SciDAS on Chameleon: Integrating Data, Networks, and the Cloud

CC*DATA ACI-1659300

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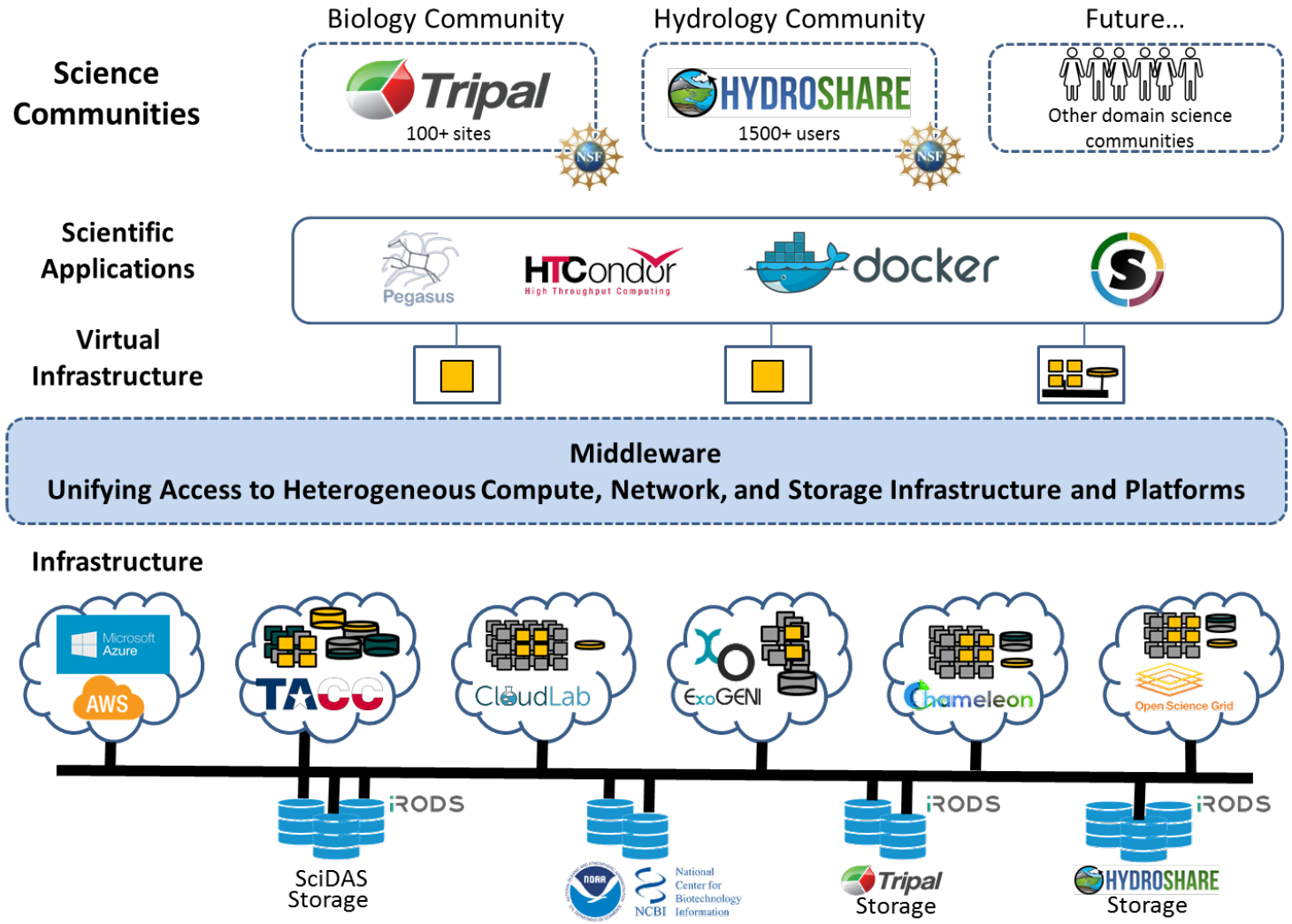
SciDAS View From High Above



