OAG All-Hands Meeting, March 20, 2019

# GlueX Experience with the Open Science Grid

past experience,
present challenges,
future prospects

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# Background: *the Gluex experiment*

**GlueX at Jefferson Lab**

- 9 GeV photons, fixed target
- *map the hybrid meson spectrum*

**installed:** 2012-2014

**commissioned:** 2014-2016

**approved physics:** 2017-2022


*This work is supported by the National Science Foundation under grant 1508238*

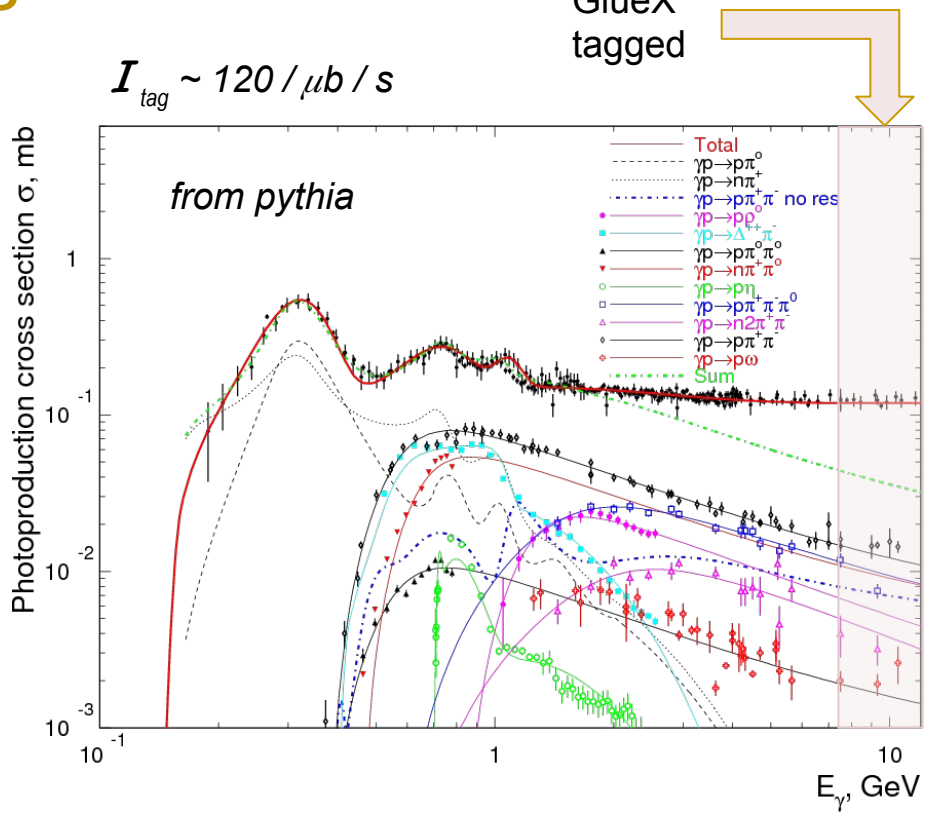
# GlueX event, data rates

## Experimental data rates

- 80 kHz trigger rate (~1.6GB/s)
- many exclusive final states
- < 50% are simple topologies

## Simulated data estimates

- based on *GlueX-doc-3813* (2018)
- **36 Mcore-hr/yr** (2020 and beyond)
- *primarily targeted for OSG*





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# OSG: *the Gluex VO*


- Gluex vo created in 2009 (10 years!)
- *NSF Physics at the Information Frontier*
- underwent an early series of data challenges
  - *data challenge I* - 2 Mcore-hr, 10 days
  - *data challenge II* - 6 Mcore-hr, 30 days
  - ***campus cluster campaign*** - 1 Mcore-hr, 15 days
- reconstruction is maturing, analysis is ramping up...



