Open Science Grid

Galaxy based BLAST submission to distributed high throughput computing resources

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Topics

- What is BLAST / Galaxy?
- Why BLAST on OSG?
- How to run BLAST on HTC?
- Conclusion and future TODO...

NCBI-BLAST

NCBI (National Center for Biotechnology Information)

BLAST (Basic Local Alignment Search Tool)

Popular application for Bioinformaticists

Compares biological sequences

- Identify unknown sequences
- Discover related organism

Database Source fasta

```
>gi|6226515|ref|NC_001224.1| Saccharomyces cerevisiae mitochondrion
TTCATAATTAATTTTTTATATATATATTATATTATAATATTAATTTATATTATAAAAATAATATTTATTATTAAAATAT
T
TATTCTCCTTTCGGGGTTCCGGCTCCCGTGGCCGGGCCCCGGAATTATTAATTAATAATAAATTATTATTAATAATTAT
T
TATTATTTTATCATTAAAATATATAAATAAAAAATATTAAAAAGATAAAAAAAATAATGTTTATTCTTTATATAAATTA
T
ATATATATATATAATTAATTAATTAATTAATTAATTAATAATAAAAATATAATTATAAATAATATAAATATTATTCTTT
A
TTAATAAATATATATTTATATATTATAAAAGTATCTTAATTAATAAAAATAAACATTTAATAATATGAATTATATATTA
T
TATTATTATTAATAAAATTATTAATAATATATCAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAA
T
... (150,000 lines)
```

```
$ makeblastdb -in
yeast.fasta -dbtype nucl -
out yeast
```

Blast DB

Input Query (Unknown Organism)

```
>CHR1.19971009 Chromosome I Sequence
CCACACCACACCCACACACCCACACACCACACCACACACCACACCCACACACACA
CATCCTAACACTACCCTAACACAGCCCTAATCTAACCCTGGCCAACCTGTCTCTCAACTT
ACCCTCCATTACCCTGCCTCCACTCGTTACCCTGTCCCATTCAACCATACCACTCCGAAC
CACCATCCATCCCTCTACTTACTACCACTCACCCACCGTTACCCTCCAATTACCCATATC
CAACCCACTGCCACTTACCCTACCATTACCCTACCATCCACCATGACCTACTCACCATAC
TGTTCTTCTACCCACCATATTGAAACGCTAACAAATGATCGTAAATAACACACACGTGCT
TACCCTACCACTTTATACCACCACCACATGCCATACTCACCCTCACTTGTATACTGATTT
TACGTACGCACACGGATGCTACAGTATATACCATCTCAAACTTACCCTACTCTCAGATTC
CACTTCACTCCATGGCCCATCTCTCACTGAATCAGTACCAAATGCACTCACATCATTATG
CACGGCACTTGCCTCAGCGGTCTATACCCTGTGCCATTTACCCATAACGCCCATCATTAT
CCACATTTTGATATCTATATCTCATTCGGCGGTCCCAAATATTGTATAACTGCCCTTAAT
ACATACGTTATACCACTTTTGCACCATATACTTACCACTCCATTTATATACACTTATGTC
AATATTACAGAAAAATCCCCACAAAAATCACCTAAACATAAAAATATTCTACTTTTCAAC
```

```
$ blastn -db mydb -query input_query.fasta -out output.txt -outfmt 1
```

```
comp10597_c0_seq1    Uextra    100.00    28 0 0 168    195    3953904    3953931    4e-06    52.8
comp10597_c0_seq1    Uextra    100.00    28 0 0 168    195    28550642   28550615   4e-06    52.8
comp12438_c0_seq1    2L        100.00    29 0 0 116    144    8509466    8509494    2e-06    54.7
comp12438_c0_seq2    2L        100.00    29 0 0 134    162    8509466    8509494    2e-06    54.7
```

Common Blast Databases

NCBI RefSeq Databases

NT/NR (10-20 parts 400-800M each compressed)

Collection of taxonomically diverse, non-redundant and richly annotated sequences.

