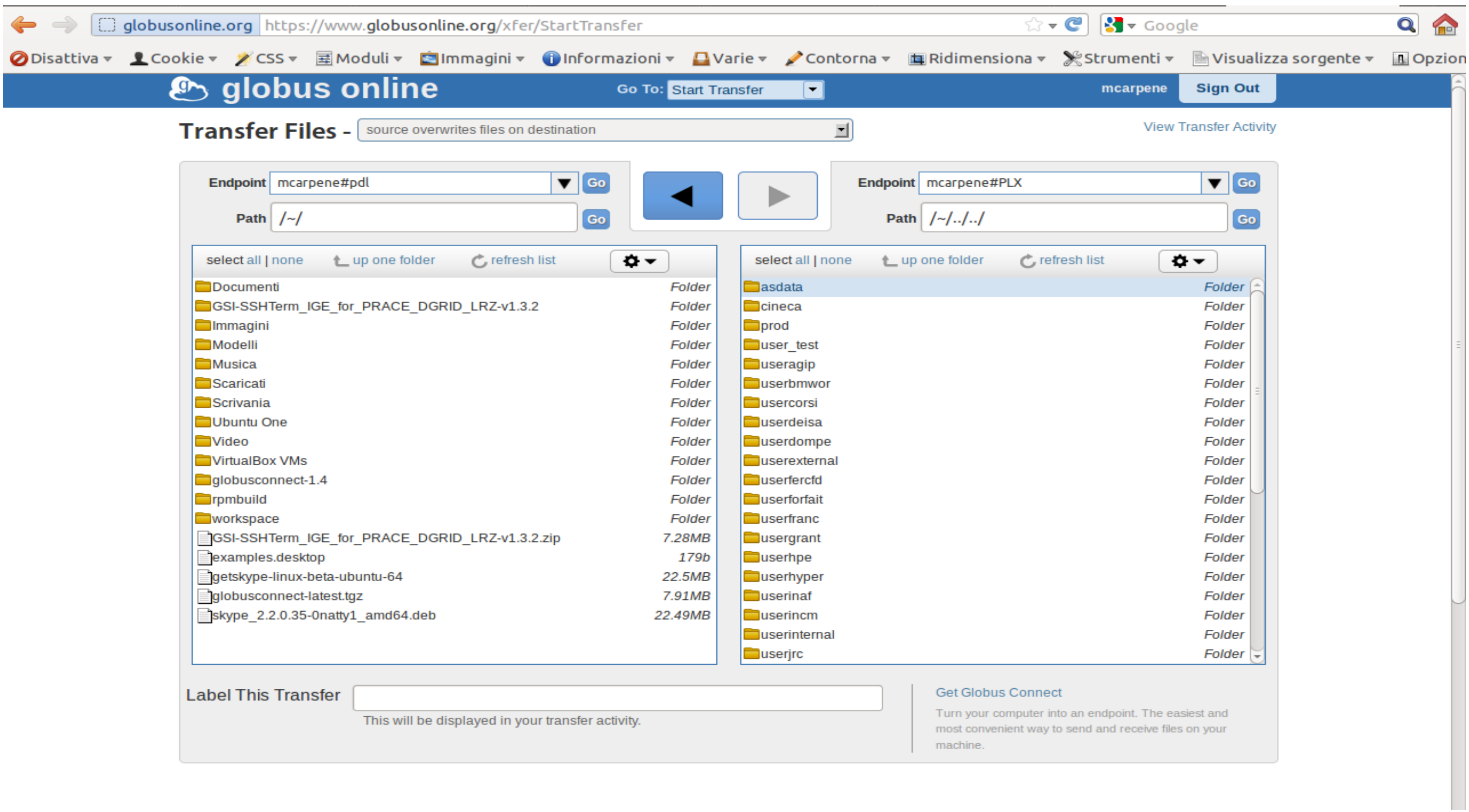
```
globus-url-copy -cc 4 -af /tmp/alias-file -f
/tmp/xfer-file
```

```
gsiftp://gridftp1.source-cluster.org/tmp/x1 gsiftp://gridftp1.destination-cluster.org/tmp/x1
gsiftp://gridftp2.source-cluster.org/tmp/x2 gsiftp://gridftp2.destination-cluster.org/tmp/x2
gsiftp://gridftp1.source-cluster.org/tmp/x3 gsiftp://gridftp3.destination-cluster.org/tmp/x3
gsiftp://gridftp2.source-cluster.org/tmp/x4 gsiftp://gridftp4.destination-cluster.org/tmp/x4
```

SuperComputing Applications and Innovation

Globus OnLine Service





http://www.globusonline.org

GridFTP bottleneck detector

- new command line option for globus-url-copy, "-nlb”
  - nlb = NetLogger bottleneck
  - Uses NetLogger libraries for analysis of network and disk I/O
    - http://acs.lbl.gov/NetLogger
- Possible "Bottleneck:" results are:
  - network: somewhere in the network
  - disk read: sender's disk
  - disk write: receiver's disk
  - unknown: disk/network are about the same and/or highly variable

GridFTP bottleneck detector (cont.)

- **Sample Output:**
  - Total instantaneous throughput:
    - disk read = 1235.7 Mbits/s
    - disk write = 2773.0 Mbits/s
    - net read = 836.3 Mbits/s
    - net write = 1011.7 Mbits/s
  - **Bottleneck: network**
- Ignore the "net write" value (strongly influenced by system and TCP buffer artifacts)
- ***instantaneous throughput is*** **the average # of bytes divided by the time spent blocking on the system call**
- ***instantaneous throughputs*** **are higher than the overall throughput of the transfer:**
  - does not include the time waiting for data to be available
  - primarily useful for comparison and not as absolute numbers

Sample Data Transfer Results

- Using the right tool is very important
- Sample Results:
  - RTT = 53 ms, network capacity = 10Gb/s.
- **Tool Throughput**
  - **scp:** 140 Mb/s
  - **HPN patched scp:** 1.2 Gb/s
  - **FTP:** 1.4 Gb/s
  - **GridFTP**, 4 streams 5.4 Gb/s
  - **GridFTP**, 8 streams 6.6 Gb/s

Other tools

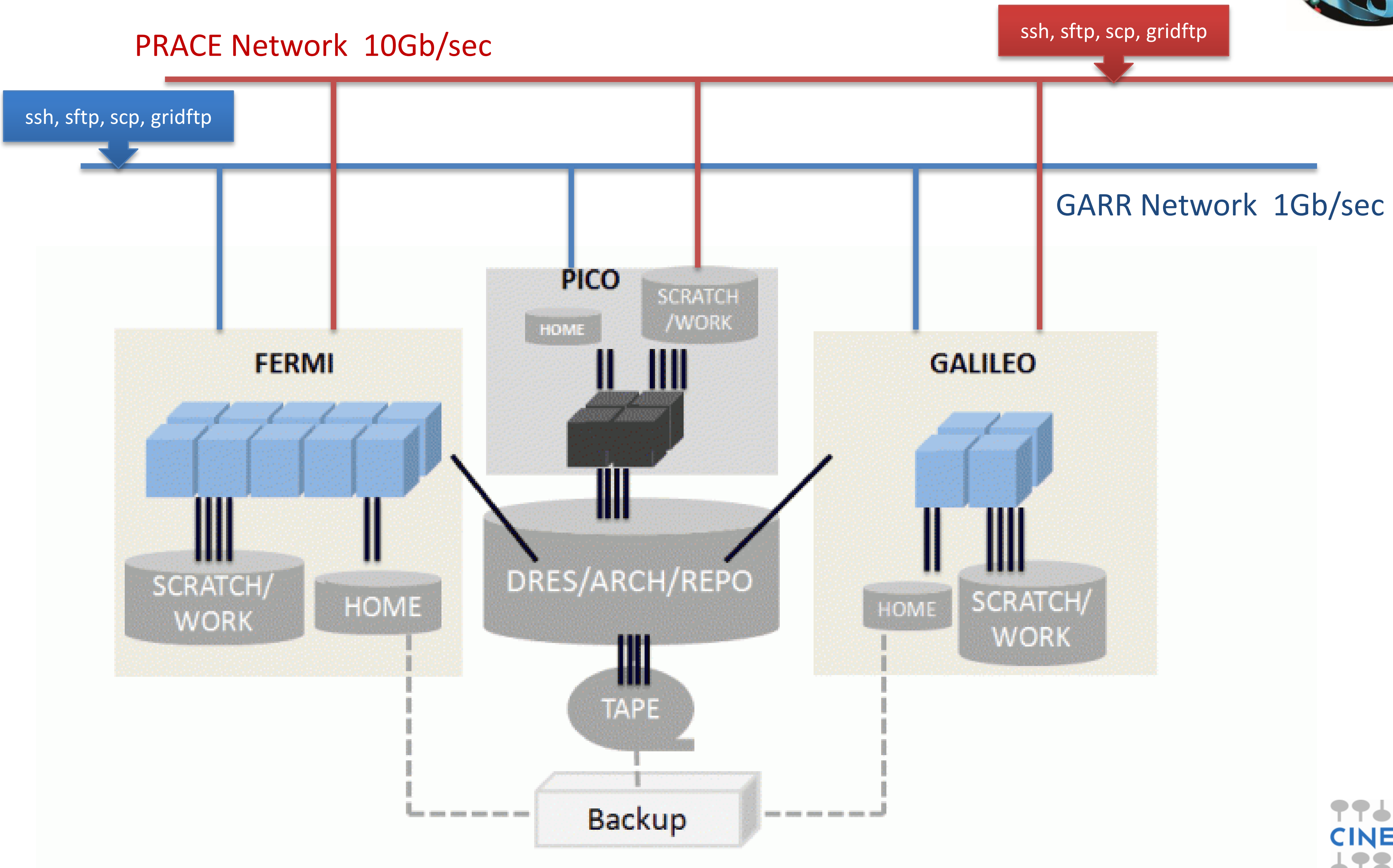
- **bbcp**: http://www.slac.stanford.edu/~abh/bbcp/
  - supports parallel transfers and socket tuning
  - `bbcp -P 4 -v -w 2M myfile remotehost:filename`
- **lftp**: http://lftp.yar.ru/
  - parallel file transfer, socket tuning, HTTP transfers, and more.
  - `lftp -e 'set net:socket-buffer 4000000; pget -n 4 [http|ftp]://site/path/file; quit'`
- **axel**: http://axel.alioth.debian.org/
  - simple parallel accelerator for HTTP and FTP.
  - `axel -n 4 [http|ftp]://site/file`
- **rsync:** http://rsync.samba.org/
  - `rsync --timeout=600 -avHS -r --numeric-ids --bwlimit=80000 --block-size=1048576  --progress $CINECA_SCRATCH/path/file $CINECA_DATA/path/`