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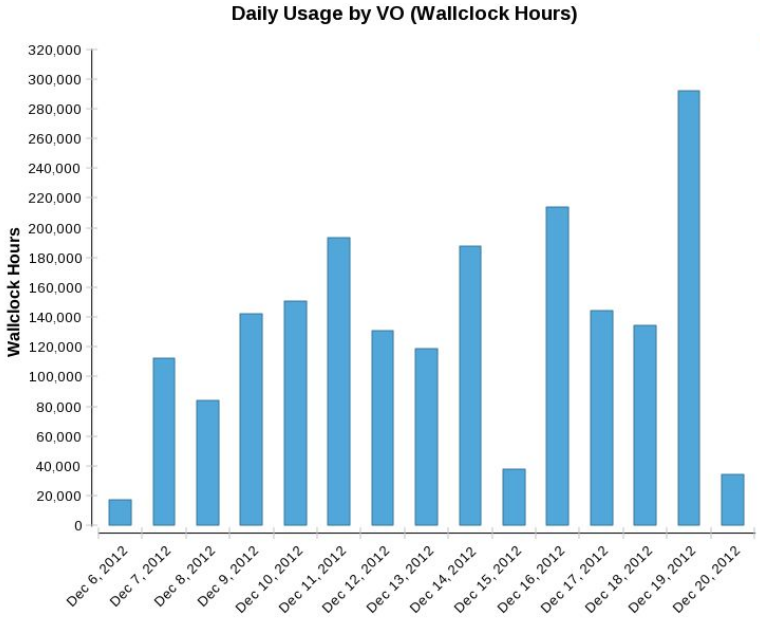
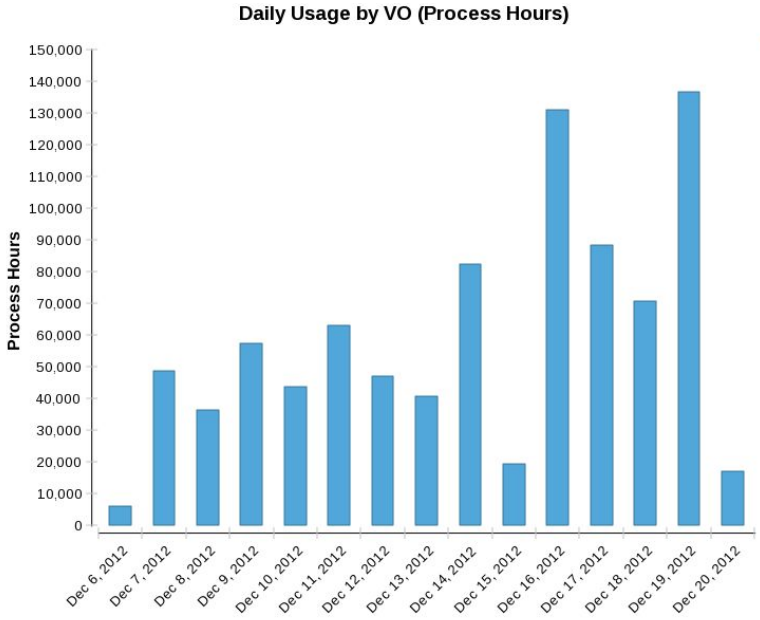
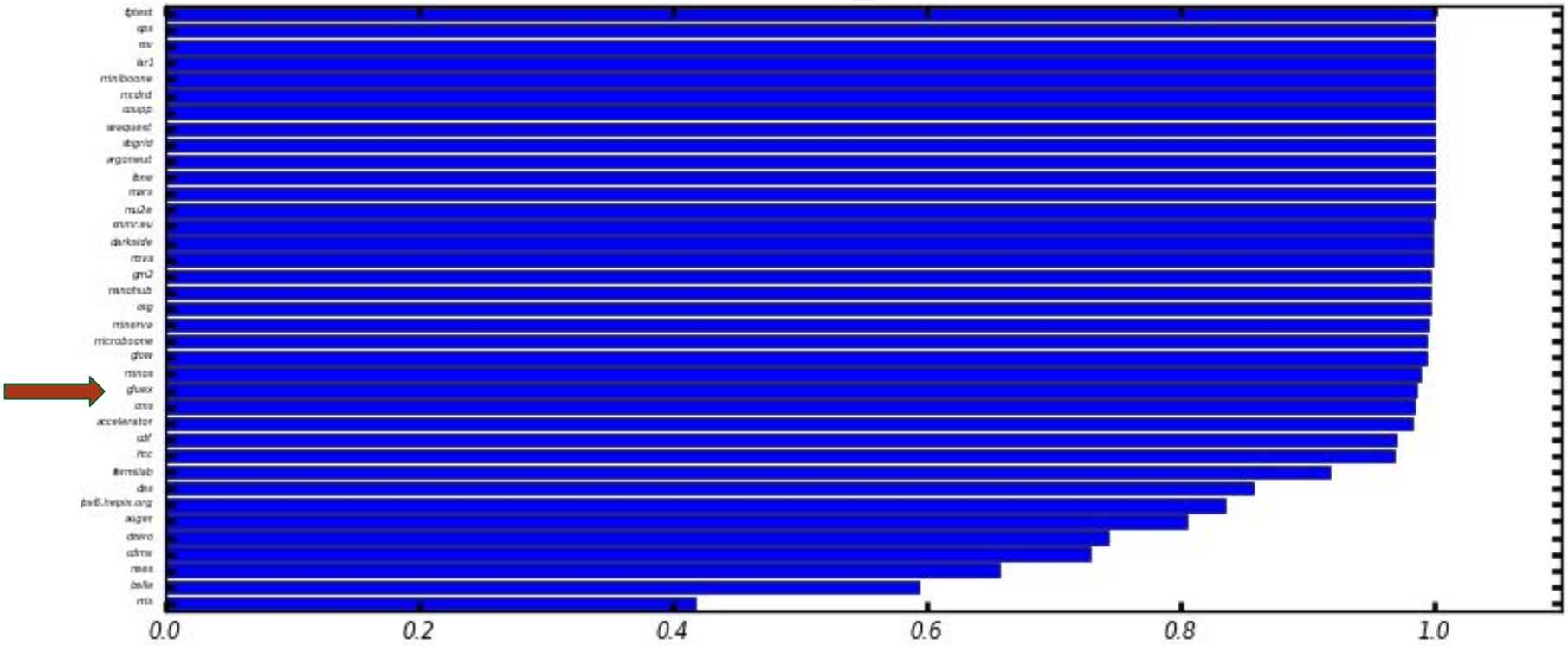
# Data Challenge 1: *results*

- cpu availability was very high (>10,000 cores peak)
- production efficiency was not great (40 – 60%)
- part of inefficiency is due to pre-emption (opportunistic)
- understanding sources of inefficiency is reason why we stopped @5B events



# Data Challenge 2: *results*




cpu time / wall clock time, daily average



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# Evolution in methodology

Open Science Grid

1. OSG_APPS, OSG_DATA ⟶ /cvmfs/oasis.opensciencegrid.org
2. singularity containers ⟶ /cvmfs/singularity.opensciencegrid.org

Big gains in opportunistic throughput seen by adapting software to run on the widest possible range of platforms.

For Gluex, this was a iterative, labor-intensive, experts-only process until ...

*All Gluex jobs containerized, can run on sites without singularity installed.*


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# Evolution in methodology (2)

Open Science Grid

1. Nightly builds inside standard container  oasis updates (as needed)
2. Software release management using github tags + *versions.xml*
3. Container rarely updated (once per year?)
4. Multiple binary releases maintained on oasis
   a. selected by demand
   b. currently on the high side - 150 GB oasis footprint
   c. *Is there a best practice to follow in this area?*


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# Evolution in *resources*

Open Science Grid

**GlueX offline computing resource needs *(GlueX-doc-3813)***

1. 130 Mcore-hr/yr - experimental data reconstruction
   - *Jefferson Lab compute facility (total 70 Mcore-hr/yr, all experiments)*
   - *NERSC (proven option, but competitive)*
   - *other ??*

2. 36 Mcore-hr/yr - Monte Carlo simulation
   - *primarily targeted for OSG*
   - *cannot live on donations alone*



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# Evolution in *resources*

Open Science Grid

## Existing OSG resources for GlueX:

1. **UConn_OSG** site: 600-core cluster
   - active on OSG since ca. 2010
   - contributed 3-4 Mhr/yr opportunistic OSG cycles over past decade
2. **GLUEX_US_FSU_HNPGRID** site: “entry-level” cluster
   - active on OSG since ca. 2017
   - contributed 100 khr/yr to OSG over the past 2 years
   - starting point for future growth in GlueX computing at FSU

*This amounts to **10%** of the projected need for GlueX simulations over past 2019.*


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# Evolution in *resources*

Open Science Grid

## *Where are the OSG resources for GlueX?*

A number of *resourced GlueX institutions* have offered to contribute:

a. Carnegie Mellon University
b. Indiana University - stanley, karst, BigRed
c. Florida State University - RACF
d. George Washington University - ColonialOne
e. College of William and Mary - vortex
f. University of Regina - computecanada
g. UConn Health Center HPC - xanadu
h. UConn Storrs HPC - hornet


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# Evolution in *resources*

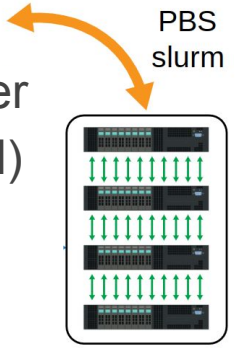
Open Science Grid

## *Where are the OSG resources for GlueX?*

A number of *resourced GlueX institutions* have offered to contribute, *but the barriers turned out to be higher than expected -- 2017 summer of setbacks.*

## *Summer 2018 -- what can be done to move forward?*

- for the time being, *skip OSG site integration*
- **implement a separate stand-alone condor pool (at UConn)**
- get access to individual user accounts on every member's cluster
- **customize a glidein** for each individual cluster (bosco, 8 in total)
- install local copy of complete GlueX stack + container
- diagnose, debug, optimize...