* plasmids, organelles, viruses, archaea, bacteria, and eukaryotes.

patnt/pataa (1-4 parts 1G each)

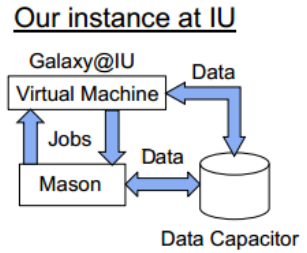
Patent database from USPTO or from EU/Japan Patent Agencies via EMBL/DDBJ

Flybase Databases

dmel-all-chromosome

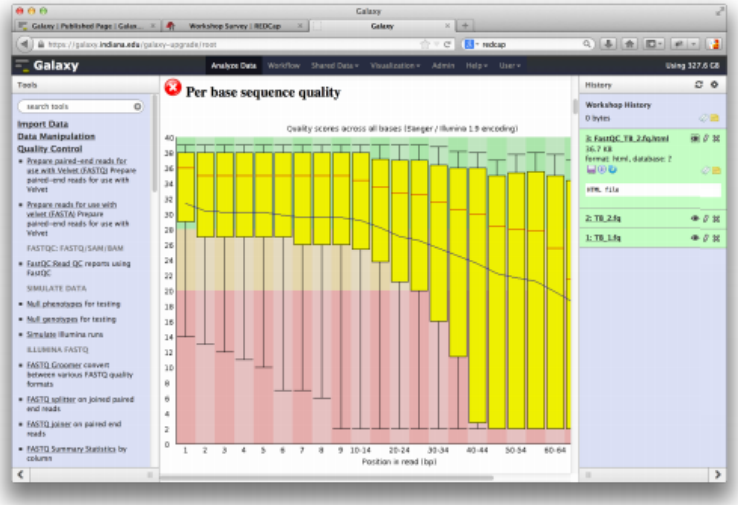
Galaxy

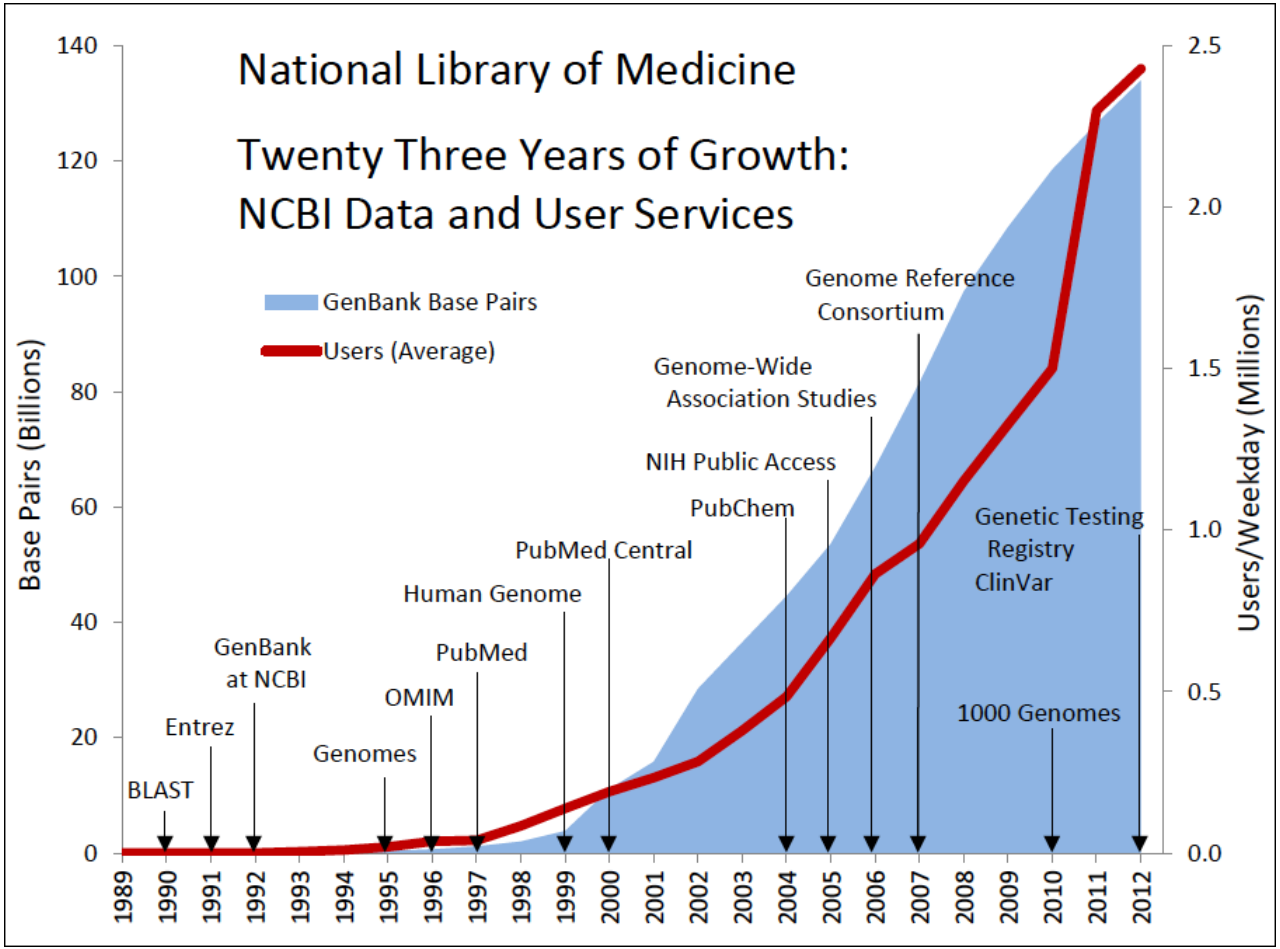
A popular Web-based platform for data intensive biomedical research