Improvements in performance
30x
25x
20x
15x
10x
5x
0x
scp
gsiscp
gt (direct)
gt (via SARA)
PRACE
1
sara
2
NERSC

Network resources

- The clusters are reachable from the public network through GARR (Italian NREN) facility (1Gb/s)
- The PRACE infrastructure has a dedicated private network which provides 10Gb/s guaranteed bandwidth (available on FERMI)

CINECA data resources



CINECA “cindata” command

- What’s about storage’s status?

```
-bash-3.2$ cindata
-----------------------------ASyncronous Data report---------------------------------
--------------------------------------|-------USER USAGE-----|------TOTAL USAGE------
USER       AREADESCR                FRESH   SPACE     QTA     QTA%   SPACE     MAX    MAX%
-------------------------------------------------------------------------------------
pr1is019   /cineca/                -15hou      1K      --      --%     78G    800G    9.8%
pr1is019   /shared/data/          -113min     32K    100G     0.0%    139T    189T   73.8%
pr1is019   /gpfs/scratch/          -15hou    256K      --      --%    286T    349T   82.1%
pr1is019   /sp6/                   -15hou    305M      2G    14.9%    895G     13T    6.4%
```

GridFTP endpoints @ CINECA

GALILEO

- gsiftp://gftp.galileo.cineca.it:2811

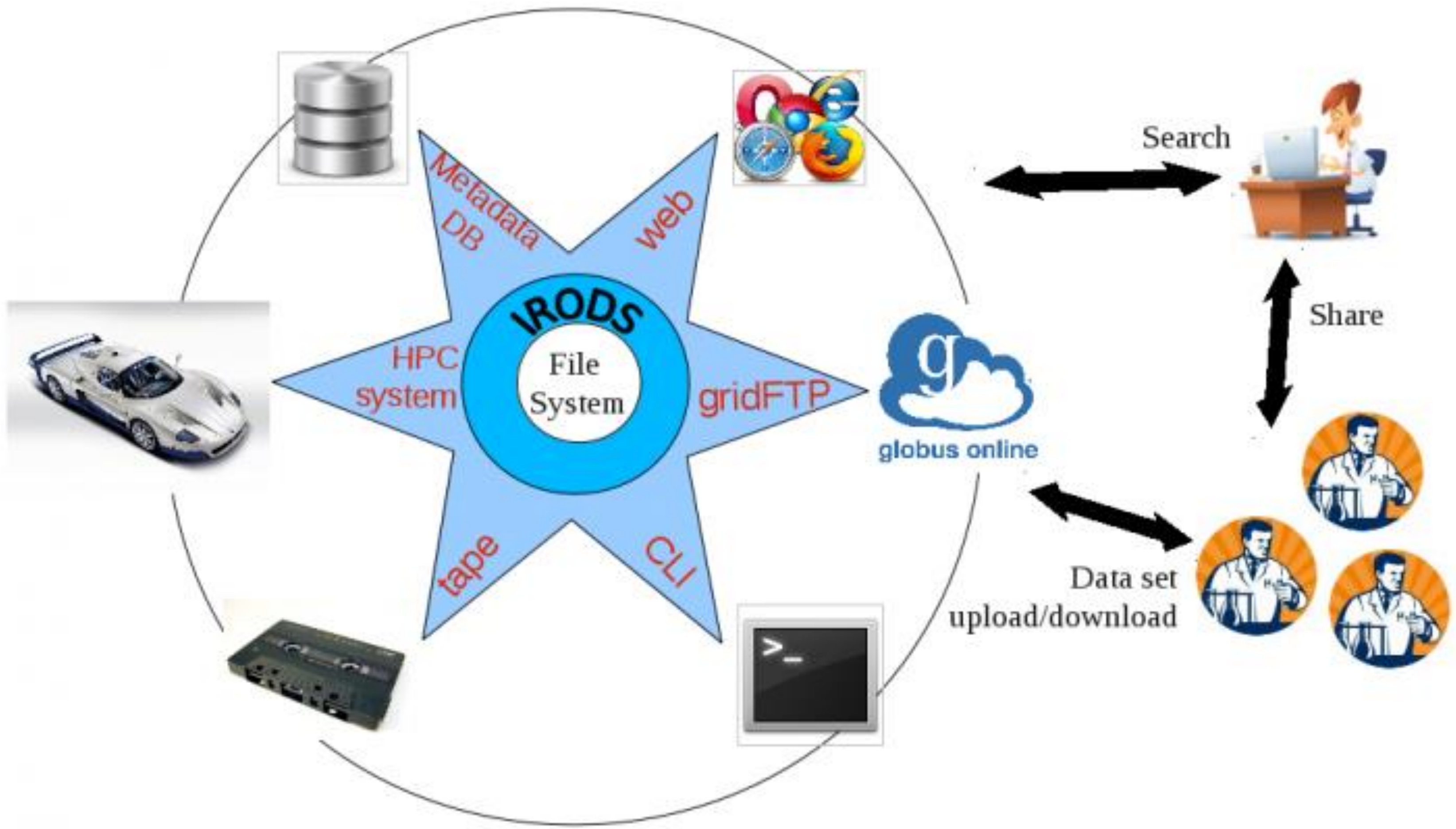
PICO

- gsiftp://gftp.pico.cineca.it:2811

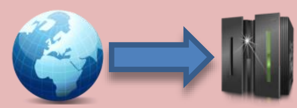
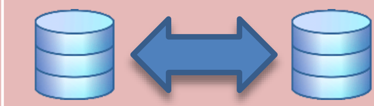
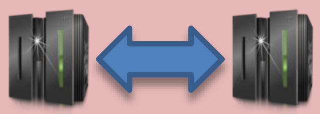
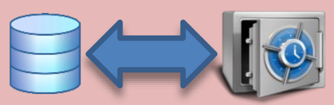
FERMI

- gsiftp://gftp-fermi.cineca.it:2811 (public network)
- gsiftp://gftp-prace.cineca.it:2811 (PRACE network)

CINECA repo resources



Tools: comparative table

				
cp/mv		✓		
scp/sftp	✓		✓	
rsync		✓✓	✓✓	
GridFTP	✓✓		✓✓	
LTFS				✓✓

Extreme solution…

PHOTO: DAVIES & STARR

Bulk Data Transfer Summary

- **TCP tuning is critical, but is now easy**
  - Four lines in /etc/sysctl.conf to give autotuning
  - Make sure you're not stuck with TCP Reno
- **Build one host for WAN data transfers, make sure it's right**
  - Make sure TCP parameters are configured
- **Plug your hosts into the right place in the network**
- **Use the right tools**
  - Parallelism is a key
  - GridFTP, BBCP, HPN-SSH

