# Diversity of Science on the OSG



### **Open Science Grid**

### Rob Gardner • University of Chicago Ken Herner • Fermilab

OSG All Hands Meeting, University of California San Diego, March 6-9, 2017



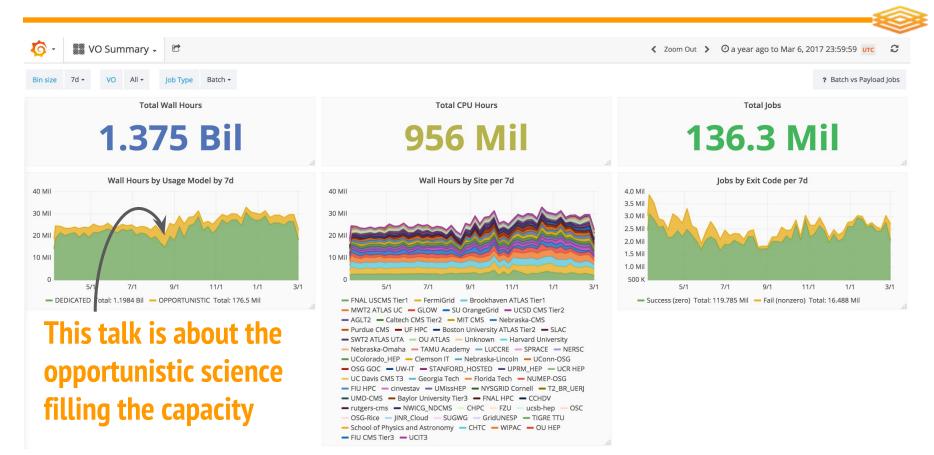
# **Overview**

# Review of opportunistic usage on OSG Highlights from electrical engineering, neuroscience, evolutionary biology, genomics, medical science & more! Summary of the Virtual Organizations

600 K

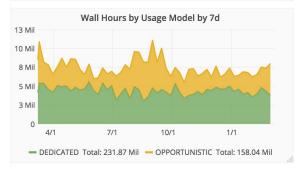
University of New Mexico — University of Pennsylvania — University of Minnesota — Texas A&M University, University of Illinois at Urbana-Champaign — Space Telescope Science Institute
 University of Washington — SUNY at Stony Brook — UT Southwestern — University of Wisconsin — University of Arizona — Brookhaven National Laboratory — University of New England — Fermilab
 University of Oklahoma — University of North Carolina at Chapel Hill — Colorado School of Mines — University of Illinois — Harvard Medical School — Georgia State University
 Washington State University — Worcester Polytechnic Institute — Southern Illinois University — Michigan State University — University of Minnesota, Duluth — Western Washington University
 University of Nebraska Lincoln — University of Nebraska - Lincoln — Rutgers, the State University of New Jersey — Las Alamos National Lab — College of Charleston — University of Wisconsin - Madison
 Hobart and William Smith Colleges — Pennsylvania State University — University of California San Diego — University of Wisconsin — University of College of Medicine
 Massachusetts Institute of Technology — Duquesne University — University of Wisconsin Madison — University of Texas — Austin — Northwestern University — Rutgers University
 Rochester Institute of Technology — University of California, San Francisco — Rutgers — Baylor College of Medicine — University of Notre Dame — International Center for Theoretical Physics
 Siena College — Fermi National Accelerator Lab — UC Riversite — Seargia Tech — SLAC — Swarthmore College — OSG — University of California Santa Cruz — University of California Santa Cruz — University of Central Florida
 New Vark — Ochababa Institute for Computational Sciences — Stanford University of Central Florida

# Total Production (VO Summary)



# VO Summary w/o ATLAS and CMS

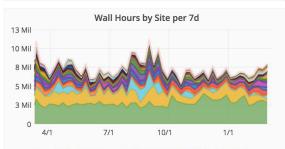
390 Mil



#### About 28% of batch hours in the past year were not ATLAS or CMS

**Total CPU Hours** 

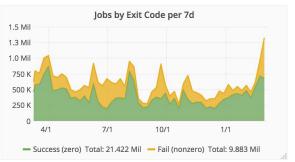
263 Mil



FermiGrid SU OrangeGrid FNAL USCMS Tier1 Unknown
 OU ATLAS Caltech CMS Tier2 MWT2 ATLAS UC
 Nebraska-CMS UCSD CMS Tier2 GLOW NERSC
 Nebraska-Omaha Brookhaven ATLAS Tier1 Clemson IT
 AGLT2 UCONNOSG OSG GOC Nebraska-Lincoln
 UW-IT Boston University ATLAS Tier2 STANFORD\_HOSTED
 MIT CMS Purdue CMS UC Davis CMS T3 NUMEP-OSG
 UCR HEP Florida Tech FIU HPC UColorado\_HEP
 UF HPC cinvestav SPRACE FNAL HPC Gregia Tech
 CCHDV SWT2 ATLAS UTA UPRM\_HEP NYSGRID Cornell
 UMissHEP NWICG\_NDCMS CHPC FZU OSC
 JINR\_Cloud SUGWG TAMU Academy GridUNESP
 TIGRE TTU CHTC WIPAC OU HEP T2\_BR\_UERJ
 FIU CMS Tier3

Total Jobs

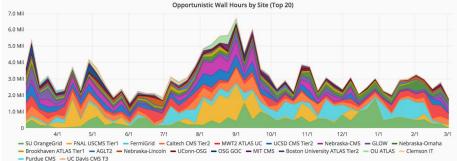
31.3 Mil

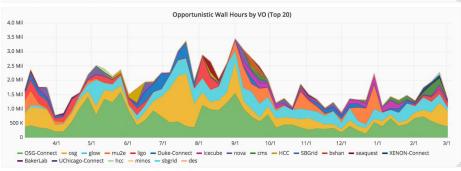




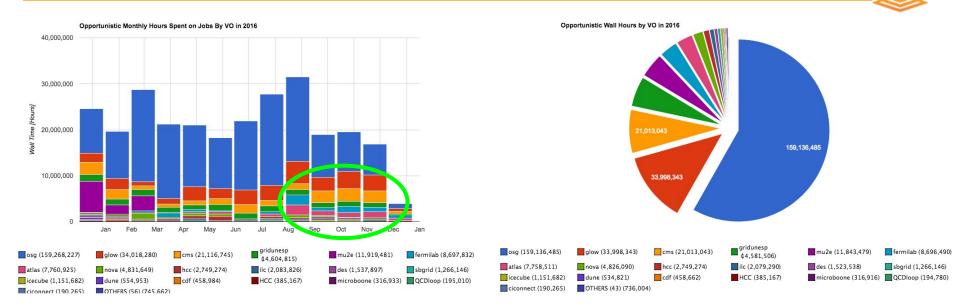
Top 20 Sites Providing Opportunistic Usage