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# Evolution in *resources*

Open Science Grid

## ***Summer 2018 -- lessons from "bosco" exercise***

1. It was successful
   - 1 Mcore-hr of simulations completed in 15 days
   - average 5k cores active during periods when not debugging
   - spanned very different types: included BigRed Cray HPC @ IU
2. It was a management headache
   - like going back to opportunistic OSG ca. 2012 *(rsync, pilot jobs, etc.)*
   - no two clusters the same, each one like a green field
   - ***whack-a-mole ops*** -- not sustainable for GlueX production long-term.


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# Evolution in *resources*

Open Science Grid

## *Where are the OSG resources for GlueX?*

A number of *resourced GlueX institutions* have offered to contribute, *and through the summer 2018 bosco exercise all have done so, except one.*

## *BUT*

- There are good reasons to go the route of full OSG site integration.
- This will require some effort from individual site admins.
- More than *technical expertise* is needed.


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# Evolution in *resources*

Open Science Grid

## *Where are the OSG resources for GlueX?*

Broader lessons from the GlueX bosco exercise:

1. Private cluster resources owned by individual groups are not keeping pace with the needs of our science.
2. Growth is happening in *shared computing resources* at universities.
3. Hurdles to executing grid jobs there are *primarily administrative*, *not technical.*
4. *In-advance discussions, agreements* with the central IT managers of these resources are needed -- they can be very helpful ***or not.***


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# Evolution in *resources*

Open Science Grid

## *Where are the OSG resources for GlueX?*

So what is the plan going forward?

1. Discussions have begun with some of our central campus IT admins (CMU, IU, UConn, Compute Canada)
2. Idea is for central cluster to be configured with a OSG glidein mechanism and accept OSG jobs, subject to administrative policies agreed among the primary stakeholders.
3. It really helps if we bring something to the table!
4. UConn -- *trying the dog food*


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# Evolution in *resources*

Open Science Grid

## *Where are the OSG resources for GlueX?*

**National Science Foundation**: Campus Computing and the Computing Continuum

***NSF 19-553 sollicitation:*** *"Local campus computing resources have emerged as an important aggregated and shared layer of scientific computing, as evidenced by the growth in* ***Open Science Grid (an NSF-funded distributed scientific computing fabric of shared computing clusters across more than 100 institutions)*** *productivity that will approach two billion CPU hours delivered in scientific computing for the calendar year 2018."*


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# Evolution in *resources*


## *Where are the OSG resources for GlueX?*


University of Connecticut proposal 1925716

- submitted February 20, 2019
- $400,000 for compute nodes (1020 cores) + storage (1 PB)
- enables a broad range of science at UConn
  - *experimental nuclear physics*
  - *geophysics*
  - *astrophysics*
  - *public health*



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# Evolution in *resources*

Open Science Grid

## *Where are the OSG resources for GlueX?*

Jefferson Lab computing review, November 2018:

- UConn - 10M core hours
- FSU - 5M core hours (so far, more on the horizon)
- Northwestern - 2M core hours
- Regina - 2M core hours (so far, asking for more)
- Indiana - 4M core hours
- Florida International - 2M core hours
- George Washington - 5M core hours (rough estimate)
- College of William and Mary - 2M core hours
- opportunistic cycles - 10M core hours


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# Evolution: *beyond simulation?*

Open Science Grid

**GlueX offline computing resource needs *(GlueX-doc-3813)***

1. 130 Mcore-hr/yr - experimental data reconstruction
   - *Jefferson Lab compute facility (total 70 Mcore-hr/yr, all experiments)*
   - *NERSC (proven option, but competitive)*
   - *other ??*

In the future, maybe OSG can contribute to the greater need here

- This is intrinsically a **HTC problem**
- To solve it we are *looking primarily to HPC resources* (technical reasons)
- These problems should be readily solvable (UConn working with WCHTC)


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# Evolution *beyond GlueX*

Open Science Grid

## Also from the November, 2018 Jefferson Lab computing review:

Plan to provision for simulation offsite ~63 M core hours per year

- OSG – pioneered by GLUEX, we will follow.
  - Submit jobs from JLab OSG submit node.
  - Collaborators contribute to OSG –in particular MIT.
- Other
  - Submit simulation in Docker container locally at the remote site using remote site's staff and batch system. Return results to Jlab.
  - INFN and others interested in this.
- NERSC
  - Submit via SWIF2 workflow tool (follow GLUEX).
  - Have requested NERSC allocation of 30M core hours.
  - Enough to cover 50% of the annual simulation workload.


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# Backup slides


*This work is supported by the National Science Foundation under grant 1508238*

# History: *slide from Oct. 2012, rtj*


- Experiment is in *construction phase until 2014*
- **Usage increasing with demand for Monte Carlo**

| run period | usage |
|---|---|
| 9/2009 – 9/2010 | 26.4 khr |
| 9/2010 – 9/2011 | 1.1 Mhr |
| 9/2011 – present | **2.1 Mhr** |

- **Growth has slowed as work turns to digesting the results**
- **Task:** simulation of background QCD photoproduction (Pythia)
- **Purpose:** develop cuts to suppress background, measure leakage from minimum-bias events into signal sample after cuts, requires very large statistics MC samples, shared between analysis tasks.
- **Plans**: saturate at the level 5-10M core-hr/yr until physics data collection begins ca. 2015.
- **Strategy**: glideinWMS – support from OSG admins *outstanding !*


