



Open Science Grid

# OSG Virtual Organizations Status and Outlook

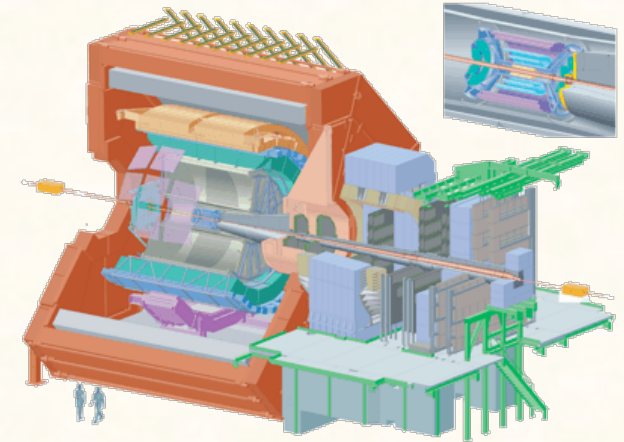
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1. ALICE – Jeff Porter
2. ATLAS – Rob Gardner
3. Belle II – Leo Piilonen
4. CDF – Rick Snider
5. CMS – Frank Würthwein
6. DZero – Joel Snow
7. Engage – John McGee
8. Fermilab – Steven Timm
9. HCC – David Swanson
10. SBGrid – Piotr Sliz



# ALICE & ALICE-USA

- **ALICE Experiment**
  - Dedicated heavy-ion experiment at the LHC
    - Study physics of strongly interacting matter at extremely high energy densities
  - 1000 physicists, 33 countries
- **ALICE-USA Collaboration**
  - Formed to manage construction & operation of ALICE EMCal
  - ~50 physicists at 11 participating US institutions
- **ALICE-USA Computing Project**
  - Build a facility to meet ALICE-USA computing obligations to provide share of computing resources for ALICE data analysis and simulations, enabling US ALICE Scientist to pursue research goals
  - Proposal developed in 2008/2009 & project approved in 2010:
    - Locate facility at two sites: LLNL/LC and LBNL/NERSC/PDSF
    - LBNL as host lab, Ron Soltz & Jeff Cunningham (LLNL), Jeff Porter & Keith Beattie (LBNL)

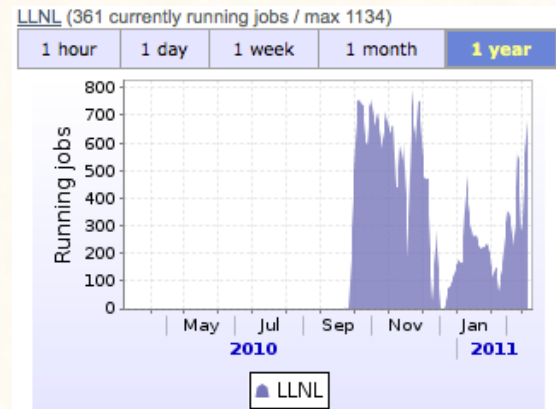




# ALICE-USA Facilities: LLNL/LC & NERSC/PDSF

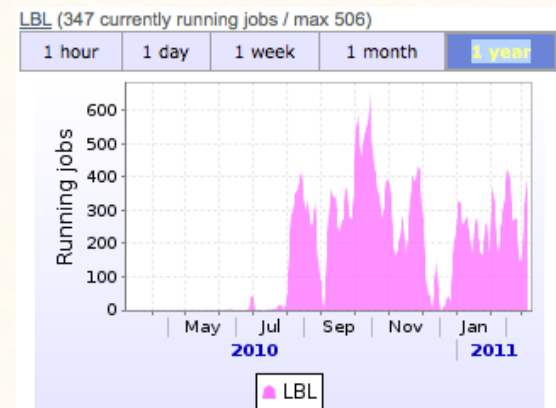
- **LLNL/LC Computing: Institutional-HPC supporting LLNL Science & Engineering projects**

- Cost effective procurement & operations model
  - large scalable unit purchases
  - In-house standard software → OS (CHAOS) & batch (SLURM)
- Pursuing external collaborations (e.g. Green Data Oasis)
- ALICE Resources
  - 800 cores, 650TB Disk space
  - Fixed resources for 3 year life cycle



- **NERSC: DOE Office of Science Flagship facility for High Performance Scientific Computing**