OIM_Site	OIM_Facility	Wall Hours 🕶
SU OrangeGrid	Syracuse University	24 Mil
FNAL USCMS Tier1	Fermi National Accelerator Laboratory	19 Mil
FermiGrid	Fermi National Accelerator Laboratory	19 Mil
Caltech CMS Tier2	California Institute of Technology	17 Mil
MWT2 ATLAS UC	University of Chicago	15 Mil
UCSD CMS Tier2	University of California San Diego	13 Mil
Nebraska-CMS	University of Nebraska	13 Mil
GLOW	University of Wisconsin	10 Mil
Nebraska-Omaha	University of Nebraska	9 Mil
Brookhaven ATLAS Tier1	Brookhaven National Laboratory	5 Mil
AGLT2	University of Michigan	4 Mil
Nebraska-Lincoln	University of Nebraska	4 Mil
UConn-OSG	University of Connecticut	3 Mil
OSG GOC	Indiana University	3 Mil
MIT CMS	Massachusetts Institute of Technology	3 Mil
Boston University ATLAS Tier2	Boston University	2 Mil
OU ATLAS	University of Oklahoma	1 Mil
Clemson IT	Clemson University	1 Mil
Purdue CMS	Purdue University	1 Mil
UC Davis CMS T3	University of California Davis	1 Mil





# Opportunistic VO usage trends in 2016

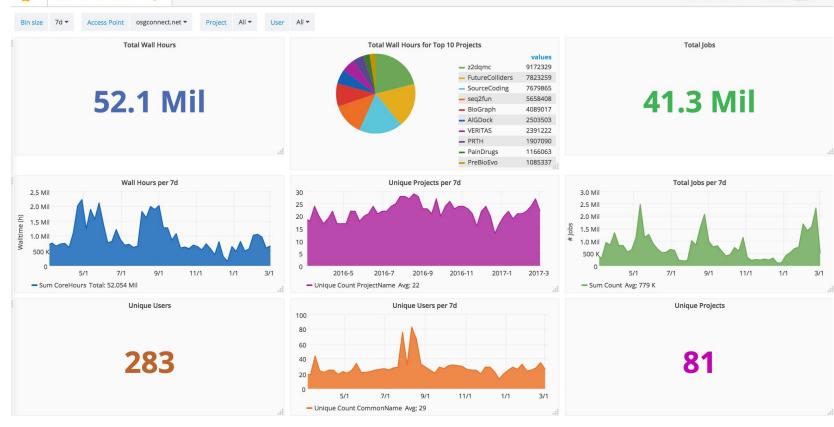


N.B. Mu2e folded into Fermilab in March Large ATLAS and CMS increases late in year: Expected to continue