SciDAS Glues NSF+ ACI

- Tripal
- Hydroshare
- BioDep-Vis
- OSG-GEM
- OSG-KINC
- SciDASH
- AHAB
- CC-RADII
- ORCA
- iRODS
- CICI-SAFE
- CC-ADAMANT
- Pegasus
- HTCONDOR
- QueryArrow
- ExoGENI
- CloudLab
- Chameleon
- COMET/XSEDE
- Open Science Grid
- Pacific Research Platform

SciDAS

renci

Scientific Data Analysis At Scale

Challenges:

- Limited storage, RAM, CPU time
- Hardware failure
- Data movement across resources

- Example: Moving data between the Palmetto Cluster and the Open Science Grid

```
------------------------------------------------------------------------------
Type           Succeeded Failed  Incomplete  Total     Retries   Total+Retries
Tasks          39997     0       3           40000     2247      42244
Jobs           40504     0       3           40507     2247      42751
Sub-Workflows  0         0       0           0         0         0
------------------------------------------------------------------------------

Workflow wall time                                       : 3 days, 1 hr
Cumulative job wall time                                 : 3 years, 133 days
Cumulative job wall time as seen from submit side        : 3 years, 131 days
Cumulative job badput wall time                          : 18 days, 10 hrs
Cumulative job badput wall time as seen from submit side : 18 days, 6 hrs
[wpoehlm@login02 statistics]$
```