Agenda

Bulk data transfer

Basic concepts, tools and techniques

Data post-processing

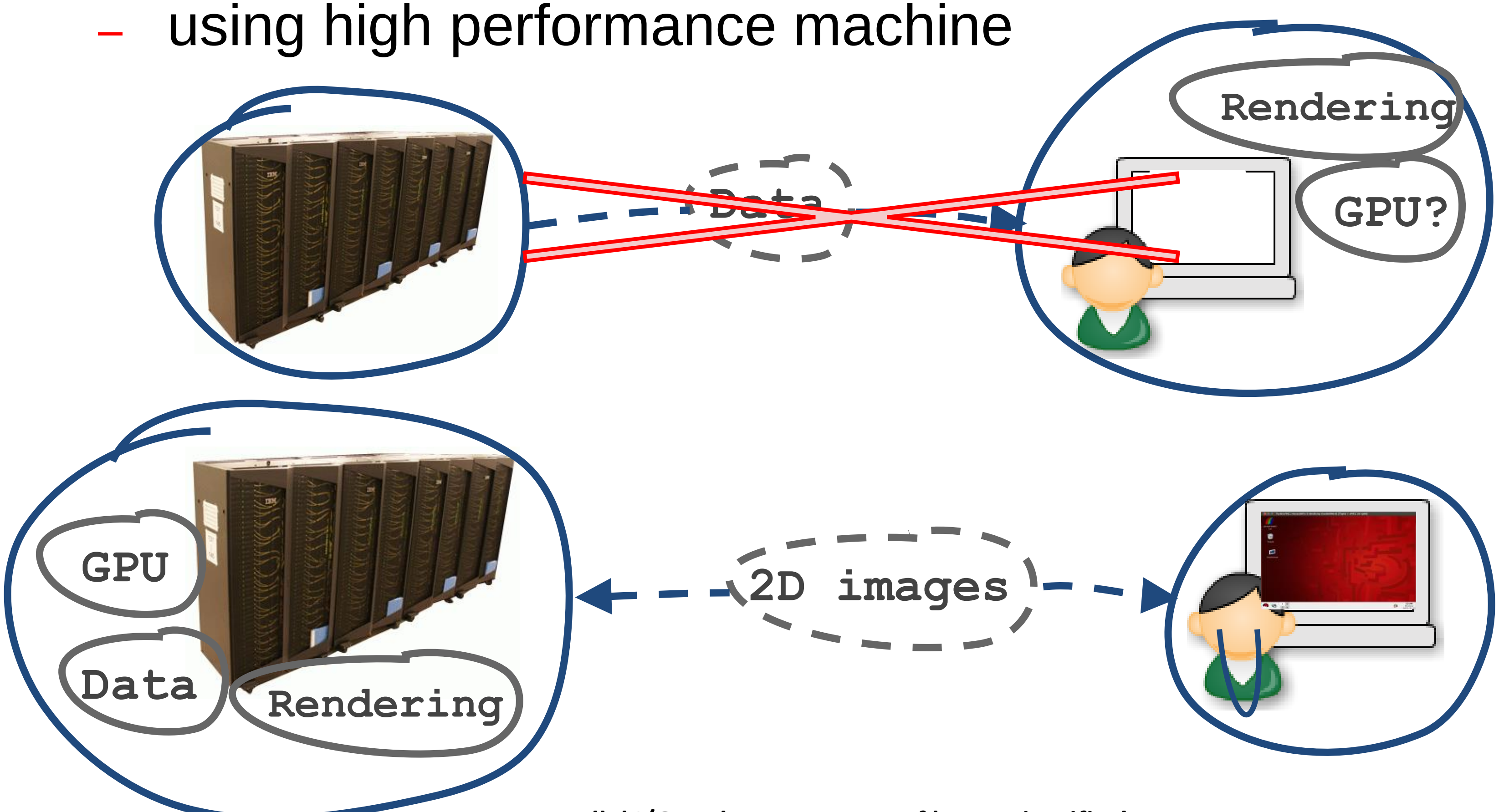
Remote visualization

Data management across the Europe

The EUDAT project overview

Remote Visualization

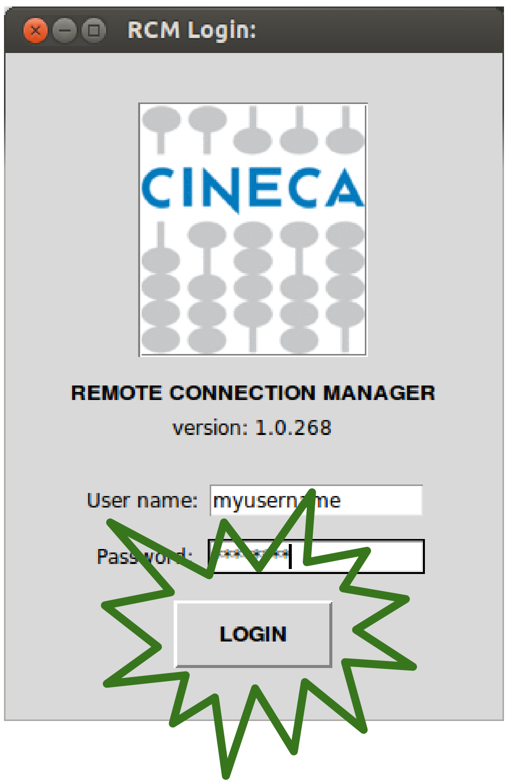
- Perform scientific visualization on large amounts of data produced on HPC systems
  - without moving data
  - using high performance machine