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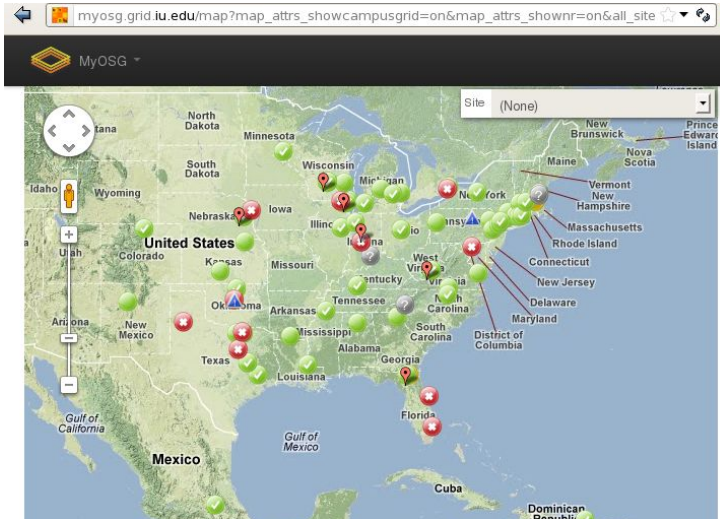
# Data Challenge 1: Dec. 2012

Open Science Grid

## Purpose of the exercise:

1. **Test** the current simulation and reconstruction tools
   - **bggen** – pythia-based background Monte Carlo generator
   - **hdgeant** – geant3-based physics simulation, base detector
   - **mcsmear** – detector efficiency and resolution models
   - **hd-ana** – reconstruction of tracks, neutrals
   - **REST** plugin – summary of reconstruction results




2. **Develop** the ability to manage simulation production and data storage at rates approaching GlueX Phase I.

3. **Produce** a large sample of background simulation data.

initial goal: 10 billion events, **60 days** at startup intensity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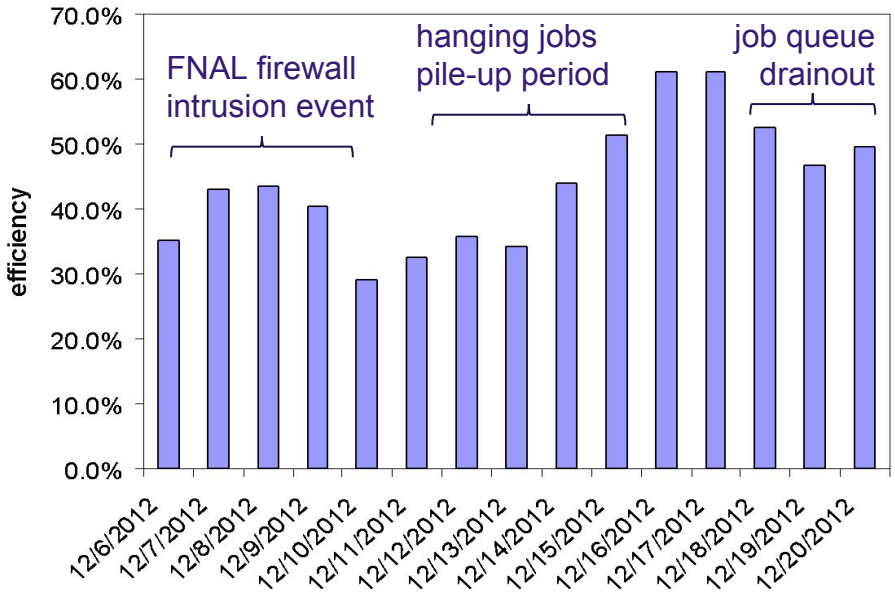
# Data Challenge 1: *results*

Open Science Grid

- total of 5.56B events simulated
  - **4.24B** on the OSG
  - **0.96B** at Jefferson Lab
  - **0.36B** at CMU
- completed over a period of 14 days

**Ran into several limiting factors:**

1. security event
2. software staging
3. freeze-ups in hd-ana
4. memory hogging in hd-ana
5. segfaults in hdgeant
6. irreproducibility in mcsmear





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# Data Challenge 2: Apr. 5-24, 2014

Open Science Grid

## Similar in purpose to DC1:

1. **Test** the current simulation and reconstruction tools, see if we fixed problems from DC1, check for new ones.

2. **Develop** the ability to manage production and data storage at rates approaching GlueX Phase I.

3. **Produce** a large sample of background simulation data, sufficient statistics to address issues.


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# Data Challenge 2: Apr. 5-24, 2014

Open Science Grid

## Similar in purpose to DC1:

1. **Test** the current simulation and reconstruction tools, see if we fixed problems from DC1, check for new ones.
   - more realistic simulation
   - include electromagnetic background
   - improved reconstruction
2. **Develop** the ability to manage production and data storage at rates approaching GlueX Phase I.
3. **Produce** a large sample of background simulation data, sufficient statistics to address issues.


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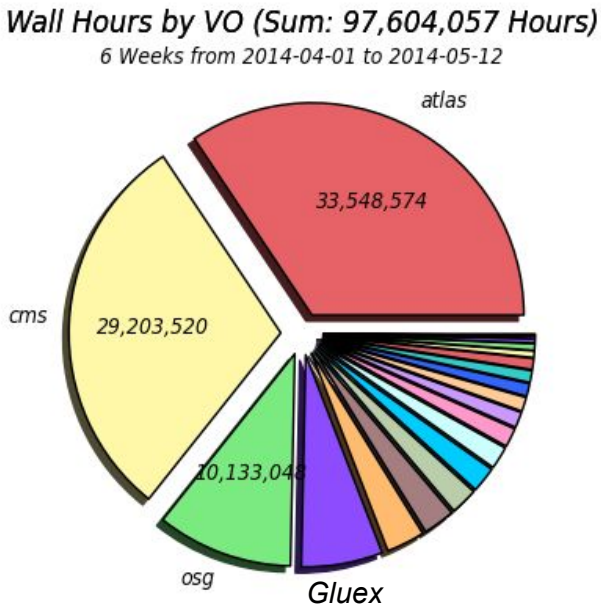
# Data Challenge 2: Apr. 5-24, 2014

Open Science Grid

## Similar in purpose to DC1:

1. **Test** the current simulation and reconstruction tools, see if we fixed problems from DC1, check for new ones.
   - more realistic simulation
   - include electromagnetic background
   - improved reconstruction
2. **Develop** the ability to manage production and data storage at rates approaching GlueX Phase I.
   - software distribution using cervnvm / oasis
   - particular focus on job efficiency
3. **Produce** a large sample of background simulation data, sufficient statistics to address issues.