globus

Requested 2017-08-13 10:28 am

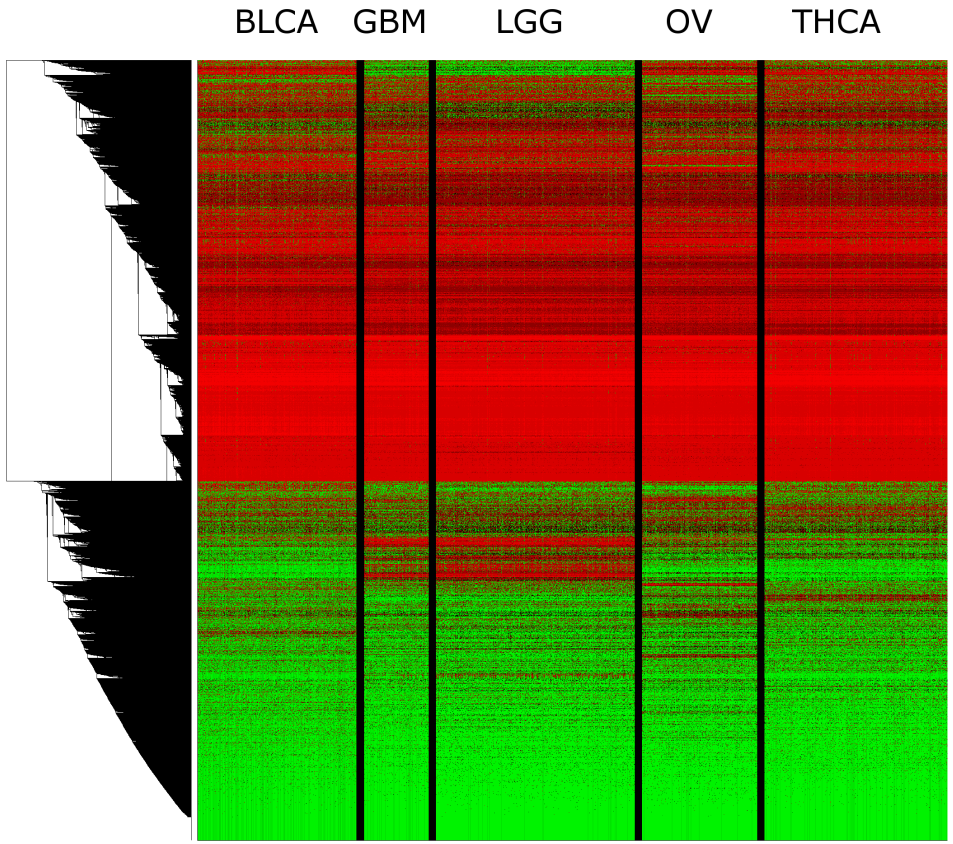
Completed 2017-08-13 07:45 pm

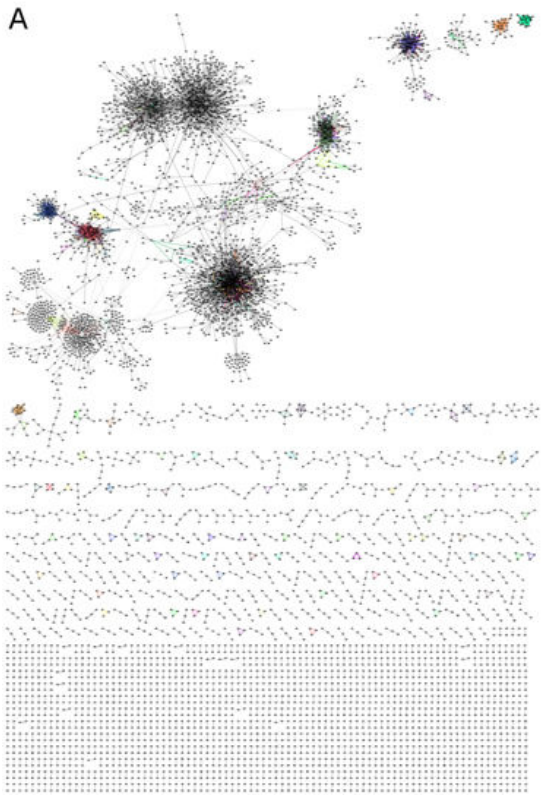
THE CANCER GENOME ATLAS
National Cancer Institute
National Human Genome Research Institute

Discovering Condition-Specific Gene Co-Expression Patterns Using Gaussian Mixture Models: A Cancer Case Study

Open Science Grid

Stephen P. Ficklin, Leland J. Dunwoodie, William L. Poehlman, Christopher Watson, Kimberly E. Roche & F. Alex Feltus