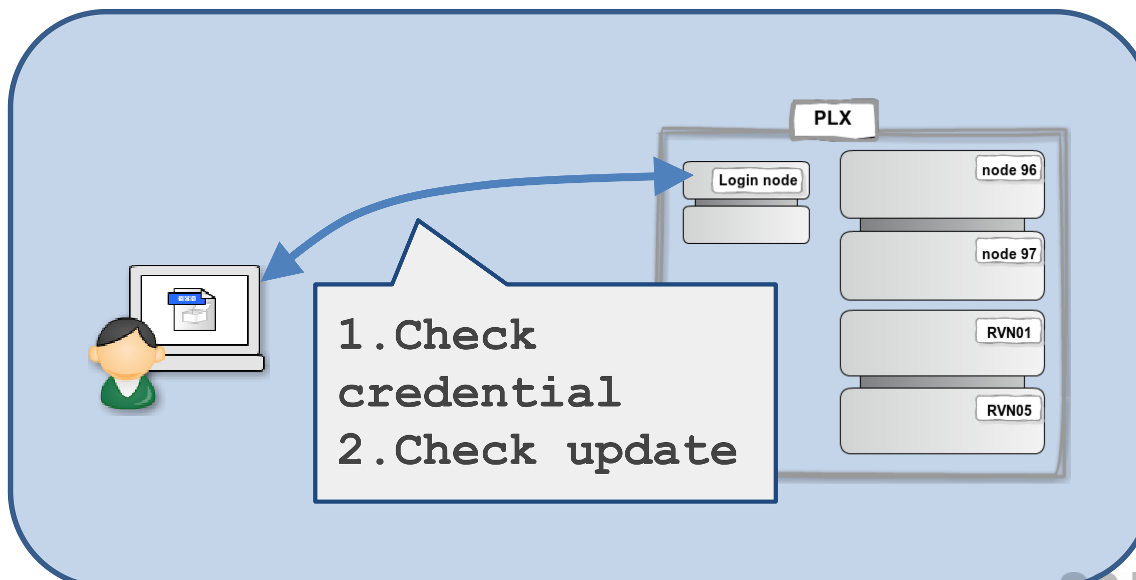


RCM - Login

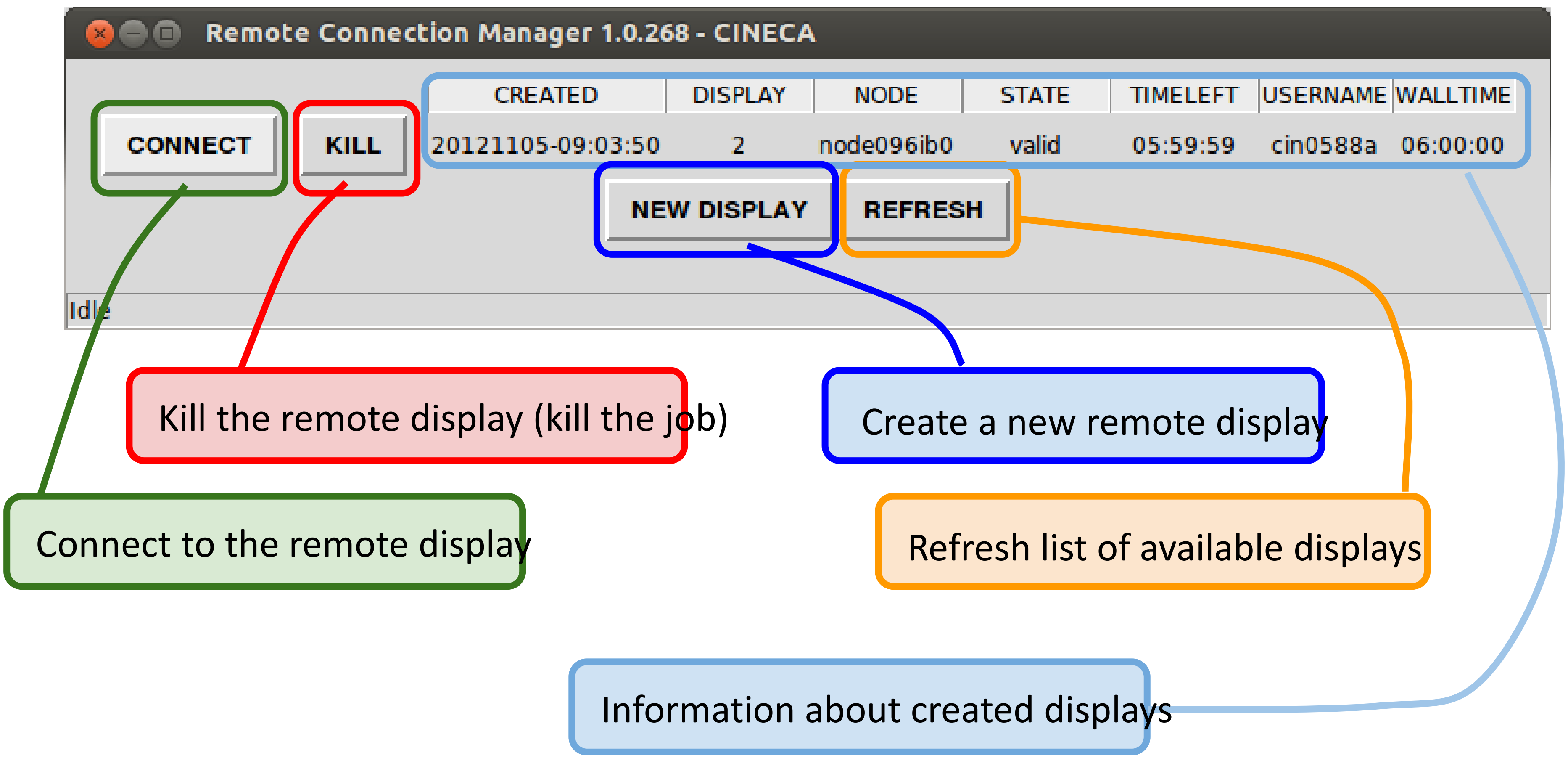
USER

SYSTEM





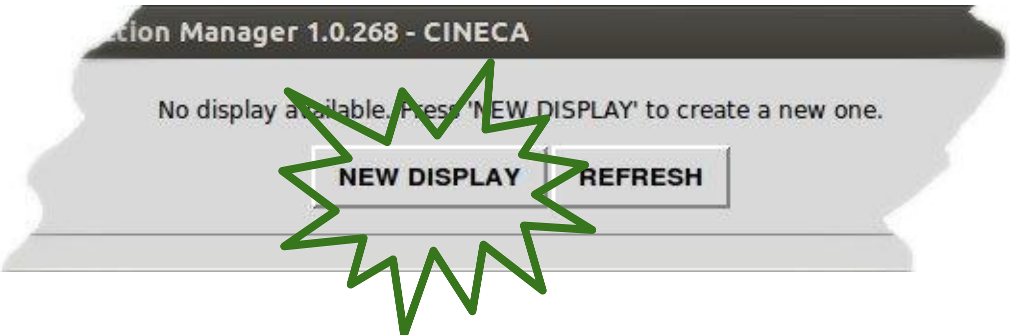
RCM - Display info

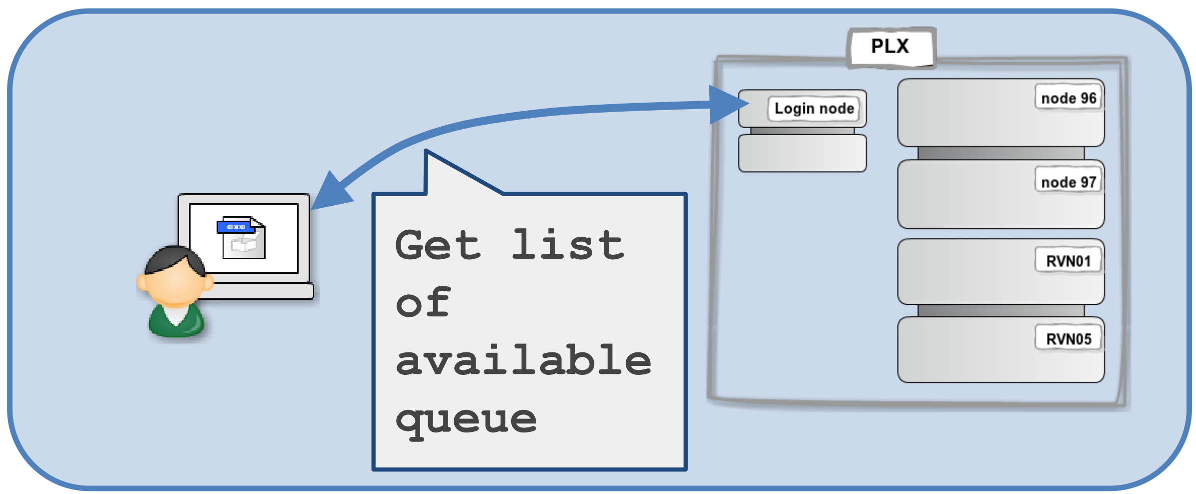


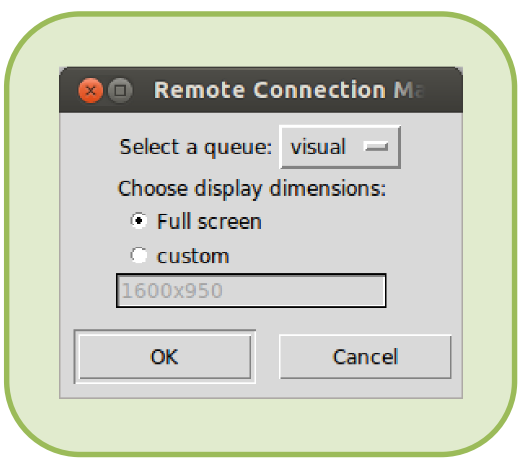
RCM - New display (1)

USER

SYSTEM



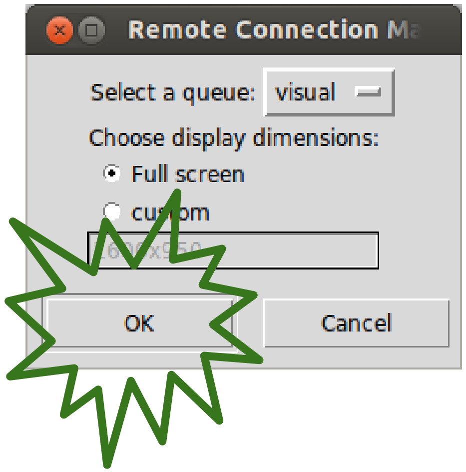




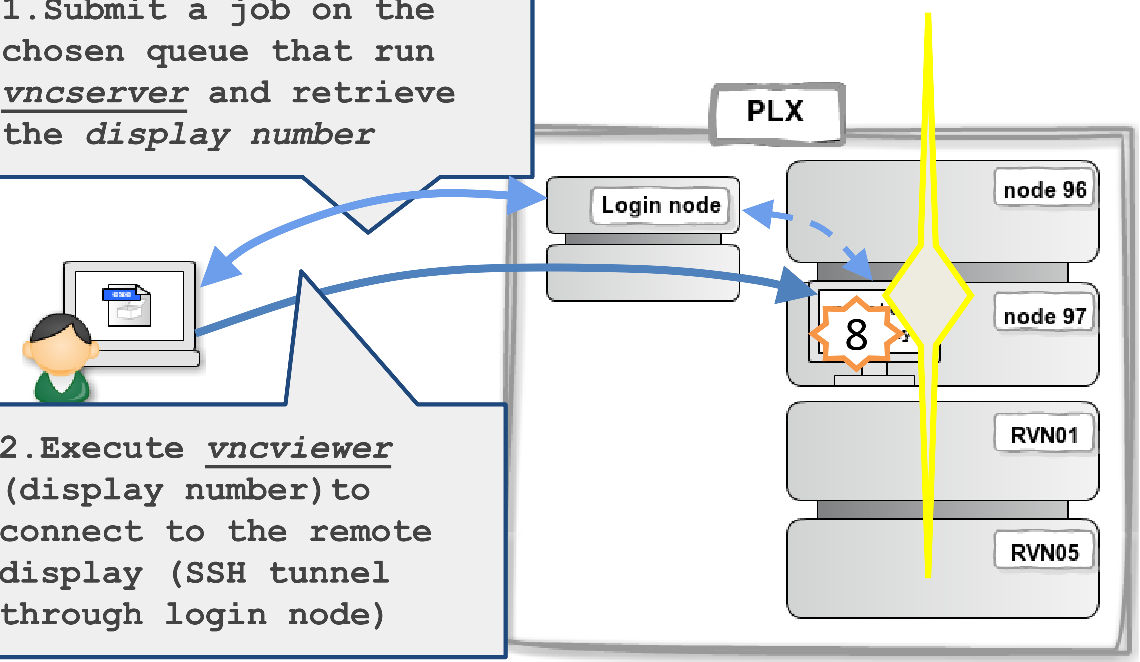
RCM - New display (2)