NCGAS (National Center for Genome Analysis Support) hosts an instance of Galaxy portal

- IU Mason Cluster (8TB-memory)
- Access to IU DC2 (3.5PB)
- Genome assembly
- Large-scale phylogenetic software
- Blast




National Library of Medicine
Twenty Three Years of Growth:
NCBI Data and User Services
GenBank Base Pairs
Users (Average)
Base Pairs (Billions)
Users/Weekday (Millions)
BLAST
Entrez
GenBank at NCBI
Genomes
OMIM
PubMed
Human Genome
PubMed Central
PubChem
NIH Public Access
Genome-Wide Association Studies
Genome Reference Consortium
Genetic Testing Registry
ClinVar
1000 Genomes
0
20
40
60
80
100
120
140
0.0
0.5
1.0
1.5
2.0
2.5
1989
1990
1991
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2004
2005
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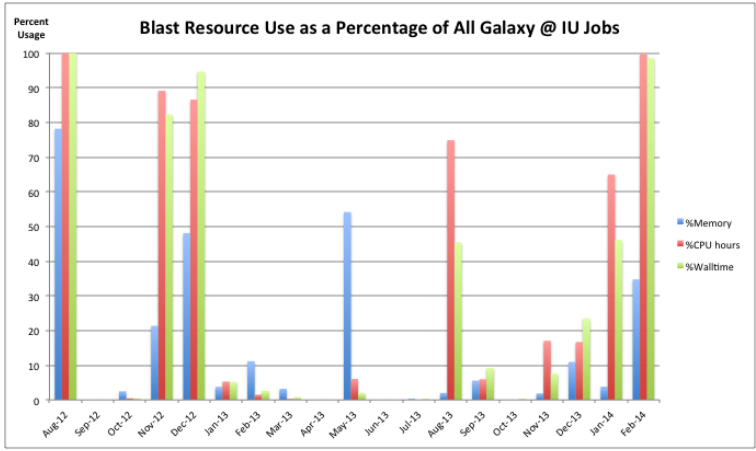
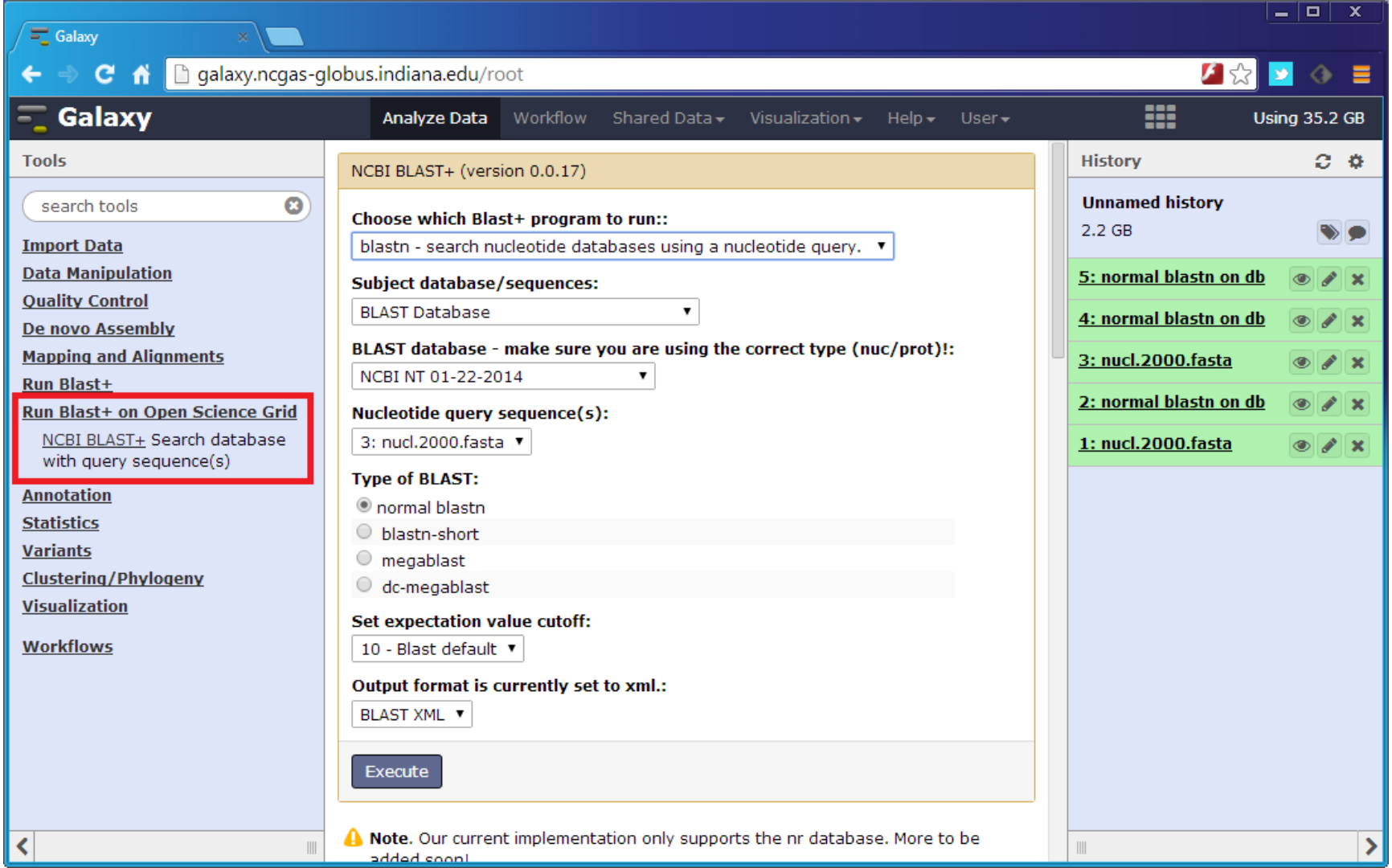
2007
2008
2009
2010
2011
2012

Why BLAST on OSG?

- BLAST is CPU intensive (not memory)
- IU/Mason is not an optimal resource to run BLAST
- Growth in data volume will squeeze available resource capacity at NCGAS in coming years.
- OSG's opportunistic resource could be used as an alternative for Mason and can provide necessary resource capacity.