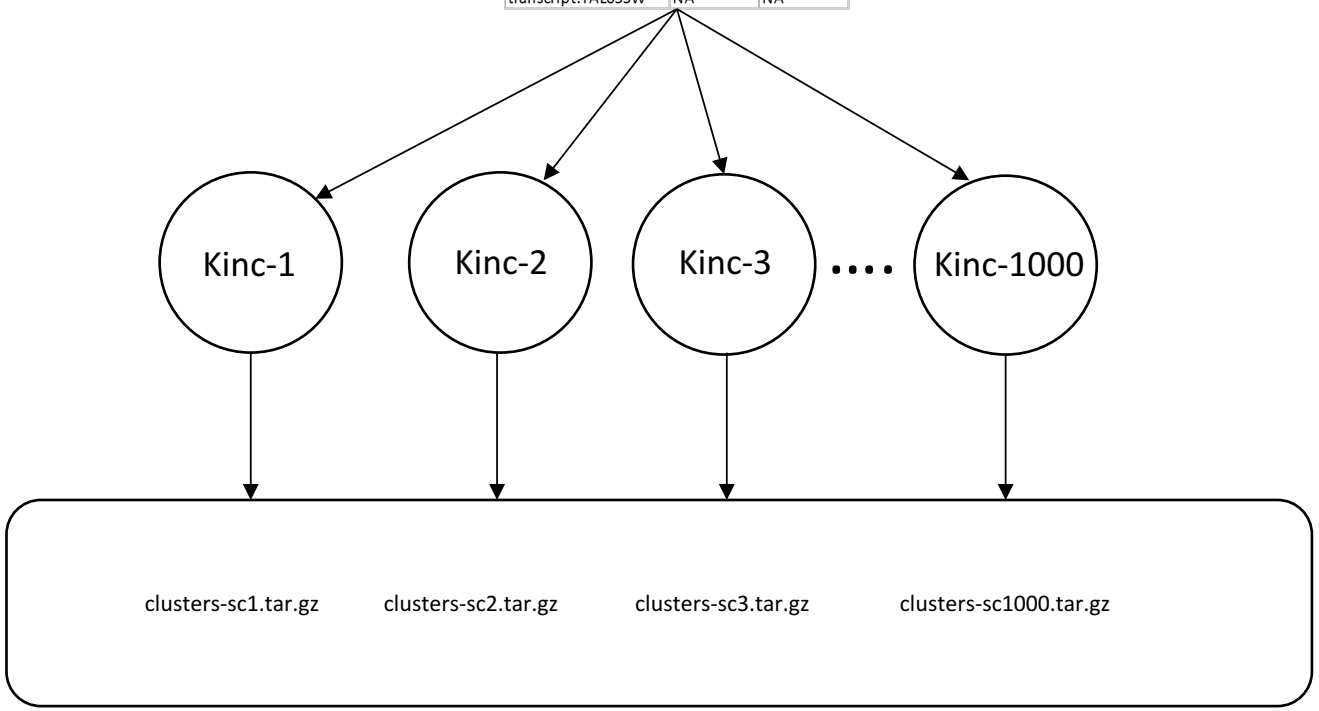


•*Scientific Reports* **7**, Article number: 8617 (2017) doi:10.1038/s41598-017-09094-4

OSG-KINC

```
[wpoehlm@login02 OSG-KINC]$ ls
pegasus.conf  README.md  sites.xml  submit  task-files  tools
[wpoehlm@login02 OSG-KINC]$ ./submit 1000
```

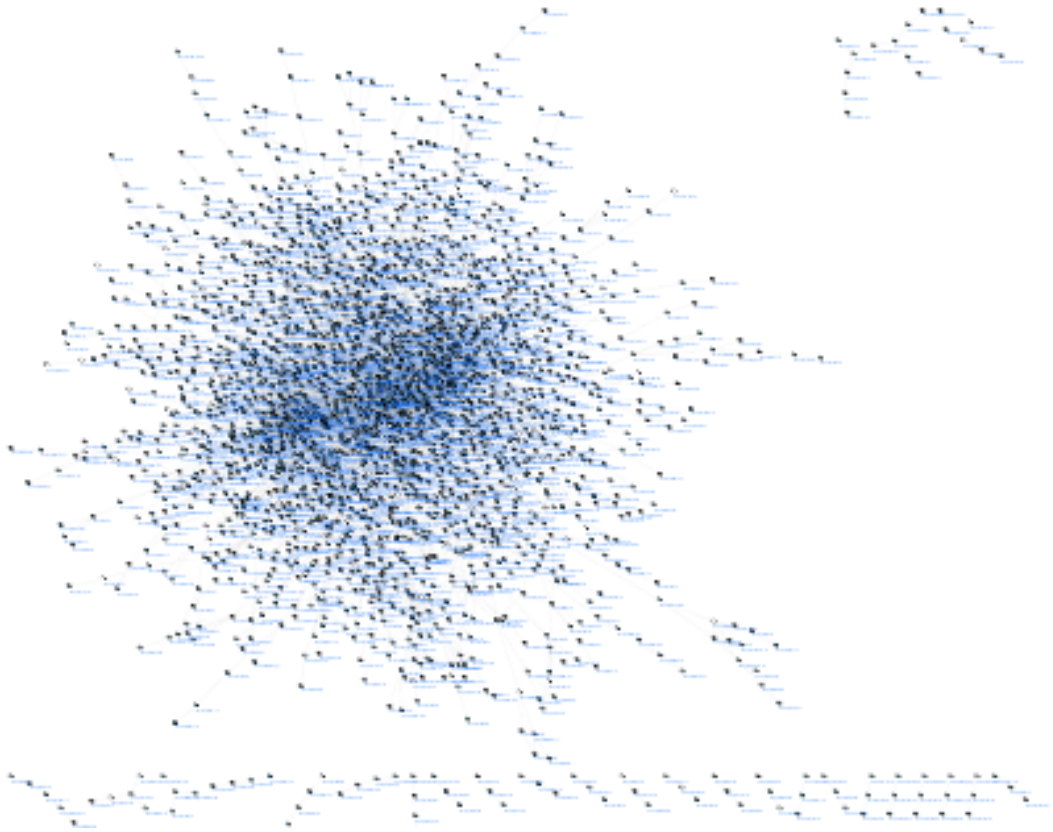
ERR472937	ERR472938	ERR472940
transcript:YAL069W	NA	NA
transcript:YAL068W-A	NA	NA
transcript:YAL067W-A	NA	NA
transcript:YAL066W	NA	NA
transcript:YAL064W-B	NA	NA
transcript:YAL064W	NA	NA
transcript:YAL062W	8.26571746	10.3418362
transcript:YAL061W	6.21383361	8.99230876
transcript:YAL060W	9.85801769	9.63639389
transcript:YAL059W	3.74150744	NA
transcript:YAL058W	3.70456386	NA
transcript:YAL056W	4.27589997	3.84691542
transcript:YAL055W	NA	NA