USER

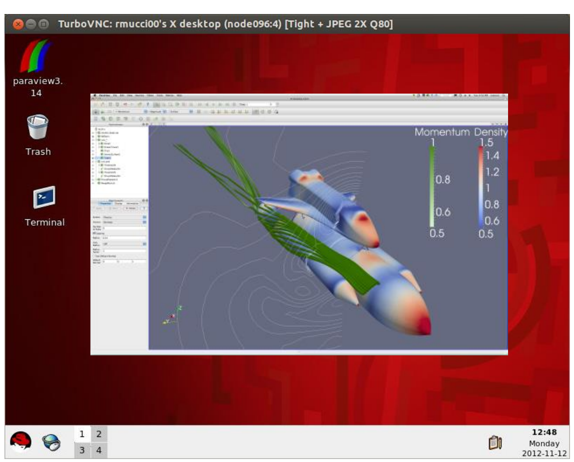
SYSTEM



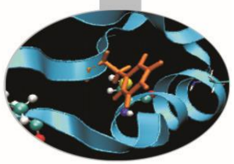
1. Submit a job on the chosen queue that run ***vncserver*** and retrieve the ***display number***



2. Execute ***vncviewer*** (display number) to connect to the remote display (SSH tunnel through login node)



Agenda



Bulk data transfer

Basic concepts, tools and techniques

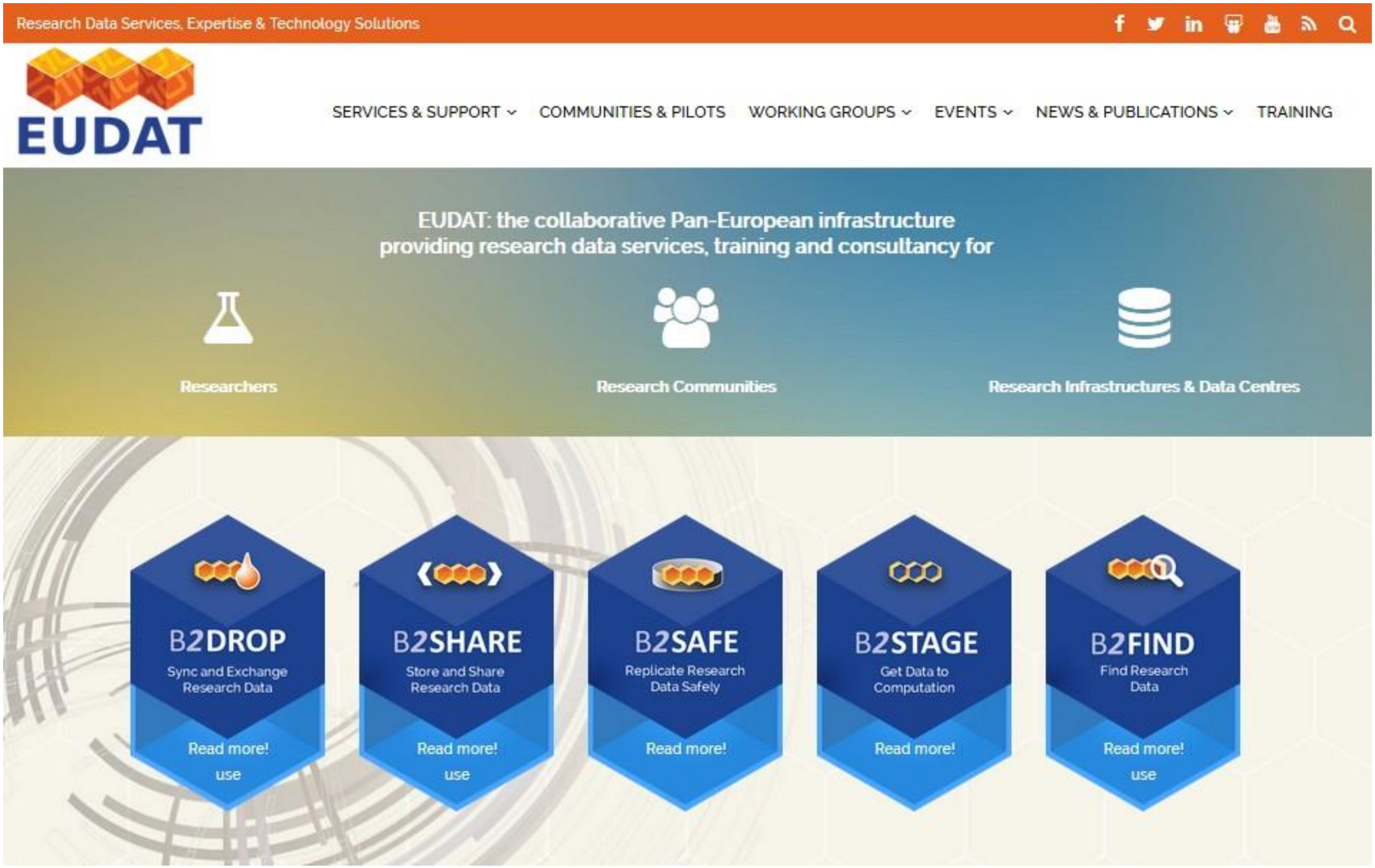