6M core-hr = DC1 x 2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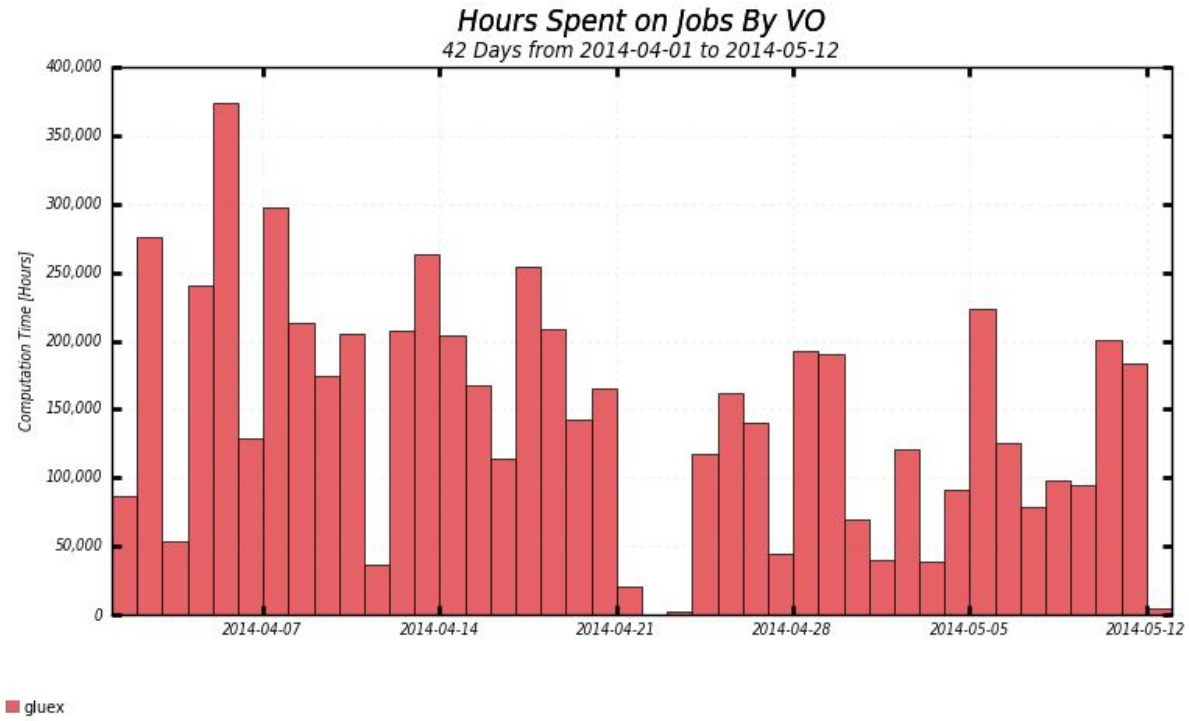
# Data Challenge 2: *results*




## Final event tally

| | | |
|---|---|---|
| **CMU** | 170M | 2% |
| **MIT** | 760M | 9% |
| **JLAB** | 2000M | 25% |
| **OSG** | 5200M | 64% |
| **total** | **8100M** | **100%** |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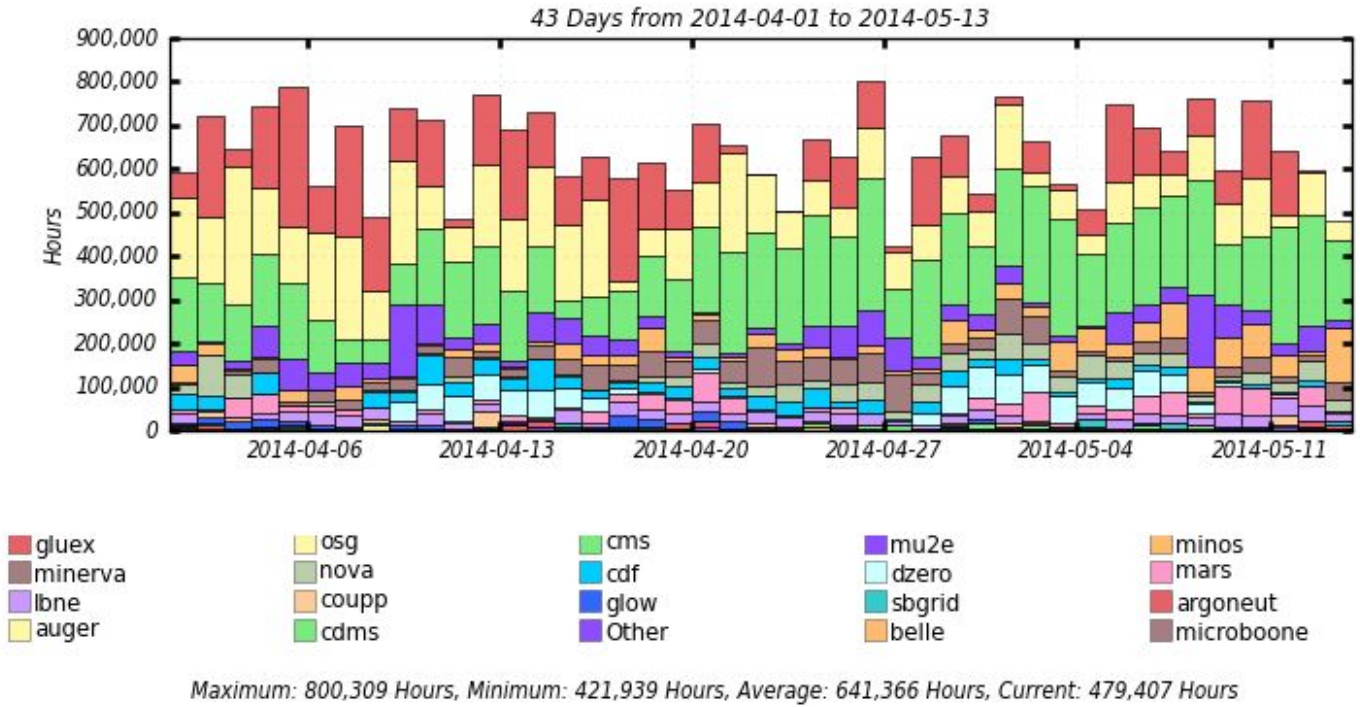
# Data Challenge 2: *results*