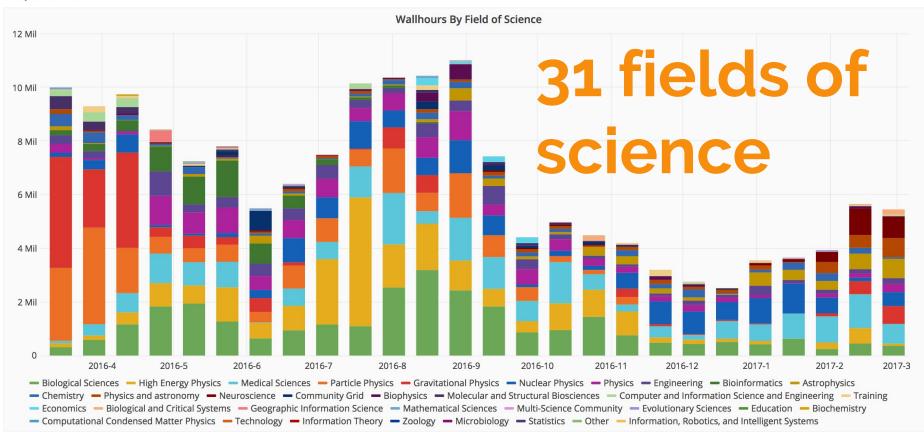
🌀 🚽 📓 OSG Connect Summary 🚽 🖻

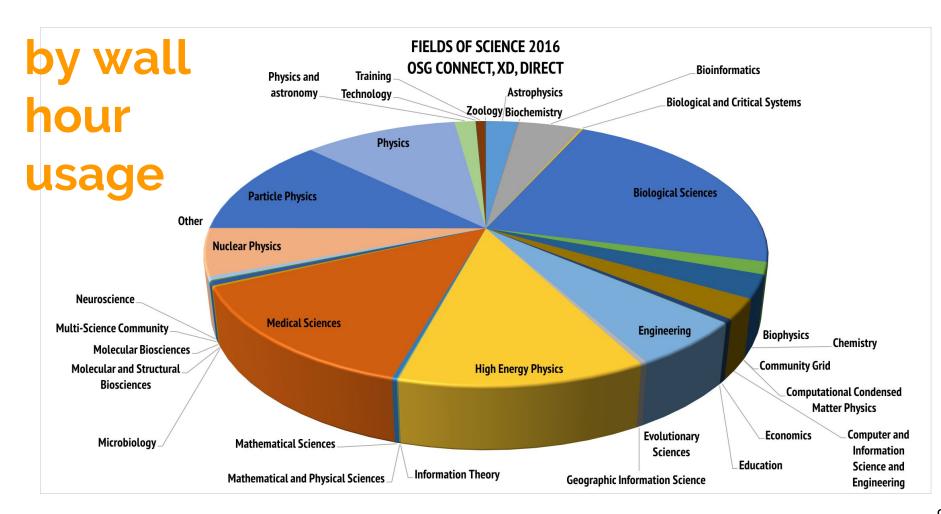
✓ Zoom Out > ② Last 1 year UTC 2



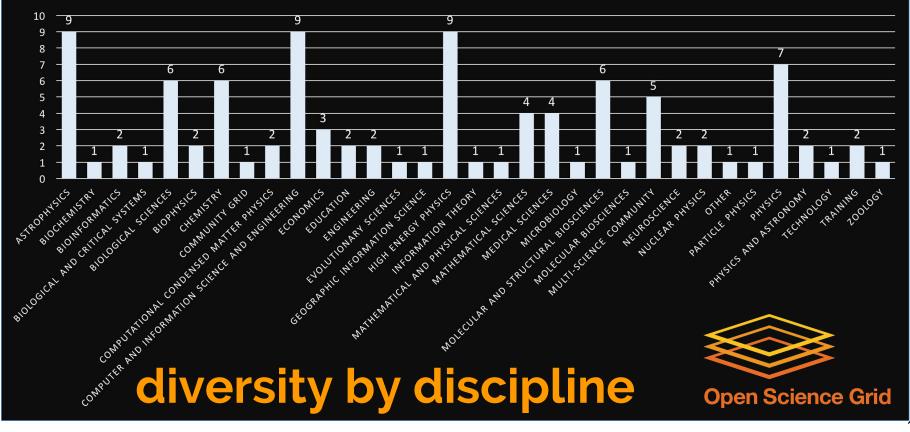
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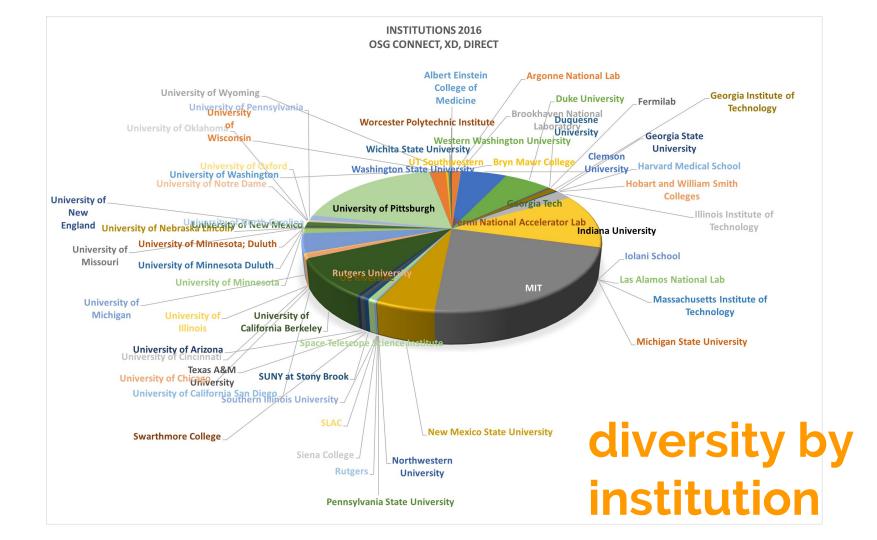
#### ✓ By Field Of Science