Data post-processing

Remote visualization

Data management across the Europe

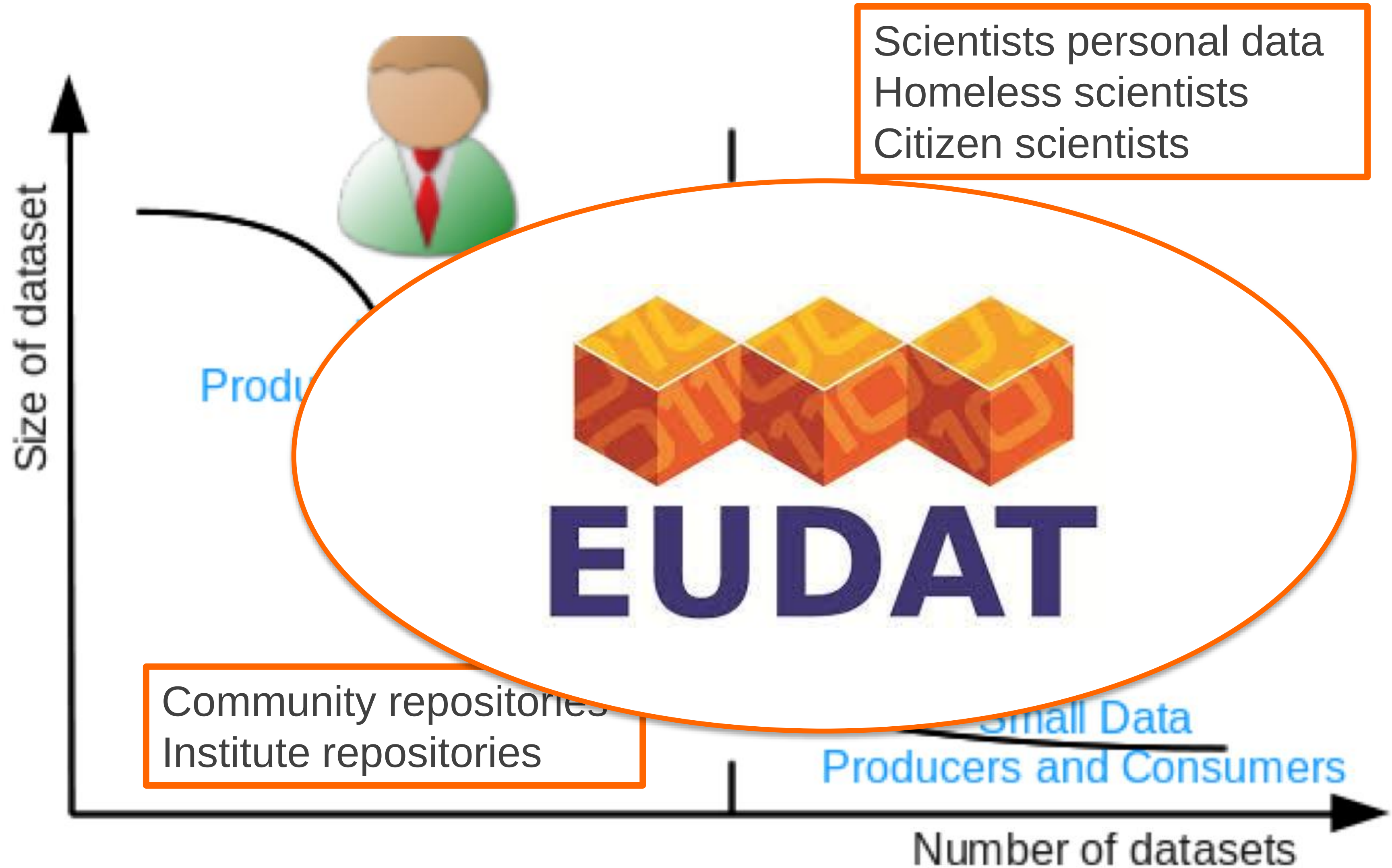
The EUDAT project overview

http://www.eudat.eu

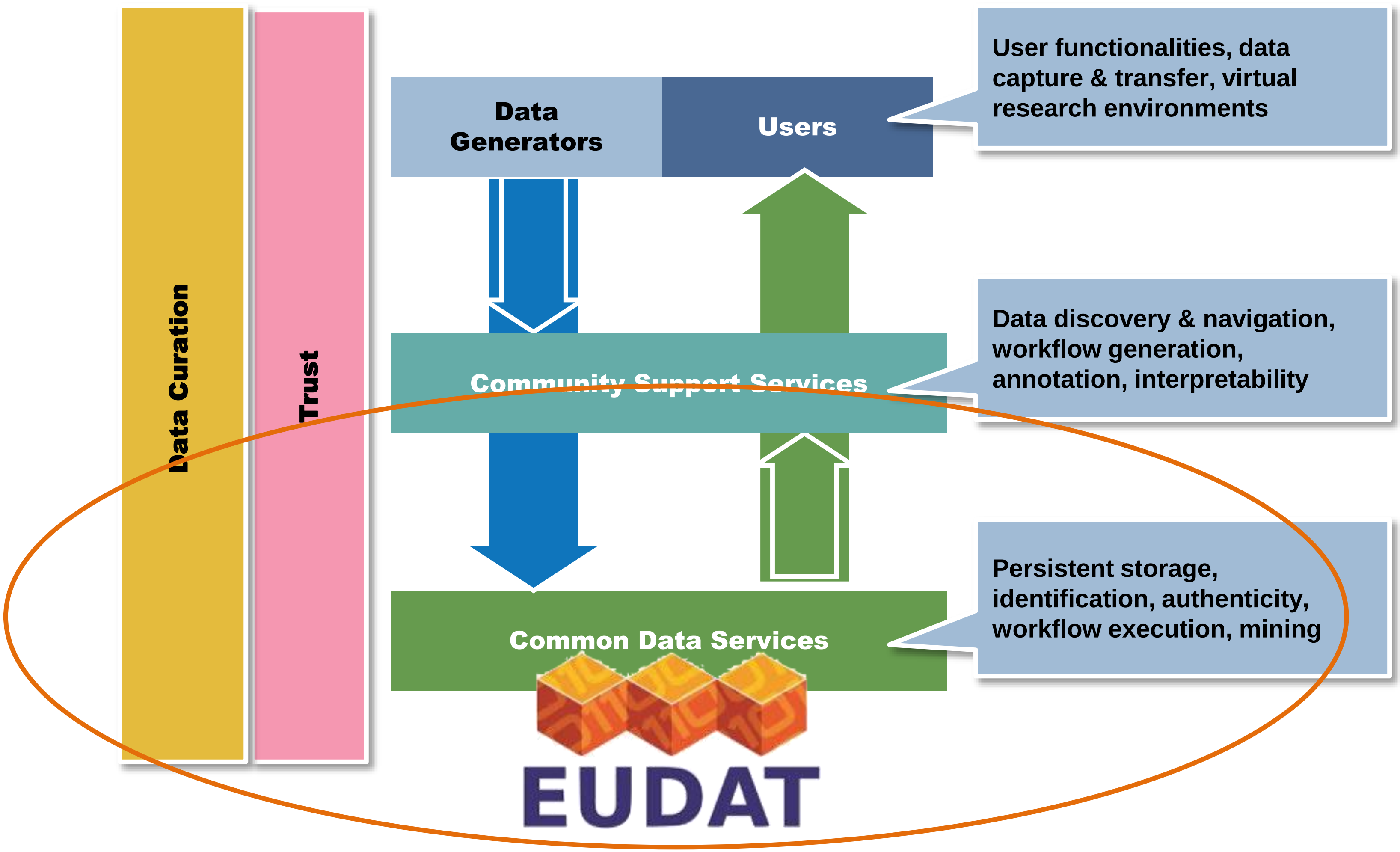


Where Does EUDAT Fit In?

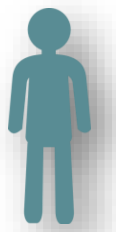
(in a Data quality view)



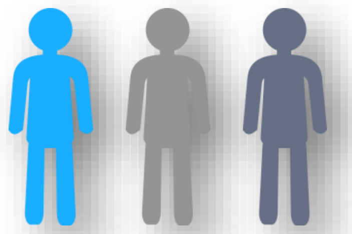
Where Does EUDAT Fit In?
(in a multilayer view of Data Management)