Open Science Grid

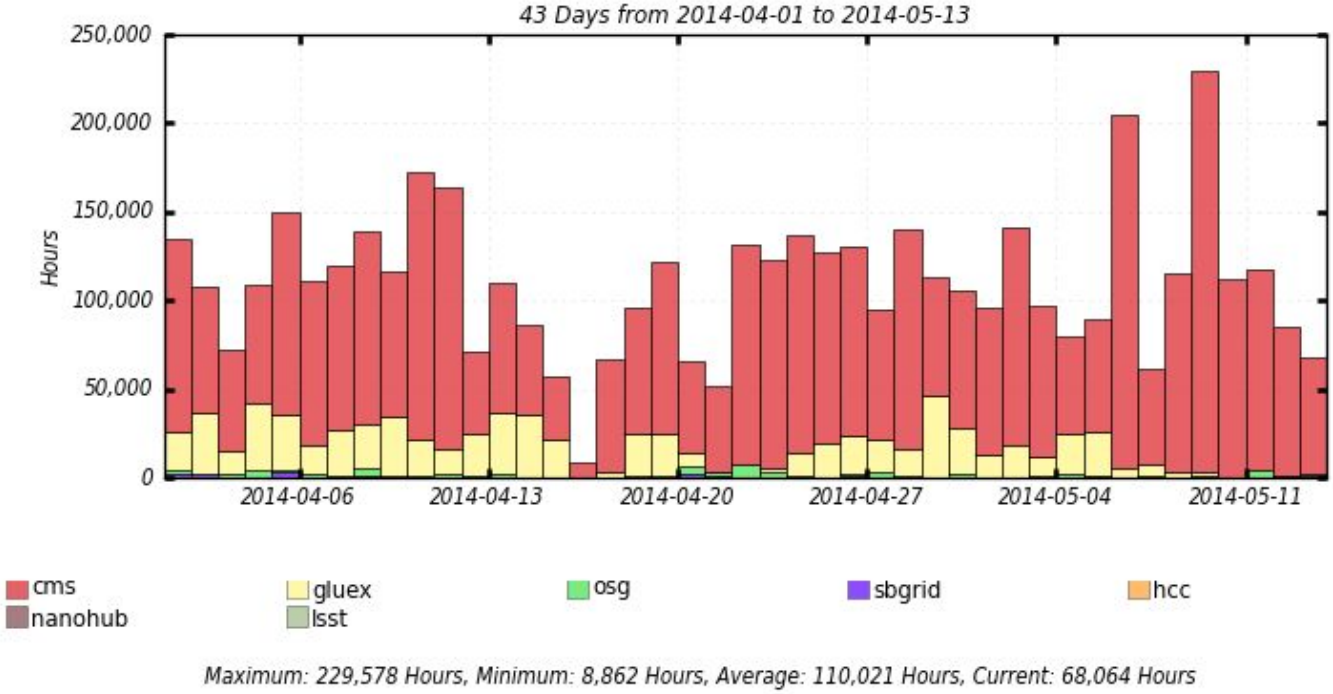
## Gluex usage on the Fermilab site



# Data Challenge 2: *results*

Open Science Grid

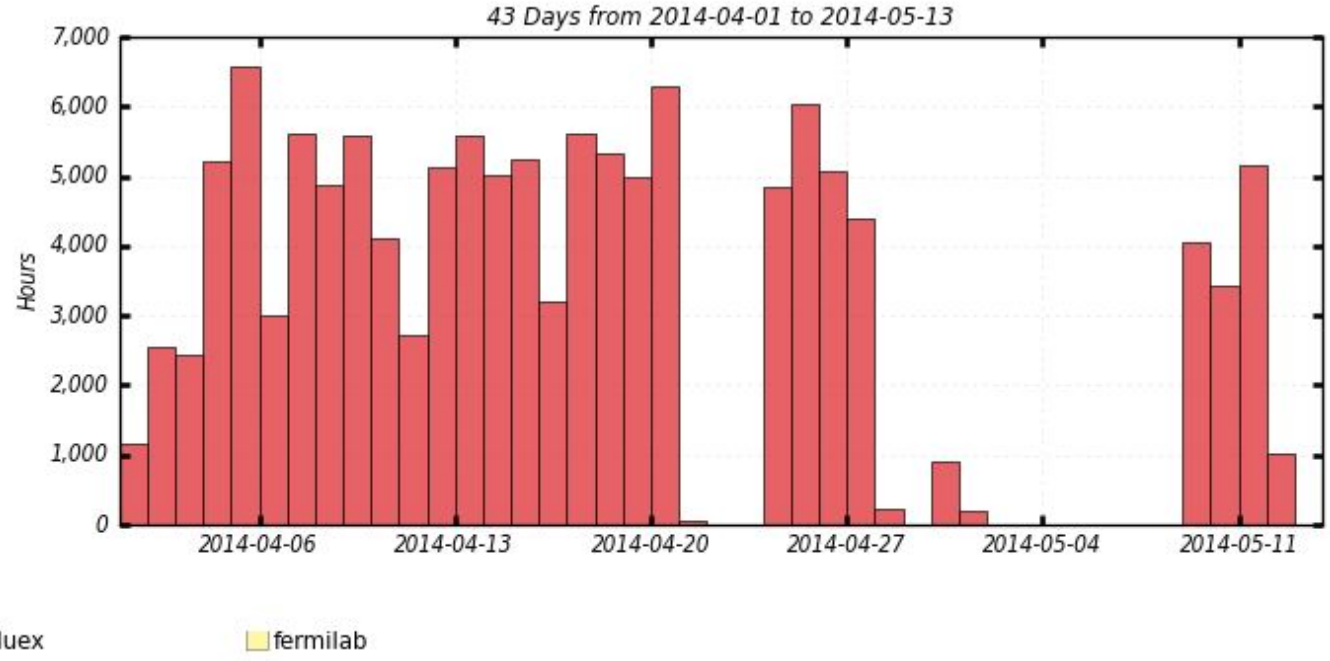
## Gluex usage on the Purdue site



# Data Challenge 2: *results*

Open Science Grid

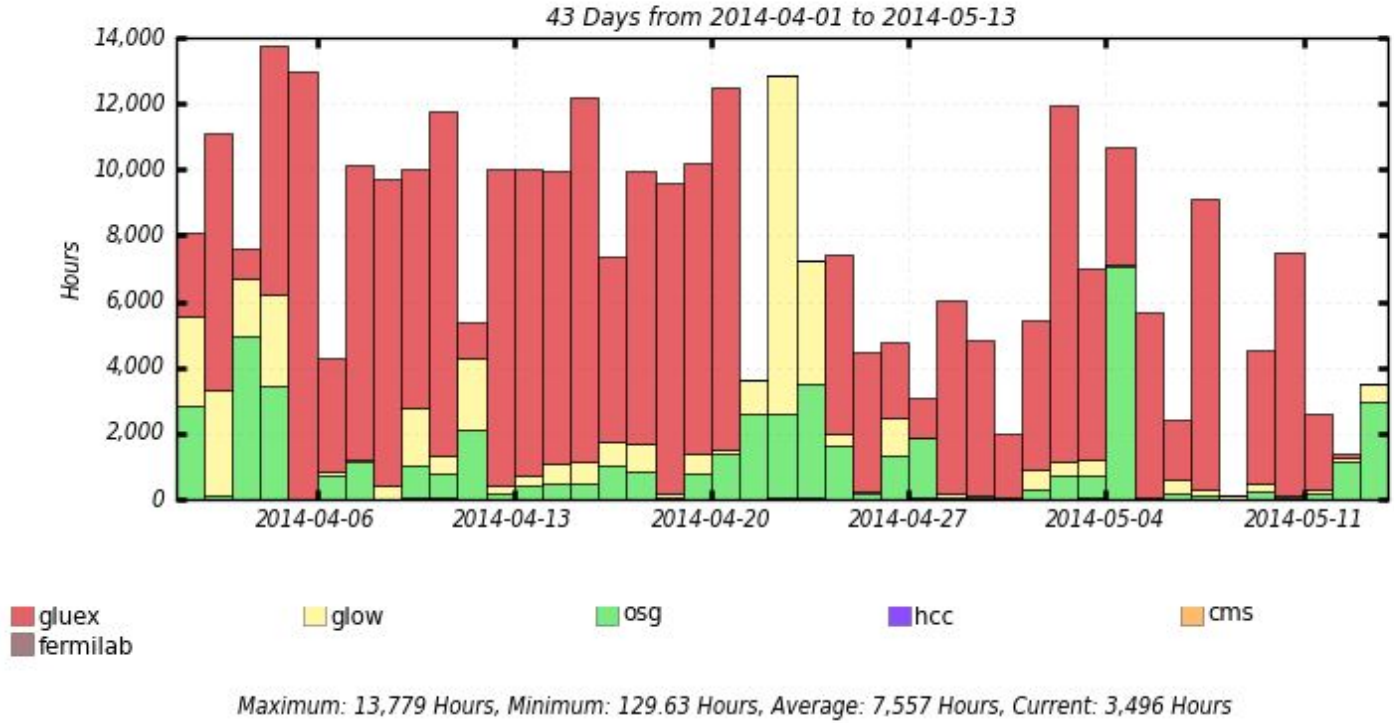
## Gluex usage on the Northwestern site



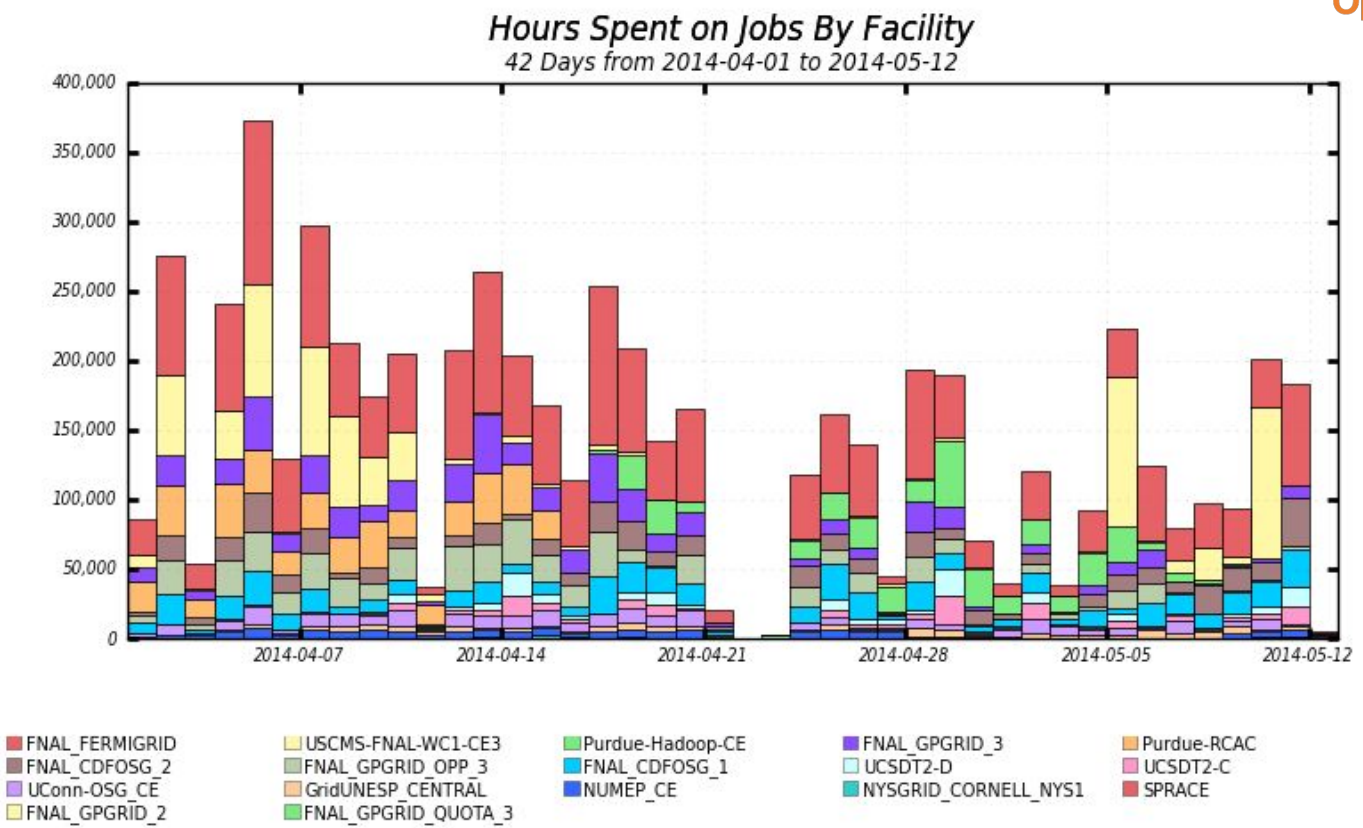
# Data Challenge 2: *results*

Open Science Grid

## Gluex usage on the UConn site



# Data Challenge 2: *results*



# Gluex activity on osg 2014-2016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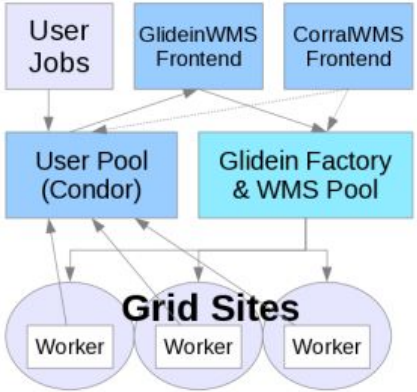
# Gluex @ – the reboot

- **OSG Executive Director, Frank Wuerthwein** speaks at *NP Computing Workshop,* Newport News, VA in March, 2016.
- **JLab CIO, Amber Boehnlein** initiates a pilot project for JLab users.