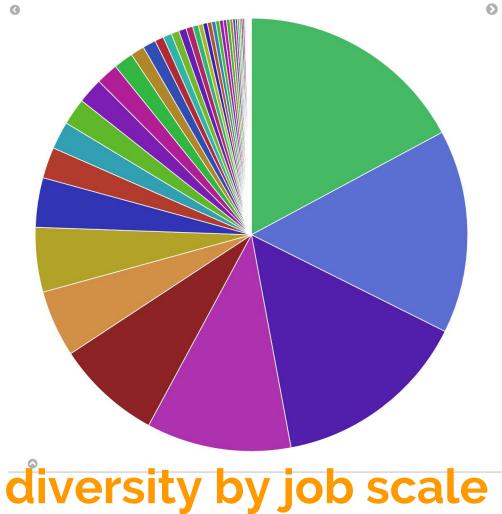


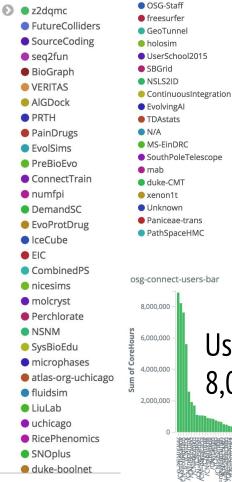


#### PROJECTS OSG CONNECT, XD, DIRECT 2016







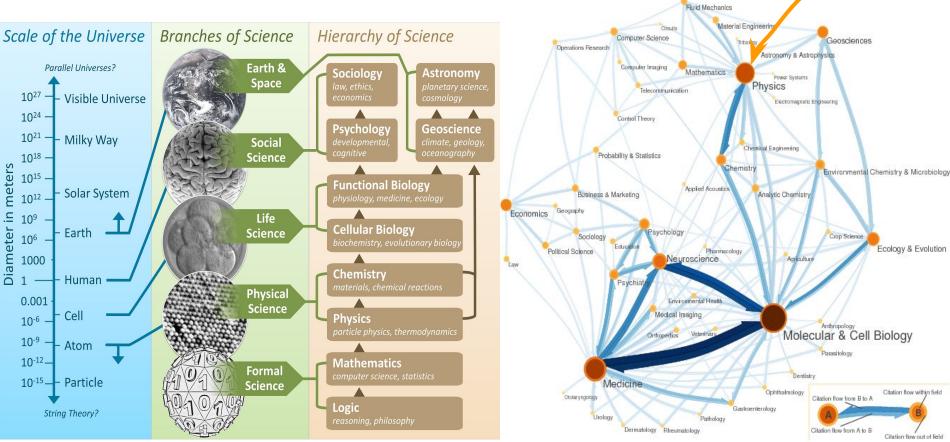


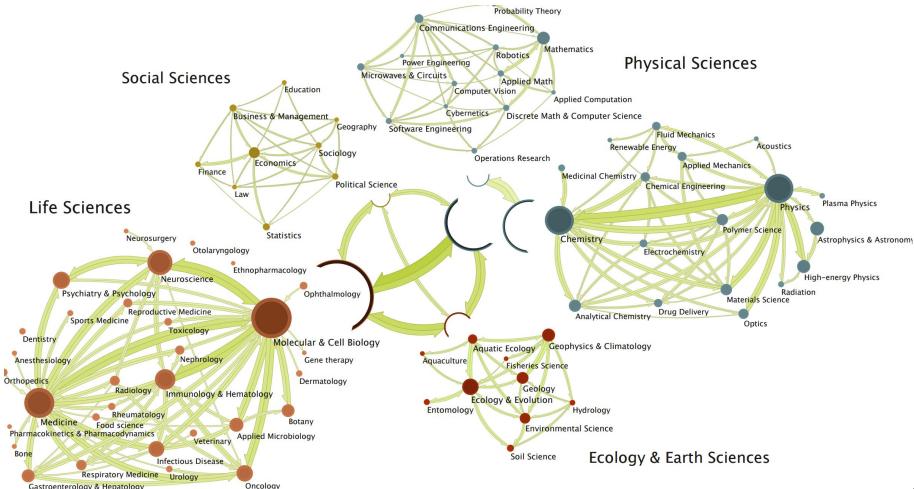
# Usage by person 8,000,000 to 1 hrs

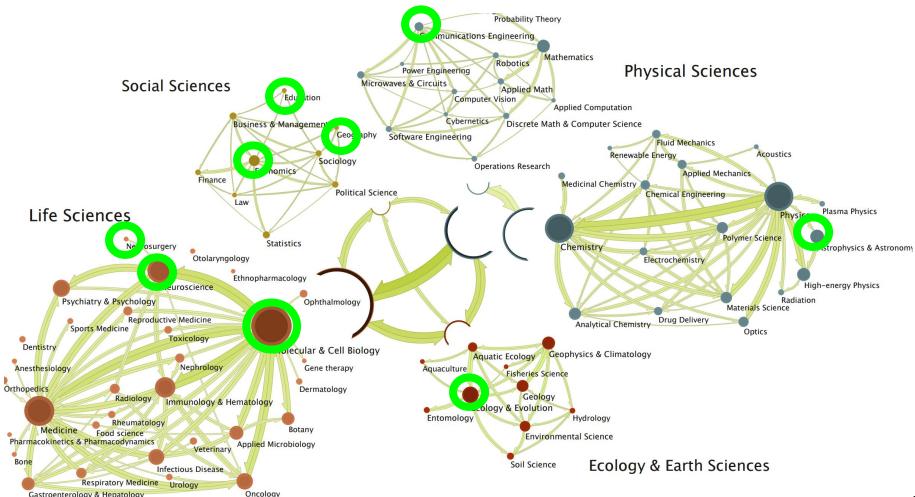
# Science sampler

With apologies for the many projects we've not included. Selection here was almost random, weighted heavily by materials supplied by speakers here.

# **Science of Science**





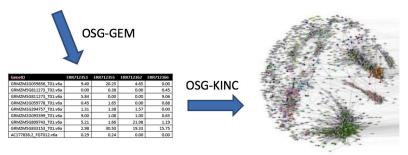


# Large Scale Genomics

#### Genomics

- FASTQ files are mapped to a reference genome and converted to a BAM alignment file.
- BAM files can be mined for gene expression vectors that can be bundled into a gene expression matrix (GEM).
- GEMs are a stable data structure that can be mined for differentially expressed genes (DEGs) or used to construct Gene Co-expression Networks (GCNs)

### Raw DNA Sequence $\rightarrow$ Gene Interaction Graph

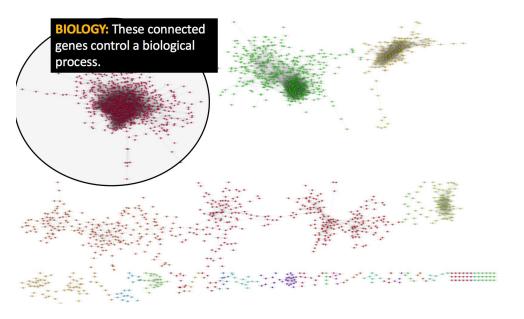


#### William Poehlman, Alex Feltus • Clemson University •• Stephen Ficklin, Washington State University 17

# Large Scale Genomics..

#### Genomics

#### COMPLEX GENETIC SYSTEMS WOVEN INTO GRAPHS



#### **Gene Expression Matrix HPC Challenges**

- Memory Intensive
  - Some Steps Require >16 GB RAM/dataset
- Storage Intensive
  - ~37 GB of intermediate files/dataset
- Dataset Size Varies Widely
  - 10M to 20M sequences/dataset
- Data Transfer Issues (Tera-/Petabytes)

#### William Poehlman, Alex Feltus • Clemson University •• Stephen Ficklin, Washington State University 18

### Student Training w/ OSG

- Introduction to Systems Biology
- WSU HORT 503 Special Topics (3 credits)
- Offered Fall 2017
- 9 Students
  - Crop & Soil Sciences
  - Molecular Plant Sciences
  - Entomology
  - Biological Systems Engineering
- Why OSG?
  - Expose students to national computing resources
  - Anticipate large-scale genomics of the future.



NEW INSIGHTS NEW BIOLOGY **HYPOTHESES** NEW BIOLOGICAL OUESTIONS NEW SOFTWARE COMPUTATION TECHNOLOGY **NEW TECHNOLOGIES** NEW C Institute for DATA Systems Biology





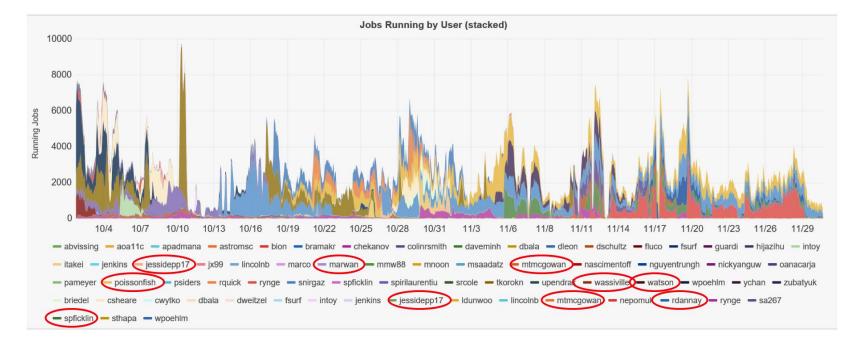
### Student Training w/ OSG

Genomics

20

Success: SysBioEdu Usage from Oct-Dec 2016

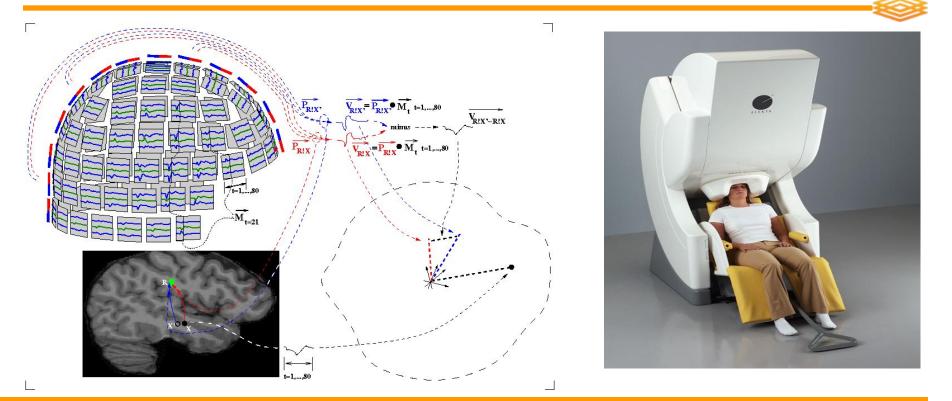
- Students launched jobs and they ran!



#### William Poehlman, Alex Feltus • Clemson University •• Stephen Ficklin, Washington State University

# **Functional Neuroimaging**

#### **Medical Science**



**Don Krieger** • **University of Pittsburgh** 

# Functional Neuroimaging..

- Don Krieger has been working with TEAM TBI at the University of Pittsburgh
  - Targeted Evaluation, Action and Monitoring of Tramatic Brain Injury
- TEAM TBI investigates the complexity of brain injury, and how targeted interventional strategies may improve outcome and function.