Who can use EUDAT service



Single researcher



Team

Community

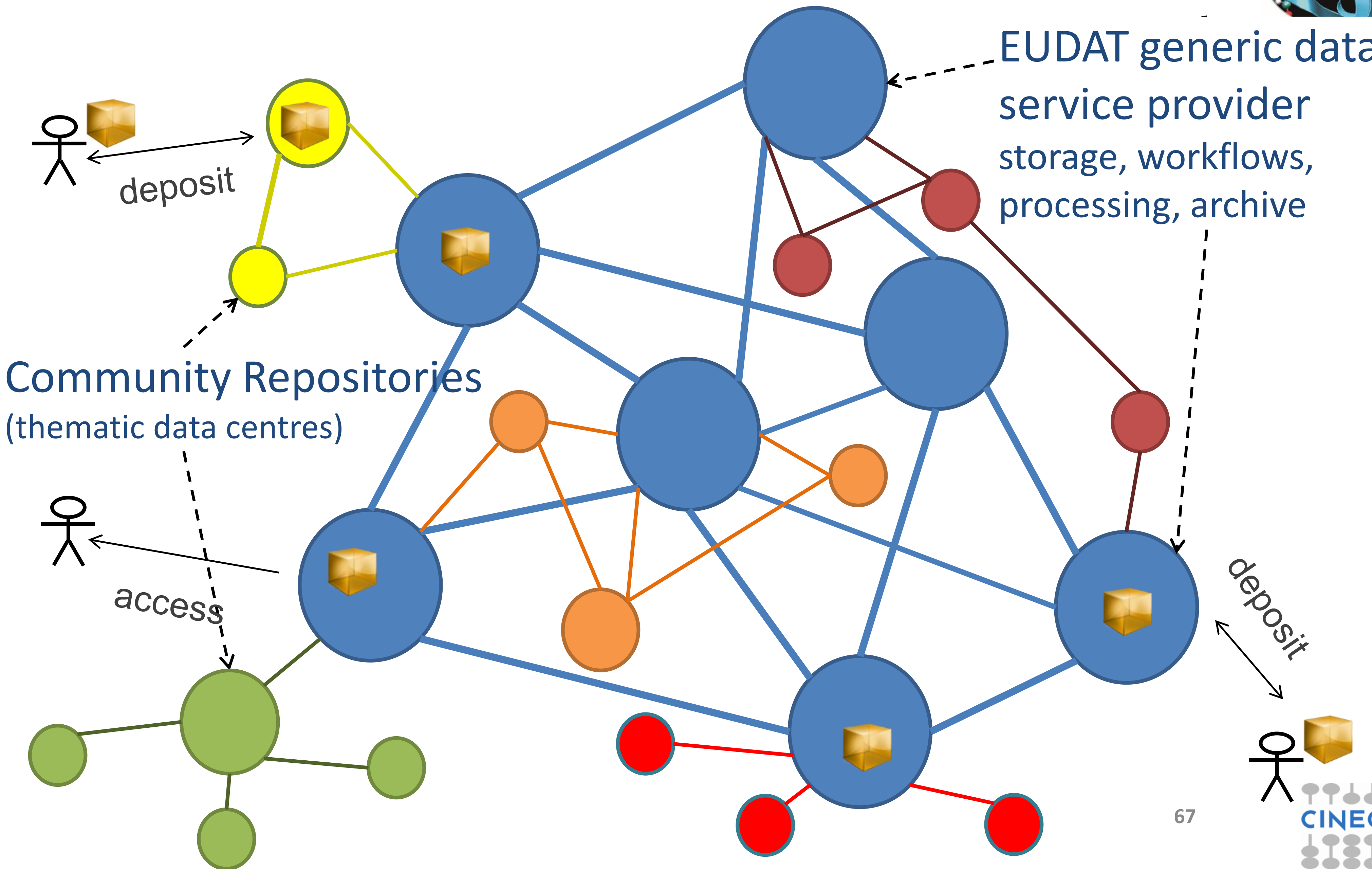
Upload and download

Upload, add metadata, share

Periodic transfers, quality checks …

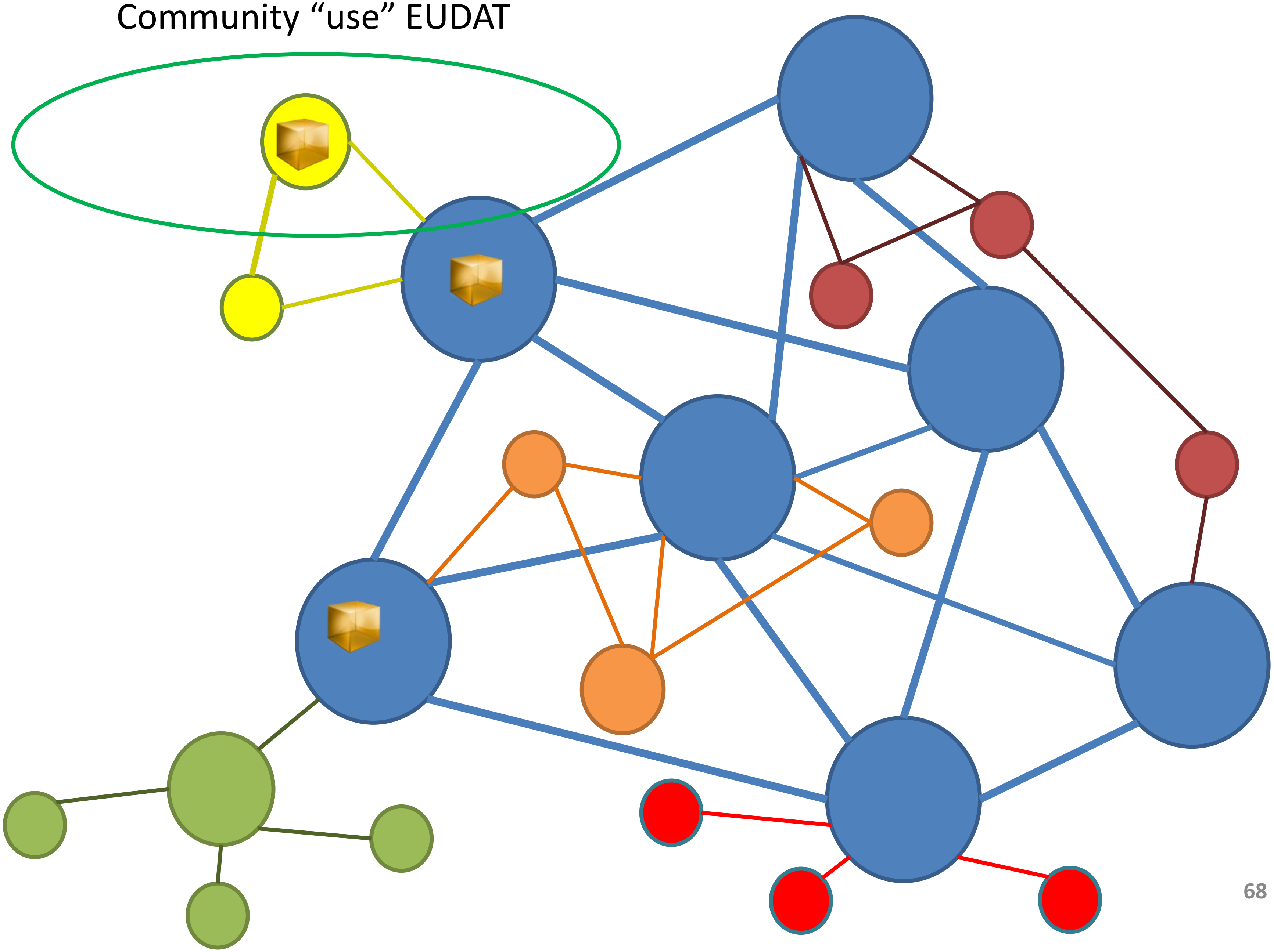
Different strategies for different usage scenarios

EUDAT Collaborative Data Infrastructure
(A general CDI architecture overview)



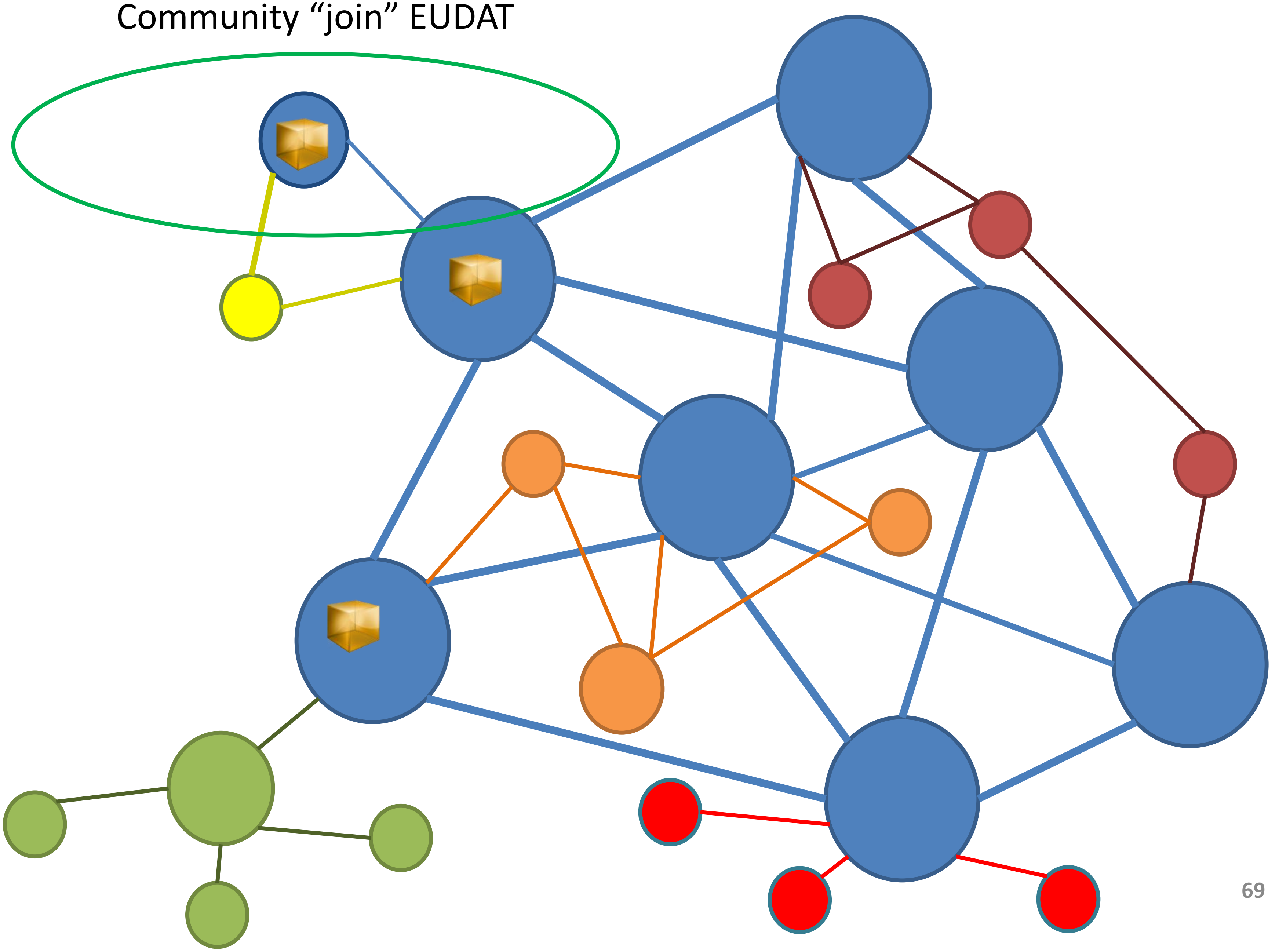
EUDAT Collaborative Data Infrastructure (Using vs. joining)

Community "use" EUDAT



EUDAT Collaborative Data Infrastructure (Using vs. joining)

Community "join" EUDAT



SuperComputing Applications and Innovation

If there are hundreds of Research Infrastructures, how many different data management systems can be sustained?