/local-scratch

Use Case: Yeast Gene Coexpression Network

- Input: Yeast Gene Expression Matrix
  - 188 Biological Samples
  - 7050 RNA transcripts
- Computation: 24,847,725 correlation tests
- Output: Gene Coexpression Network
  - 2996 Nodes
  - 6766 Edges



OSG-KINC: Chameleon vs Open Science Grid

48 Chameleon Compute Nodes

```
------------------------------------------------------------------------------
Type           Succeeded Failed  Incomplete  Total     Retries   Total+Retries
Tasks          8000      0       0           8000      0         8000
Jobs           8037      0       0           8037      0         8037
Sub-Workflows  0         0       0           0         0         0
------------------------------------------------------------------------------

Workflow wall time                                       : 2 hrs, 50 mins
Cumulative job wall time                                 : 43 days, 1 hr
Cumulative job wall time as seen from submit side        : 48 days, 7 hrs
Cumulative job badput wall time                          :
Cumulative job badput wall time as seen from submit side :
```

Open Science Grid

```
------------------------------------------------------------------------------
Type           Succeeded Failed  Incomplete  Total     Retries   Total+Retries
Tasks          8000      0       0           8000      99        8099
Jobs           8607      0       0           8607      99        8706
Sub-Workflows  0         0       0           0         0         0
------------------------------------------------------------------------------

Workflow wall time                                       : 10 hrs, 47 mins
Cumulative job wall time                                 : 44 days, 5 hrs
Cumulative job wall time as seen from submit side        : 47 days, 23 hrs
Cumulative job badput wall time                          : 1 day, 20 hrs
Cumulative job badput wall time as seen from submit side : 1 day, 20 hrs
```

Scientific Workflow Execution on Chameleon

Pegasus → DAGMan → HTCondor High Throughput Computing

- Software dependencies accessed from OSG CVMFS: read-only, cached, distributed filesystem
- Condor pool created from Chameleon nodes: each CPU on a node can be used as a compute site
- One node configured as “master node” where the workflow is submitted

- Transfer raw DNA sequencing files from National Center for Biotechnological Information(NCBI) database