#### Don Krieger • University of Pittsburgh

#### **Medical Science**

David Okonkwo, Jim Becker, Sue Beers, Mickey Collins, Anthony Kontos, Malcolm McNeil, Walt Schneider





The Department of Neurological Surgery at the University of Pittsbury

David Okonkwo, Jim Becker, Sue Beers, Mickey Collins, Anthony Kontos, Malcolm McNeil, Walt Schneider

Supported by: Department of Defense, Open Science Grid (NSF,DOE), Extreme Computing Environment for Science and Engineering (NSF).





The Department of Neurological Surger at the University of Pittsbur

We record the magnetoencephalogram (MEG) from an array of 306 magnetometers sampled at 1 KHz typically for 30 minutes.





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The solver requires about 40 core hours per second of data. It typically yields about 500 simultaneously active sources for each 40 msec step through the data stream, i.e. 20,000,000+ sources from a single 30 minute recording session.

nt of Neurological Surgery at the University of Pittsburg





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We utilize a unique deconvolution solver to identify and validate ( $p<10^{-12}$ ) each neuroelectric source within the brain with mm resolution.



# The quantity and resolution of these measurements is unprecedented.



The Department of Neurological Surger at the University of Pittsbur

In December, we gained access to the CamCAN lifespan normative cohort in collaboration with the University of Cambridge (UK). These recordings were obtained from 628 volunteers ages 18-87.





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The Department of Neurological Surgery at the University of Pittsbury

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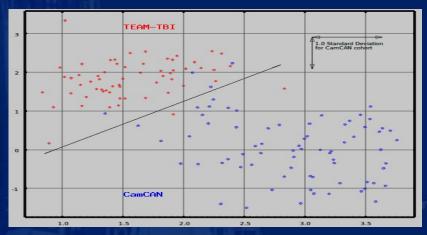
The brain patterns found in MEG recordings from volunteers with history of head injury are sufficiently different to classify them with 95% accuracy.



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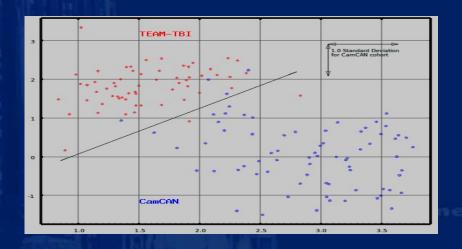


ent of Neurological Surgery at the University of Pittsburg



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One of these two brain patterns used to classify the cohorts is specific to depression, the other to somatization. These are common symptoms of PTSD.



# Large Scale Metagenomics.

#### Computational Biology



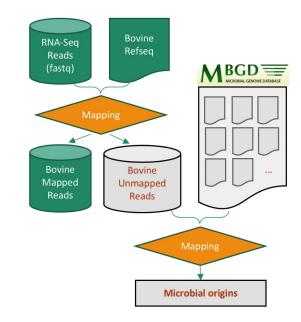
#### **Motivation**

- In a pervious project, we have isolated exosomes from the commercial cow's milk and assessed the bovine molecules inside the exosomes.
- Moreover, we also found many unmapped reads are from microbial species.
- Thus, we designed a follow-up study to understand the origin of microbial sequences in bovine milk exosomes.
  - Metagenomics analysis





Pseudomonas cedrina



#### Jiang Shu • University of Nebraska Lincoln

# Large Scale Metagenomics..

#### Computational Biology

#### Computational challenges

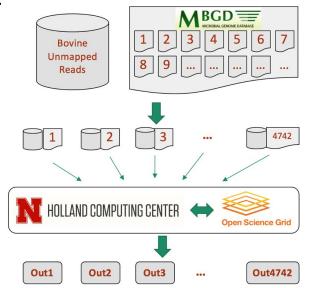
- A large number of target genomes
  - 4,742 genomes (size: 100KB ~ 58MB)
- Six samples contain over 100 million of bovine unmapped reads
  - Increasing the computing time
- In total, 6 x 4,742 = 28,452 mapping tasks

#### Question: Where to execute this many of jobs?

- Impossible for the lab-server (32 cores)
- Long pending time if submitted it to HCC clusters
  - Dynamic priority scheduling of users/groups
  - More jobs completed -> longer queue time

### Perfect Fit of Open Science Grid (OSG)

- The tasks are independent to each other
- Limited file transfer
  - Total size of transferred files ~1GB
- Small memory consumptions
  - Memory < 2GB</li>
- Short running time for each task
  - Maximum: 3 hours (HCC@UNL-Crane)
- Software is available on OSG
  - Pre-installed Bowtie and Tophat
  - No further configuration needed



#### Jiang Shu • University of Nebraska Lincoln

### Large Scale Metagenomics...

### Results

- Several microbial species were identified in bovine milk exosomes:
  - Pseudomonas fluorescens, Pseudomonas chlororaphis, Pseudomonas poae, Enterobacter cloacae, etc.
- Although some species have been reported in cow's milk before, this is the first time of identifying microbial sequences in milk exosomes
  - Potential transportability to other species through exosomes
- Based on the findings from this analysis, we have designed two experiments to further our understanding in this subject

Computational

Bioloav

### Counterfactual Analysis.

#### **Economics**

- Economic analysis
  & public policy
- Considering "what if" scenarios in microeconomics
- Simulate firm/consumer behaviors

Using OSG to Evaluate Policy

We need to solve

$$\frac{\partial \Pi_{jt}}{\partial \boldsymbol{p}_{jt}} + \beta \left[ \frac{\partial \boldsymbol{s}_t}{\partial \boldsymbol{p}_{jt}} \right]' \mathbb{E}_t \left[ \frac{\partial V_j(\boldsymbol{s}_t, \boldsymbol{X}_t)}{\partial \boldsymbol{s}_t} \right] = 0,$$

for every firm and combination of  $s_t$  and  $X_t$ .

Need to compute  $\mathbb{E}_t \left[ \frac{\partial V_j(s_t, X_t)}{\partial s_t} \right]$ . How? Forward simulation.

OSG is what makes this possible for large state spaces.

### Counterfactual Analysis..

#### **Economics**



#### Using OSG to Evaluate Policy

Outcome: making people more active decreases prices and it does not affect returns.

Case	Mean and 95% CI
Base simulation	6.195% [6.181%,6.210%]
No enrollment cost	3.666% [3.660%,3.671%]
No decision cost	3.837% [3.833%,3.842%]
No switching costs	2.607%

Note: The table reports the mean expected fees and 95% confidence intervals for the different scenarios under study using 10,000 random initial states.