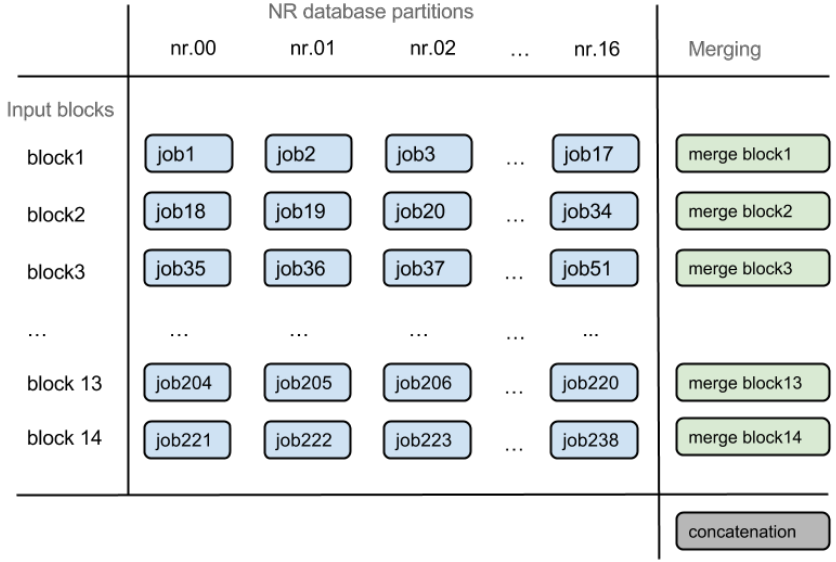

Galaxy
galaxy.ncgas-globus.indiana.edu/root
Galaxy
Analyze Data
Workflow
Shared Data
Visualization
Help
User
Using 35.2 GB
Tools
search tools
Import Data
Data Manipulation
Quality Control
De novo Assembly
Mapping and Alignments
Run Blast+
Run Blast+ on Open Science Grid
NCBI BLAST+ Search database with query sequence(s)
Annotation
Statistics
Variants
Clustering/Phylogeny
Visualization
Workflows
NCBI BLAST+ (version 0.0.17)
Choose which Blast+ program to run::
blastn - search nucleotide databases using a nucleotide query.
Subject database/sequences:
BLAST Database
BLAST database - make sure you are using the correct type (nuc/prot)!:
NCBI NT 01-22-2014
Nucleotide query sequence(s):
3: nucl.2000.fasta
Type of BLAST:
normal blastn
blastn-short
megablast
dc-megablast
Set expectation value cutoff:
10 - Blast default
Output format is currently set to xml.:
BLAST XML
Execute
Note. Our current implementation only supports the nr database. More to be added soon!
History
Unnamed history
2.2 GB
5: normal blastn on db
4: normal blastn on db
3: nucl.2000.fasta
2: normal blastn on db
1: nucl.2000.fasta

osg-blast (v2)

- Written in nodejs / node-osg & node-htcondor modules
- Can be installed on any OSG submit hosts via “npm install osg-blast”
- Hosted databases (NT/NR) distributed via OASIS (CVMFS)
- Needs to be highly reliable and autonomous
  - Handle unexpected issues well
  - Needs to figure out the best configuration by itself.
  - Report site specific issues to GOC (and recover)
  - Cleanup after itself (removing temp files, canceling jobs)

osg-blast (v2)

- Splits both input queries / databases and run all jobs in parallel.
- Results are merged to create a single output sorted by e-value.