NCBI → SRA toolkit / wget →

```
@SRR1298817.4432 GWZHISEQ02:47:C2F09ACXX:3:1101:8258:5198 length=101
CATCCTTCTCTAGAGGCTTTTGTTTCTCTCCTGGTCTACGGATTTCTGCAACTCTATTTGCACAAGCTCTACCAAAAACAACAATATCGAGAAGTGAATTT
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@SRR1298817.4435 GWZHISEQ02:47:C2F09ACXX:3:1101:8522:5043 length=101
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+SRR1298817.4435 GWZHISEQ02:47:C2F09ACXX:3:1101:8522:5043 length=101
CCCFFFFFHHFHHJJJJJJJJJJJJJJJJJJJJJJJJIJJJJJJJJJBFHIIJJJJJJJJJJJJJJJJJJJJJHHHEHHFFFFFEEEDEDDDDDDDDDD^C
```
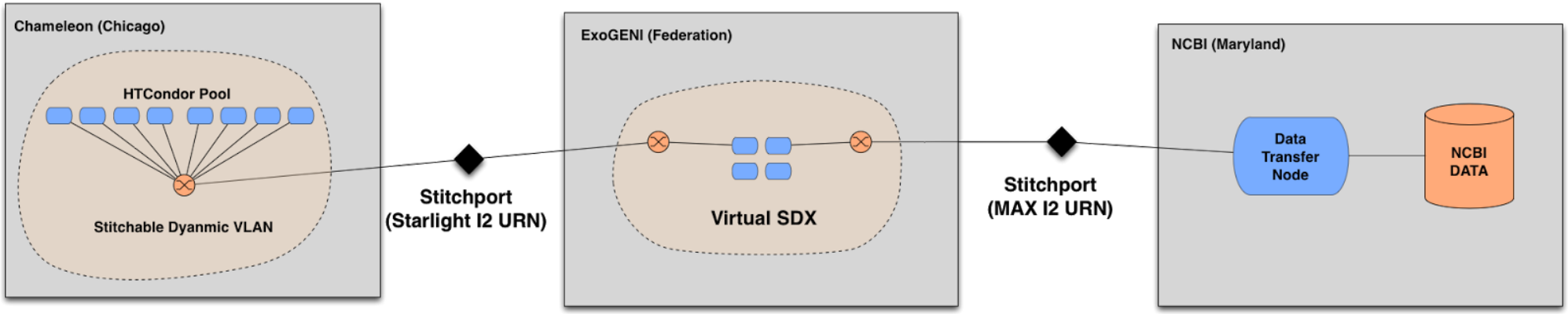
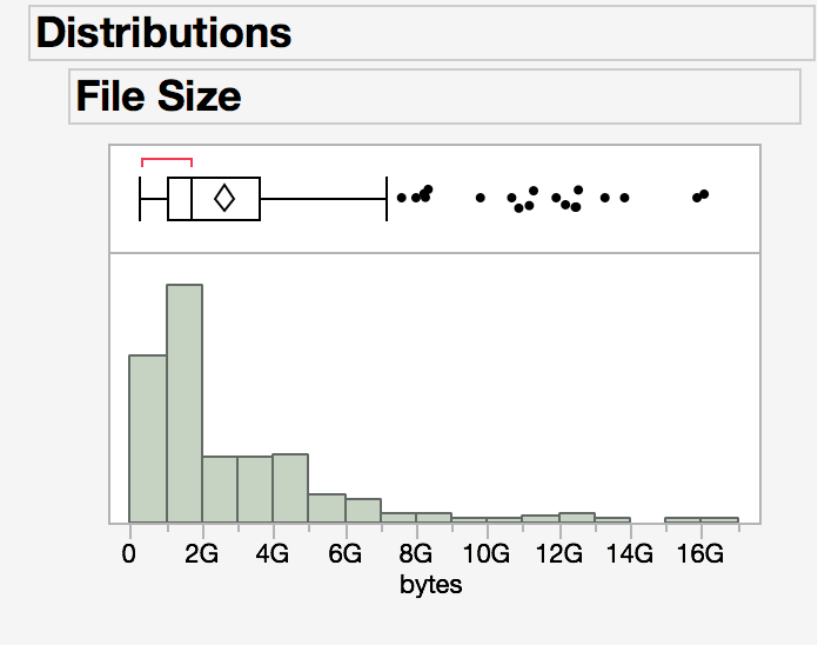