B2 Service (modular) Suite

B2DROP
Sync and Exchange Research Data

B2SHARE
Store and Share Research Data

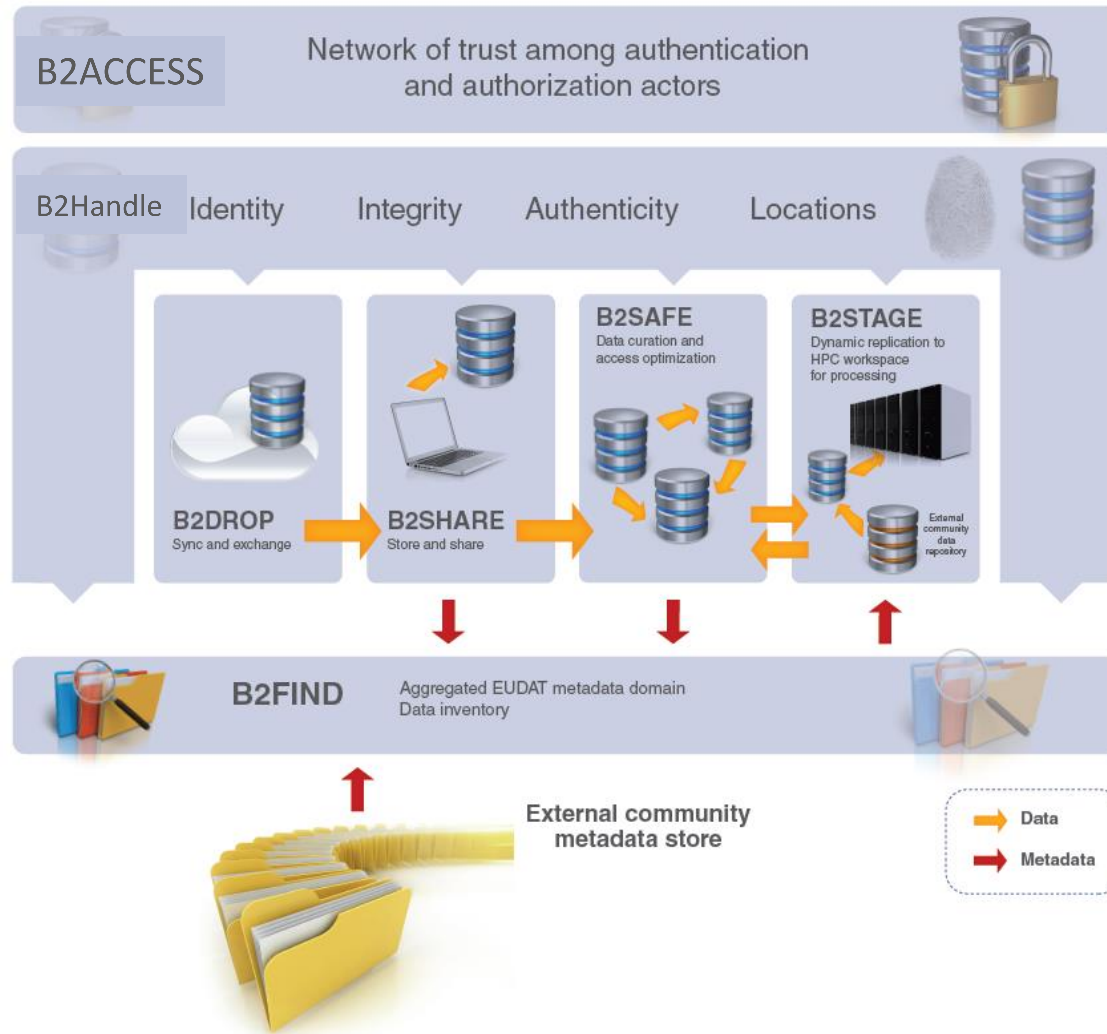
B2SAFE
Replicate Research Data Safely

B2STAGE
Get Data to Computation

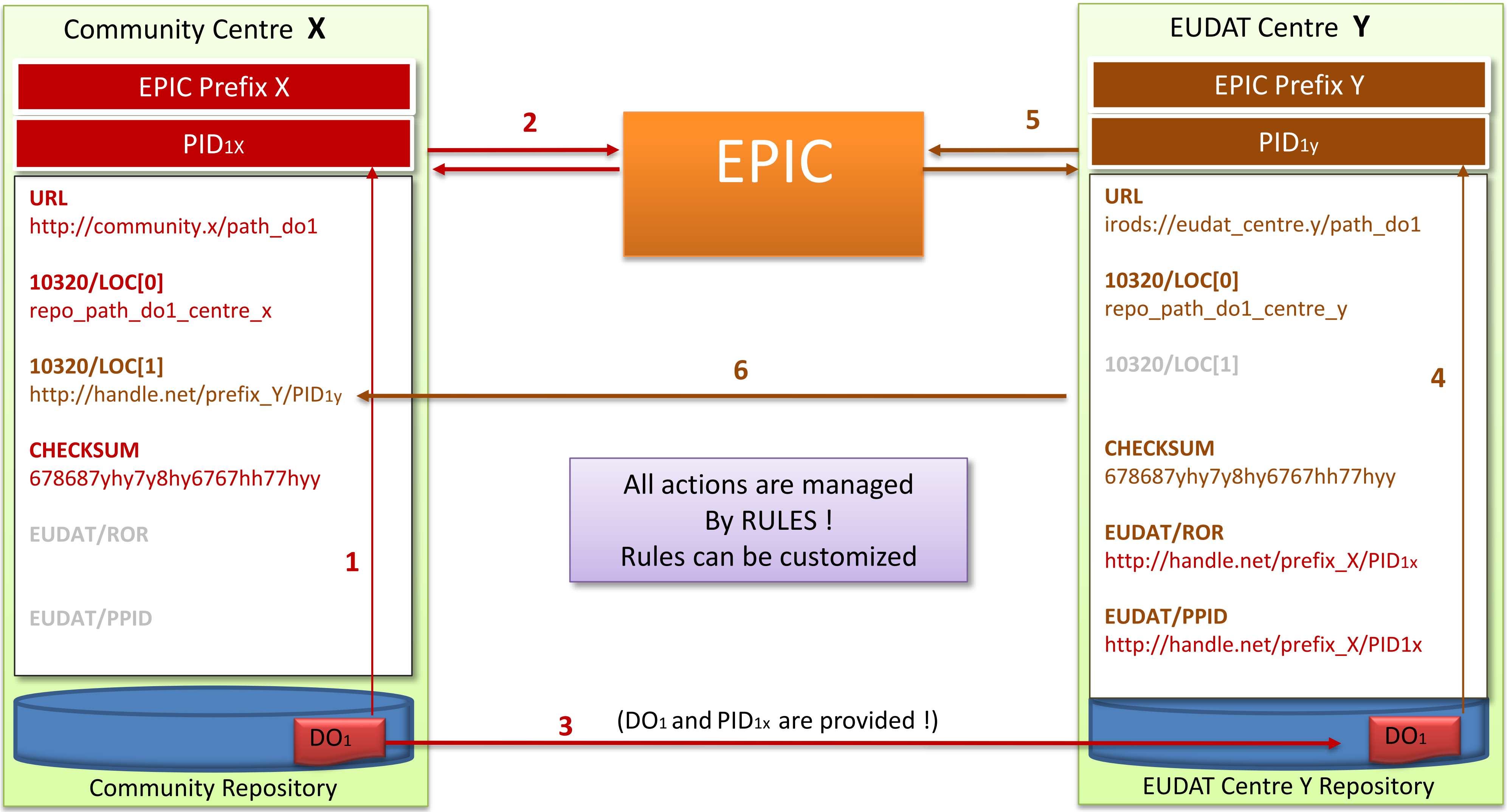
B2FIND
Find Research Data

B2HANDLE
Register your Research Data

B2ACCESS
Identity & Authorisation



B2SAFE: move and register data across EUDAT CDI



B2SAFE: move and register data across two EUDAT centres

Community Centre X

EPIC Prefix X

PID$_{1x}$

URL
http://community.x/path_do1

10320/LOC[0]
repo_path_do1_centre_x

10320/LOC[1]
http://handle.net/prefix_Y/PID$_{1y}$

CHECKSUM
678687yhy7y8hy6767hh77hyy

EUDAT/ROR

EUDAT/PPID

DO$_1$

Community Repository

EUDAT Centre Y

EPIC Prefix Y

PID$_{1y}$

URL
http://eudat_centre.y/path_do1

10320/LOC[0]
repo_path_do1_centre_y

10320/LOC[1]
http://handle.net/prefix_Z/PID$_{1z}$

CHECKSUM
678687yhy7y8hy6767hh77hyy

EUDAT/ROR
http://handle.net/prefix_X/PID$_{1x}$

EUDAT/PPID
http://handle.net/prefix_X/PID$_{1x}$

DO$_1$

EUDAT Centre X Repository

EUDAT Centre Z

EPIC Prefix Z

PID$_{1z}$

URL
http://eudat_centre.z/path_do1

10320/LOC[0]
repo_path_do1_centre_z

10320/LOC[1]

CHECKSUM
678687yhy7y8hy6767hh77hyy

EUDAT/ROR
http://handle.net/prefix_X/PID$_{1x}$

EUDAT/PPID
http://handle.net/prefix_Y/PID$_{1y}$

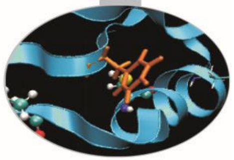
DO$_1$

EUDAT Centre Z Repository

References

- CINECA services and documentation
  - http://www.hpc.cineca.it/services
- Get in touch
  - hpc-service-int@cineca.it

Credits



- NICS Scientific Computing Group
  - http://www.nics.tennessee.edu/
- Energy Sciences Network
  - http://fasterdata.es.net
- Lawrence Berkeley National Laboratory
  - http://www.lbl.gov/
- Argonne National Laboratory
  - www.anl.gov