## scosg16: a GWMS submit host for JLab users




- ➢ located at JLab
- ➢ supported by JLab IT staff
- ➢ GlueX to be among the first users
- ➢ only out-flow of work is currently envisioned
- ➢ server configuration recommended, tested by OSG expert
- ➢ server installed, configured in 2Q 2017, testing by GlueX is now underway.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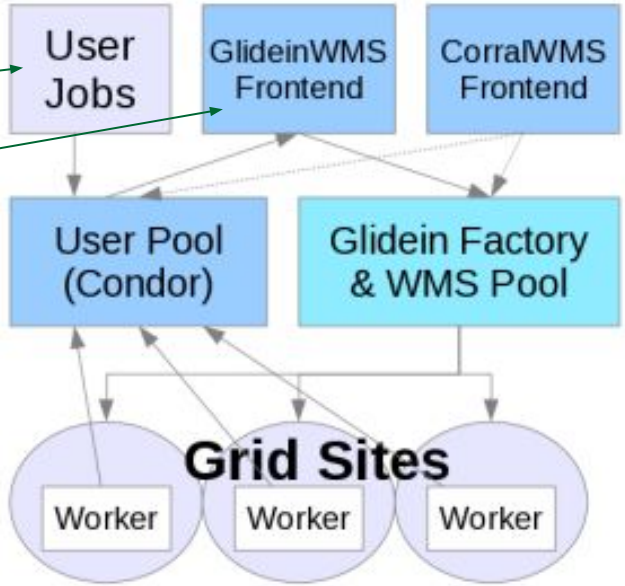
# Gluex @ – the reboot

## New infrastructure for osg @ jlab:

1. scosg16: GWMS submit host for JLab users
2. GWMS Frontend service provided by OSG ops





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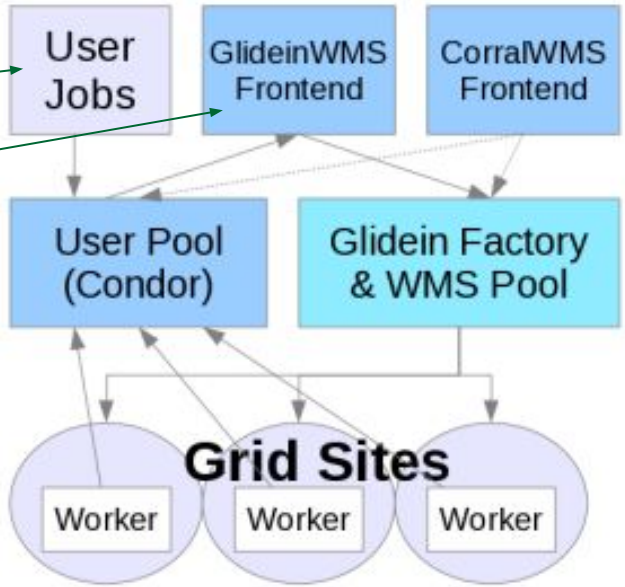
# Gluex @ – the reboot

## New infrastructure for osg @ jlab:

1. scosg16: GWMS submit host for JLab users
2. GWMS Frontend service provided by OSG ops
3. Opportunistic cycles on OSG continue to grow
4. Two new member universities in Gluex moving this summer to stand up local resources on osg
5. Software distribution is now greatly simplified by the use of the new ***Gluex singularity container***:
   - **singularity.opensciencegrid.org**
   - **oasis.opensciencegrid.org**





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# GlueX @ - opportunity cost

- osg represents a new way of working for JLab users
- lab IT management conscious of *user support issues*
- JLab collaborations are small, developing new expertise can be expensive


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# GlueX @ - opportunity cost

- osg represents a new way of working for JLab users
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***BUT***

- grid production is a good match to GlueX needs for simulations
- recent work by ***OSG + JLab*** staff has been ***a real boost***
- new effort is underway to enable us to exploit OSG for Gluex


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# Backup slides


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# Support for Gluex users

Open Science Grid

- Support for resource consumers (15 users registered)
  - howto get a grid certificate
  - howto access data from DC
  - howto test your code on osg
  - howto run your skims on osg

Quickstart users guide for Gluex
https://halldweb.jlab.org/wiki/index.php/Using_the_Grid

Gluex OSG HOWTO series (R.Jones)
https://halldweb.jlab.org/wiki/index.php/HOWTO_get_your_jobs_to_run_on_the_Grid

- Support for resource providers (UConn, NWU, FIU, FSU, CMU, IU, MIT?)
  - NOT a commitment to 100% allocation to OSG jobs
  - OSG site framework assumes that the local admin retains full control over resource utilization (eg. supports priority of local users)
  - UConn Gluex site running for 8 years
  - Northwestern Gluex site running for 3 years


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# GlueX Data Challenge #1

- total of 5,561,650000 events *successfully* generated
  - 4G events produced on the OSG (~2M core-hours)
  - 0.9G events at Jefferson Lab
  - 0.3G events at CMU
- completed over a period of 14 days in Dec., 2012
- output data saved in REST format
  - Reconstructed Event Summary Type (no hits information)
  - approx. 2.2 kB/event, including MC generator event info
  - hadronic interaction in every event (pythia 8.4 – 9.0 GeV)
  - no em beam background or hadronic pile-up included
  - 111236 files stored, 50k events each
  - typical run time 8 hours / job on Intel i7


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# Problems encountered in OSG production

1. GlueX software environment staging
   - 20 packages to install (counting all of sim-recon as 1)
   - production spread over 8 sites (fnal.gov, cornell.edu, purdue.edu, ucllnl.org, ucsd.edu, unesp.br, org.br, uconn.edu)
2. freeze-ups in hd-ana
   - occurred any time an event took >30s to process
   - dependent on other things happening at the site
   - tended to occur in clusters, many jobs at once
3. memory hogging in hd-ana (feeds into 2)
4. segfaults in hdgeant
   - artifact from one node at UConn – bad SDRAM chip
5. irreproducibility in mcsmear


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# Production inefficiency

- 10% jobs would hang in hd_ana, up to 24hr.
- 24hr is 300% inflation of normal job time
- Ejected jobs would get requeued for later execution.
- Some fraction of these would hang 2nd, 3rd time around…
- Ad-hoc scripts were written to prune jobs that were stuck looping.
- Other known factors (store output to SRM, thrashing on memory hogs…) not quantified.

FNAL firewall intrusion event

hung job script development

job queue drainout


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