- 1. Policy/transaction evaluation is critical in modern microeconomics.
- 2. Evaluations often require simulating consumer/firm behavior over a large state space.

Conclusions

3. In particular in the case of dynamic games, OSG could become a crucial tool, making the difference between being able to do something and not.

# Simulating Source Coding.

#### Engineering

- Data deluge much of it mobile traffic
- Optical data compression
- Important for digital space and satellite communication & wireless data transmission

Monte Carlo Simulation for Next Generation Source and Channel Coding on OSG Connect

Ahmad Golmohammadi\*, David G. M. Mitchell\*, Joerg Kliewer<sup>†</sup>, and Daniel J. Costello, Jr. <sup>‡</sup>

\* Klipsch School of ECE, New Mexico State University

<sup>†</sup> Dept. of Electrical and Computer Engineering, New Jersey Institute of Technology

<sup>‡</sup> Dept. of Electrical Engineering, University of Notre Dame







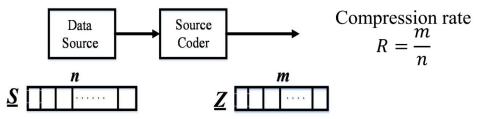
March 7, 2017

# Simulating Source Coding..

- Whole system simulations: transmitter, decoder, receiver & stochastic noise
- Data compression & reconstruction algorithms

### Data Compression

□ In order to handle the vast amounts of data society will produce, we need efficient and low-complexity algorithms to reliably compress and reconstruct data.



□ We want to reconstruct the sequence with as little distortion as possible with a practical scheme (lossy source coding)

□ The ultimate limit of compression is known (Shannon 1958)

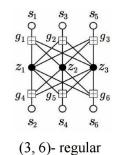
# Simulating Source Coding...

#### Engineering

- Sparse graphs can approach fundamental limits
- To verify the results, large Monte Carlo samples needed - "not possible without the OSG"

### LDGM Codes for Lossy Source Coding

- □ We construct codes for lossy source coding using a small structured graph (protograph)
- $\Box$  A large graph can be obtained from a protograph by graph lifting with lifting factor *M* 
  - > The graph is copied *M* times and the edges randomly permuted following the graph structure
- □ Low complexity algorithms based on belief propagation can be defined for the sparse graph
  - > Here, messages are passed iteratively forward and backward in the graph until we converge to a codeword  $\underline{z}$



#### Ahmad Golmohammadi • New Mexico State University • Project:SourceCoding

# Evolving Strategies for Life.

### **Evolutionary Biology**



- Understanding evolution at molecular scale in DNA with combination of mathematical modeling and simulation
- How quickly does a genome fix a mutation?
- Role of randomness versus natural selection?

Environmental variation is commonplace yet unpredictable across biological systems from the adaptive immune system, the microenvironment in cancerous neoplasms, to populations of pathogens under drug pressure.

How do populations survive environmental stochasticity? How do they manage to persist and keep one's footing on an ever-changing landscape?

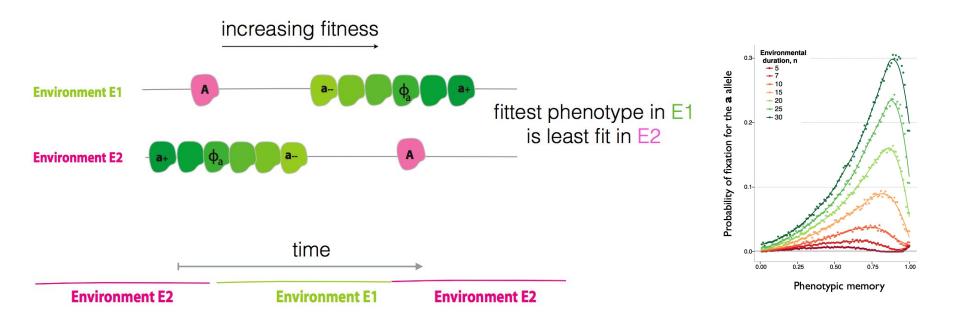
Can organisms prepare for this environmental stochasticity?

Can evolution prepare populations for this environmental stochasticity?

#### **Oana Carja** • University of Pennsylvania • Project:EvolSims

### Evolving Strategies for Life..

#### **Evolutionary Biology**



#### **Oana Carja** • University of Pennsylvania • Project:EvolSims

#### Ben Intoy • University of Minnesota • Project:PreBioEvo

aabaa

aaba

 $L_{max} = 8$ 

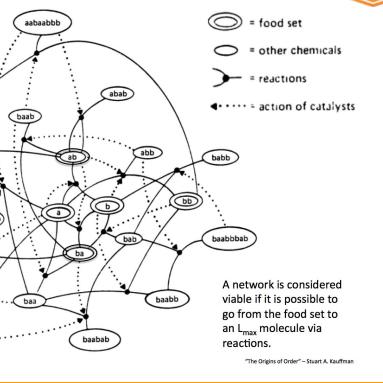
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# Models of Prebiotic Evolution

- Protein first origin of life model
- Network of interacting molecules assumed to be polymers
- Perhaps solve Eigen's paradox (low probability of randomly constructing "starter gene")



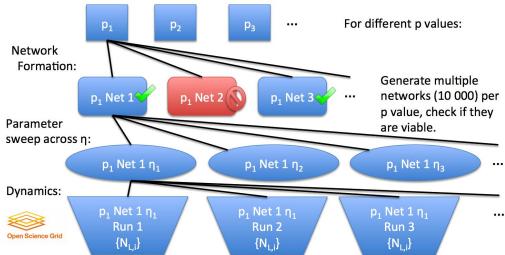
#### **Biophysics**

### Models of Prebiotic Evolution..

### **Biophysics**

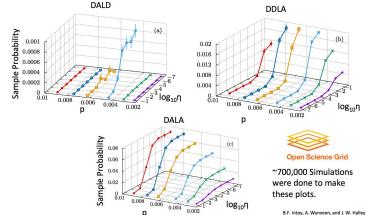


**Simulation General Structure** 



- Do multiple dynamic simulations with random initial conditions using a given viable network generated by parameter p combined with reaction rates and diffusive value η.
- A steady state is then reached with polymer length and spatial distribution {N<sub>Li</sub>}.
- Analyze the {N<sub>L,i</sub>}'s to determine whether the run was lifelike or not.