Stitching: Chameleon to NCBI



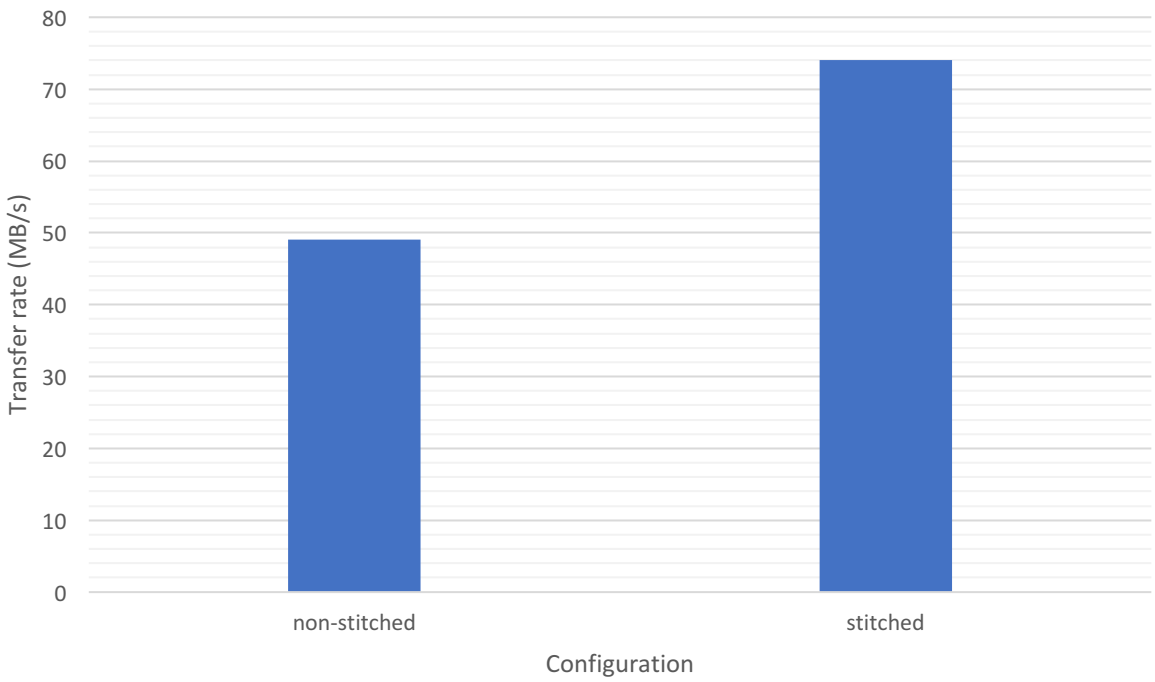
Credit: Paul Ruth

- Connect through a virtual SDX (Pittsburgh Supercomputing Center)
- Layer2 circuits from Chameleon to ExoGENI
- ExoGENI to NCBI (Maryland)

Transfer rate: Non-Stitched vs Stitched



Total dataset size 1.15 TB in 439 files.

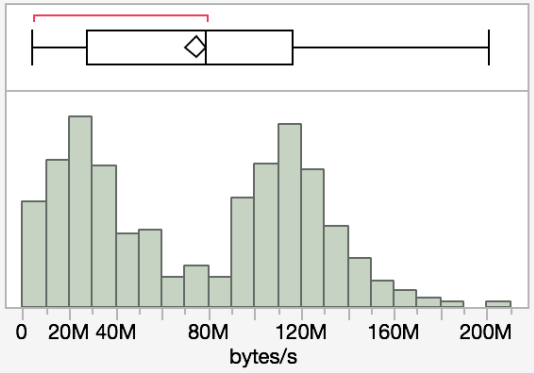


49 MB/s **74 MB/s**

Stitched transfer details

Distributions

Transfer rate



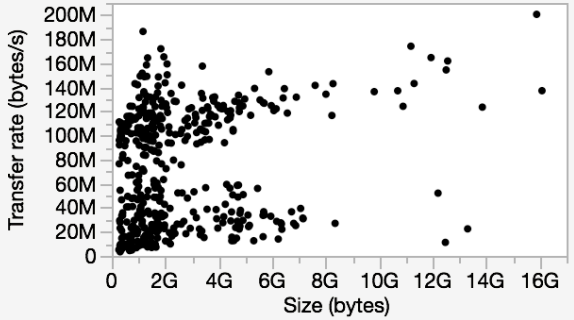
Quantiles

100.0%	maximum	200583399.37
99.5%		183916382.43
97.5%		157570379.34
90.0%		131850041.01
75.0%	quartile	115752720.55
50.0%	median	78907109.228
25.0%	quartile	27037383.898
10.0%		12699976.654
2.5%		7282925.022
0.5%		4534122.7031
0.0%	minimum	3411966.0621