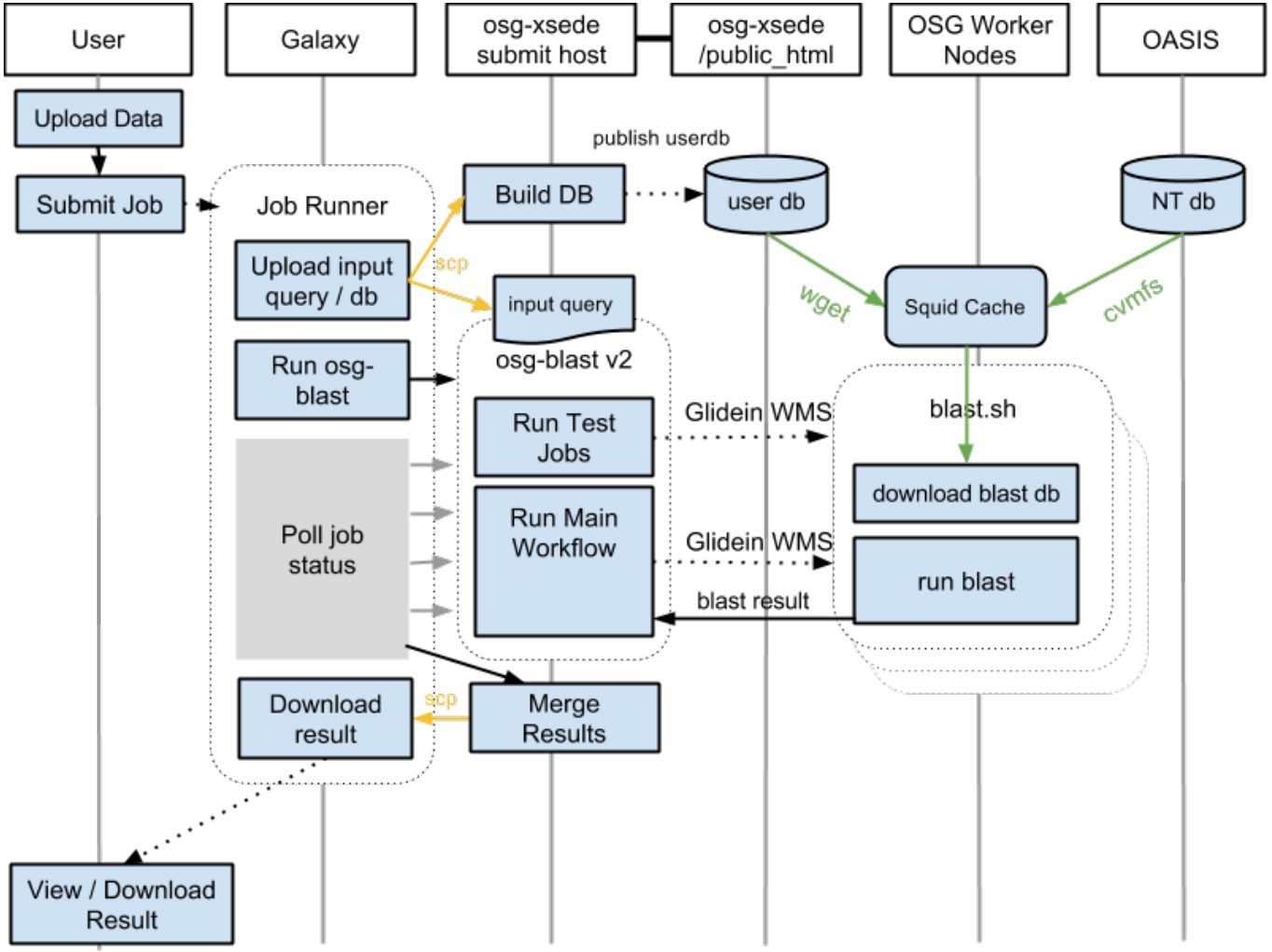


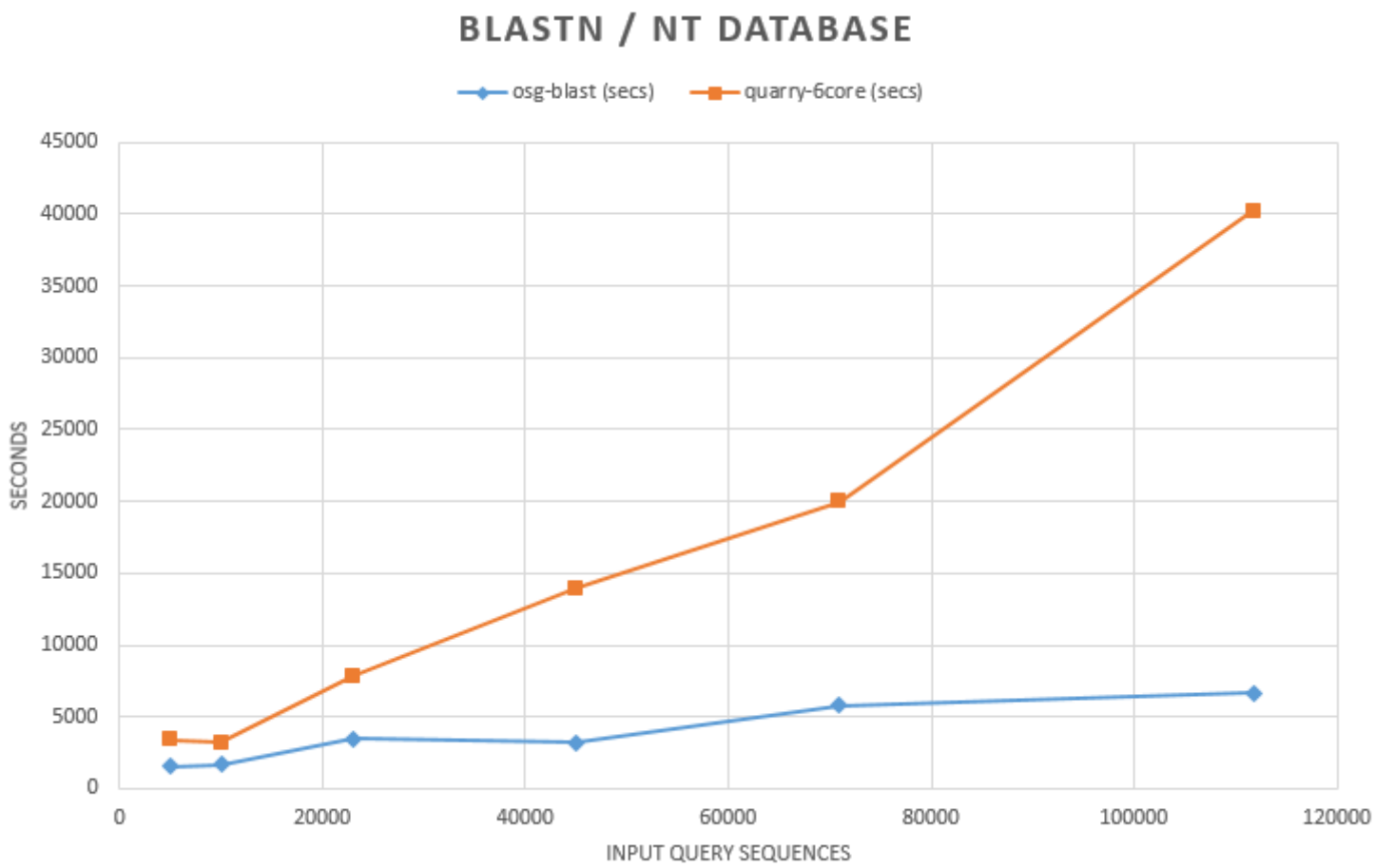
Test Stage

- Determine best input block size
- Detects issue with user input / OSG environment.

Main Stage

- Submit all jobs using information gathered during the test stage.
- Use -dbsize to correct e-value


User
Galaxy
osg-xsede submit host
osg-xsede /public_html
OSG Worker Nodes
OASIS
Upload Data
Submit Job
Job Runner
publish userdb
Build DB
user db
NT db
Upload input query / db
scp
input query
wget
Squid Cache
cvmfs
Run osg-blast
osg-blast v2
Run Test Jobs
Glidein WMS
blast.sh
download blast db
Poll job status
Run Main Workflow
Glidein WMS
run blast
blast result
Download result
scp
Merge Results
View / Download Result


BLASTN / NT DATABASE
osg-blast (secs)
quarry-6core (secs)
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
SECONDS
0
20000
40000
60000
80000
100000
120000
INPUT QUERY SEQUENCES

Conclusions

- Clearly, we will need more computing resources to run BLAST in coming years, and OSG's opportunistic environment can provide that need.
- Galaxy allows bioinformatics community to use existing UI to submit BLAST jobs.
- BLAST works well in HTC environment, and it seems to scale as expected using OSG's opportunistic resources.

Challenges / Future Goal

- osg-blast workflow needs to be highly robust (error-tolerant), reliable, and self-diagnosing to be practical (can't rely on users to fix problems)
- osg-blast output merger needs to be implemented for other output formats.
- Might need to explore alternative to CVMFS for hosting BLAST DBs.

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