### Probabilities of DALD, DDLA, DALA states as a function of p and $\eta$



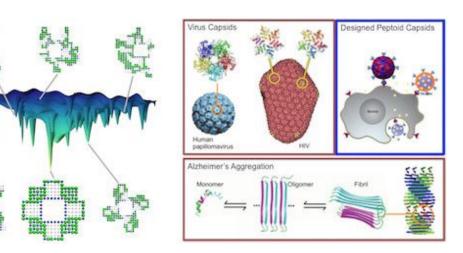
#### Ben Intoy • University of Minnesota • Project:PreBioEvo

Physical Review F 94 042424 (2016)

#### Milo Lin • UT Southwestern • Project:EvProtDrug

### **Protein Evolution**

Understand the fundamental physical bottlenecks and dynamical behavior of protein evolution. Important questions include the extent of dominant pathways (convergent evolution) and phase transitions in evolutionary rates (punctuated equilibrium). These principals and their structural underpinnings can also be used to inform rational design of antibiotics that exploit bottlenecks in pathogen mutational response.





Biophysics

### Analysis of Brain Rhythms

#### Neuroscience

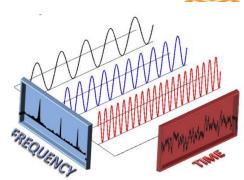
### Large-scale brain recordings

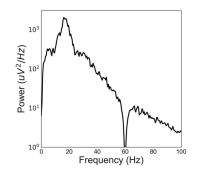
- Healthy humans
- Patients
- Animals

- Sampling: 500-30000 Hz
- Duration: 1 hour 1 week
- Channels: 1 250+
- Several GB per subject









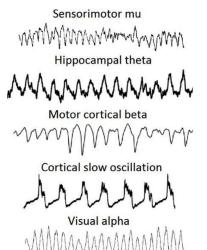
#### Scott Cole • UCSD • Project:NeurOscillation

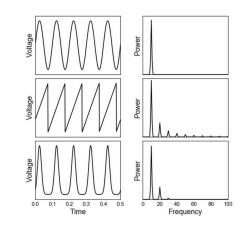
## Analysis of Brain Rhythms..

#### Neuroscience



#### Fourier Transform-based analysis





### Free supercomputing for research: A tutorial on using Python on the Open Science Grid

Jan 3, 2017

Supercomputing resources typically cost money, but the Open Science Grid (OSG) provides high-throughput computing to any researcher in the US **for free**. Briefly, OSG users can run jobs on servers owned by dozens of academic institutions, whenever those servers are not actively running a job for its owners.

Besides cost, a second major barrier to entry for those who are new to supercomputing (or, specifically, Condor) is the necessary troubleshooting before we can actually run our jobs. The purpose of this tutorial is to provide a complete example for running Python jobs on the OSG. This example is nontrivial, in that it includes multiple data sets, public libraries (e.g. scipy), private libraries, and analyzing output. In complement to this tutorial, the OSG has tutorials, a structured class, and extremely helpful online support when you get stuck.

This tutorial goes through the steps of manually connecting to and running commands on the remote server, but see the **Fabfile** section at the bottom for how this can be automated on your local machine.



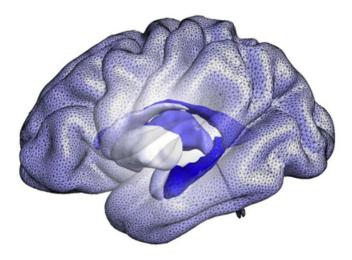




#### Scott Cole • UCSD • Project:NeurOscillation

### A FreeSurfer Workflow Service

- Widely used software suite for analysis of human brain MRI scans.
- Neurophysiology of depression, examining possible anatomical differences involved in ADHD, and studying autism



Computational model of the cortical and subcortical brain structures that form the basis of the BrainPrint, a system for representing the whole brain based on the shape, rather than the size of structures. (Martin Reuter, PhD, and Christian Wachinger, PhD, Martinos Center for Biomedical Imaging)

#### Suchandra Thapa • University of Chicago • Project:fsurf

Neuroscience

#### Working with Don Front-end user interface Command line script 0

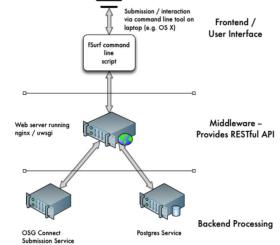
A FreeSurfer Workflow Service

- Krieger (Pittsburgh) to develop an OSG-based execution service
- Uses Pegasus
- Handles "standard" transforms and user options
- To be released this week!

- - Communicates to the execution service via RESTful-API commands
  - Allows user to submit, view, and remove workflows as well as download results
- Middleware 0
  - NGinx / uwsgi server provides RESTful API
- Backend services (running on a single VM)
  - Postgres database 0

Suchandra Thapa • University of Chicago • Project:fsurf

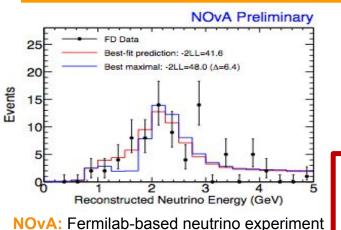
- Tracks workflow status, locations of inputs and results
- Stores user information
- Pegasus submission service (using same 0 infrastructure as OSG Connect) to



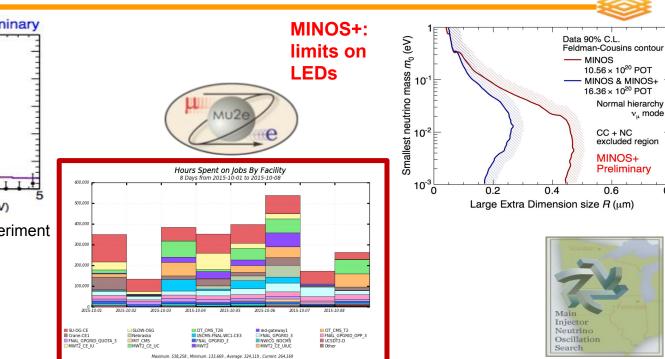




# VO Highlights: From the smallest scales...

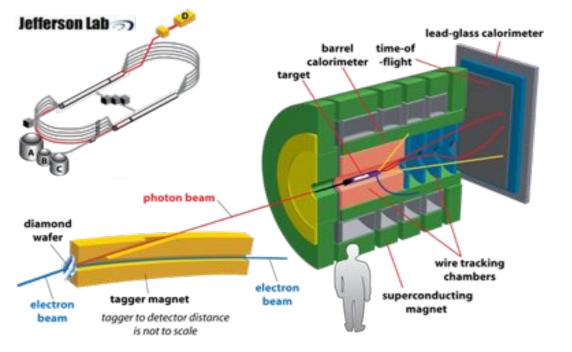






Mu2e: Lepton-flavor violation experiment Nearly 60M opportunistic hours on OSG and counting >500,000 in one day! 0.8