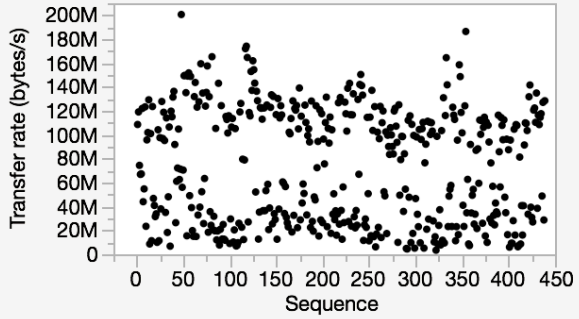
Summary Statistics

Mean	74202138
Std Dev	47583139
Std Err Mean	2271019.3
Upper 95% Mean	78665587
Lower 95% Mean	69738688
N	439

Bivariate Fit of Transfer rate By Size



Bivariate Fit of Transfer rate By Sequence



Automation of lease creation and node setup

1. Create a new lease for the master and workers.
2. Start the worker instances with a boot script to set up SSH keys.
3. Start the master instance.
4. Build a hosts file with the internal IP address of all instances and copy the file to the master.
5. Run the master boot script to finish configuration.

User experiences

- CLI tools store passwords in environment variables or on the command line.
- Adding two minutes to the lease start time is awkward.
- Compute nodes and storage nodes require separate leases.
- Storage nodes don't erase disk drives between experiments.
- Storage nodes can't connect to the ExoGENI VLAN network.

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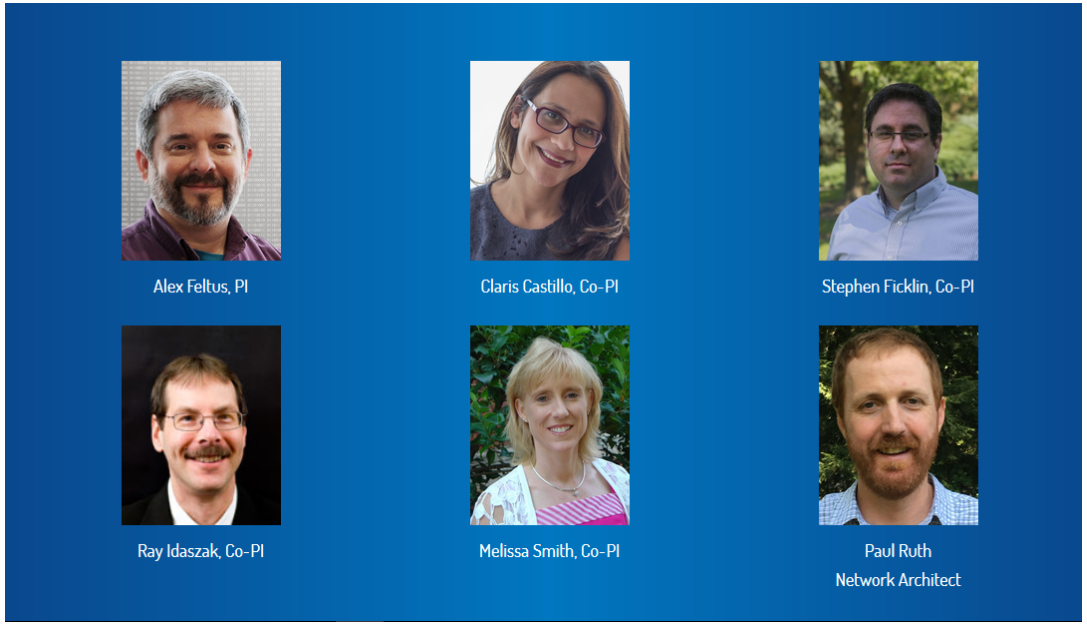
scidas.org



Open Science Grid

Mats Rynge (ISI)

NSF

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