# VO Highlights: From the smallest scales...

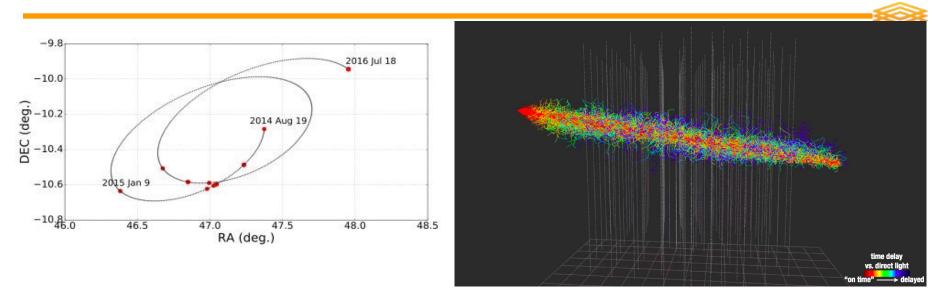


#### Au+Au event

**STAR:** Heavy Ion Physics

GlueX: probing exotic mesons predicted by LQCD

### ...to the largest...



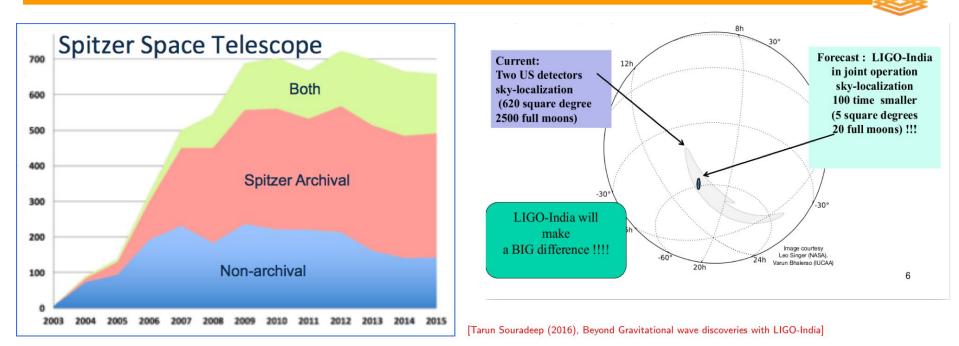
#### **Dark Energy Survey:**

Discovery of dwarf planet-Second-most distant known object in solar system Techniques applied to ongoing Planet 9 search

#### Ice Cube:

Neutrino Observatory, also sensitive to extremely high energy cosmic rays

### ...the completed to the still in planning...



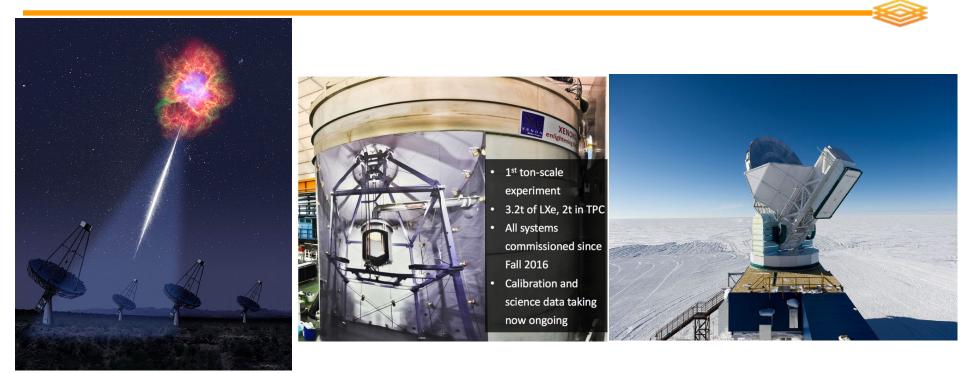
#### **Infrared Processing and Analysis Center:**

NASA's archive for a host of IR/sub-mm astronomy missions, galaxy catalogs, Keck Observatory, and more!

#### LIGO India:

Additional detector will greatly Improve localization of gravitational wave sources

# ...and working in all corners of the globe.



VERITAS: 4 12m Cerenkov telescopes for gamma ray astromony: Arizona, USA

#### XENON1T:

Dark matter detector at Gran Sasso National Laboratory, Italy

#### **South Pole Telescope:**

Microwave-millimeter telescope

### And in space!



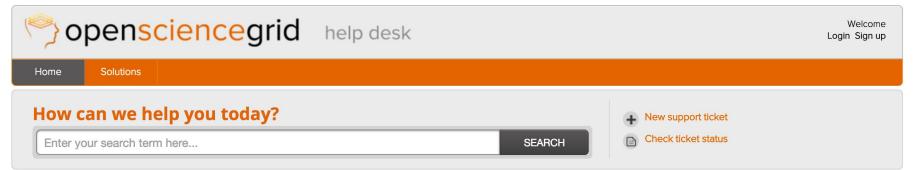
Alpha Magnetic Spectrometer (AMS) mounted at the ISS Photo credit: NASA

### **OSG User Support**





http://support.opensciencegrid.org/



### User Support

Training



Intro to HTC on OSG Connect in Synthesis Center tomorrow

# software carpentry









user-support@opensciencegrid.org

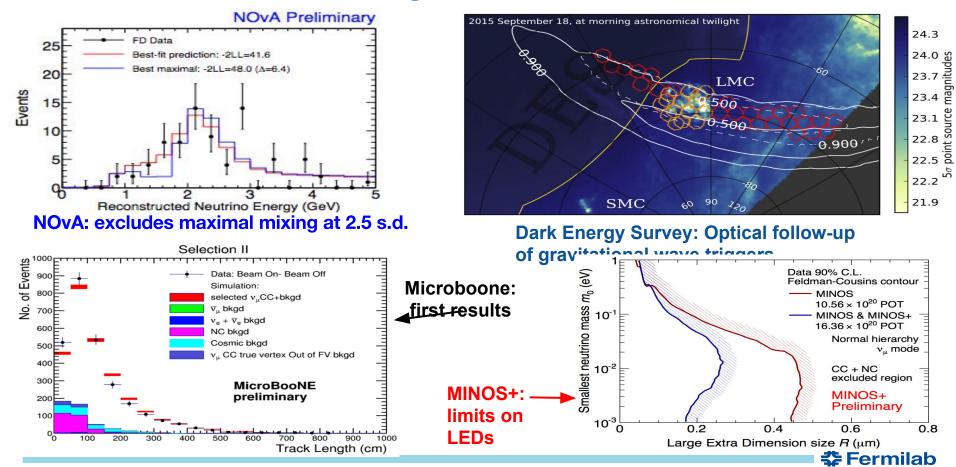


Support.opensciencegrid.org



# Extra slides

### **Selected results using the FIFE Tools**



Ken Herner | FIFE: Computing for Experiments

8/4/16

0.8