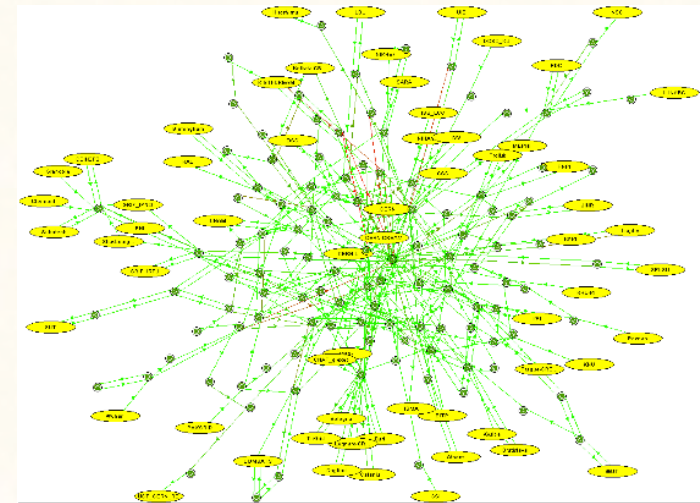
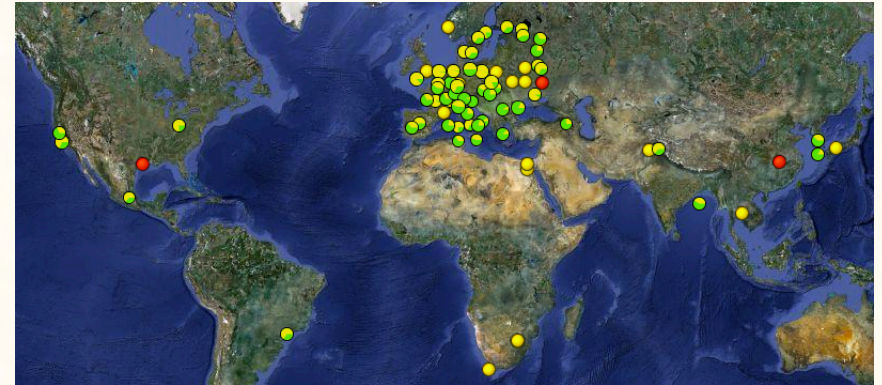
- Supports DOE sponsored research by competitive allocations
  - Two Cray Systems: Hopper & Franklin: ~200k cores
  - Special Clusters: Visualization, Analytics, HENP (PDSF)
  - Evaluation Systems: GPU and Cloud Clusters
  - PB-scale Global File System (GPFS), Tape Storage (HPSS ~40 PB)
  - Data Transfer, Science Gateways & Grid Services
- PDSF: HENP funded cluster operated by NERSC
  - STAR Tier 1, ALICE Tier 2
  - ATLAS, IceCube, Daya Bay,
- ALICE Resources
  - 320 cores, 400TB disk space , PB-scale tape storage allocation in NERSC/HPSS
  - Annual growth plan of 400 cores, 500TB disk





# ALICE Grid Computing Model

- ALICE Grid framework in production for since 2004
- AliEn, “Alice Environment”
  - VO Box at each site manages
    - Job submissions (CEs or LRMA directly)
    - Proxy renewal
    - Software deployment (AliRoot, Geant, ...)
    - Monitoring
  - Central Task Queue at CERN
  - JobAgents (pilot jobs) submitted to WNs
    - Evaluates local resources
    - pull jobs from the task queue (for 1 user)
- Data Management
  - AliEn FileCatalog
  - Xrootd-based SEs with global redirector
- Grid monitoring with MonALISA
  - Job/site status: ~30k concurrent jobs
  - SE capacities & availability: ~10PB
  - Dynamic network topology mapping



network topology map

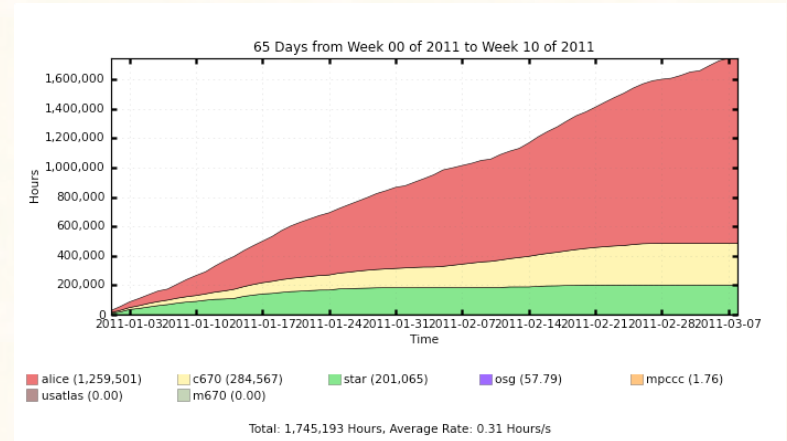




# ALICE-USA & OSG: 2011-2012

- ALICE-USA Project Plan: leverage OSG capabilities

- OSG RA participation
- Resource Accounting Reports to WLCG
  - Very good response from OSG support
    - Thanks to John W., Brian B., Chander, ...
  - WLCG-registration waiting final MOU signatures
- Disposition of unused resources
  - PDSF is already an OSG resource
  - LLNL currently hidden OSG resource, full support for limited VO set is planned this year



- Opportunistic use of OSG resources

- ALICE requirements
  - 2-4GB/core, 10GB local scratch, WN outgoing network connectivity
  - RHEL5/SLC5 or newer
- Need to relax current on-site VO-box requirement
  - Will deploy a test ALICE VO-box at LBNL to submit to remote OSG resources
  - Software distribution into \$OSG\_APPS via modified AliEn tools

# ATLAS Computing on OSG

Rob Gardner  
VO Session, OSG All Hands Meeting  
Boston March 9, 2011



- 37 countries, 174 institutions, >3000 physicists, >1000 grad students
- US: 39 universities, 4 DOE labs, 21 states involved, > 700 physicists, >200 students



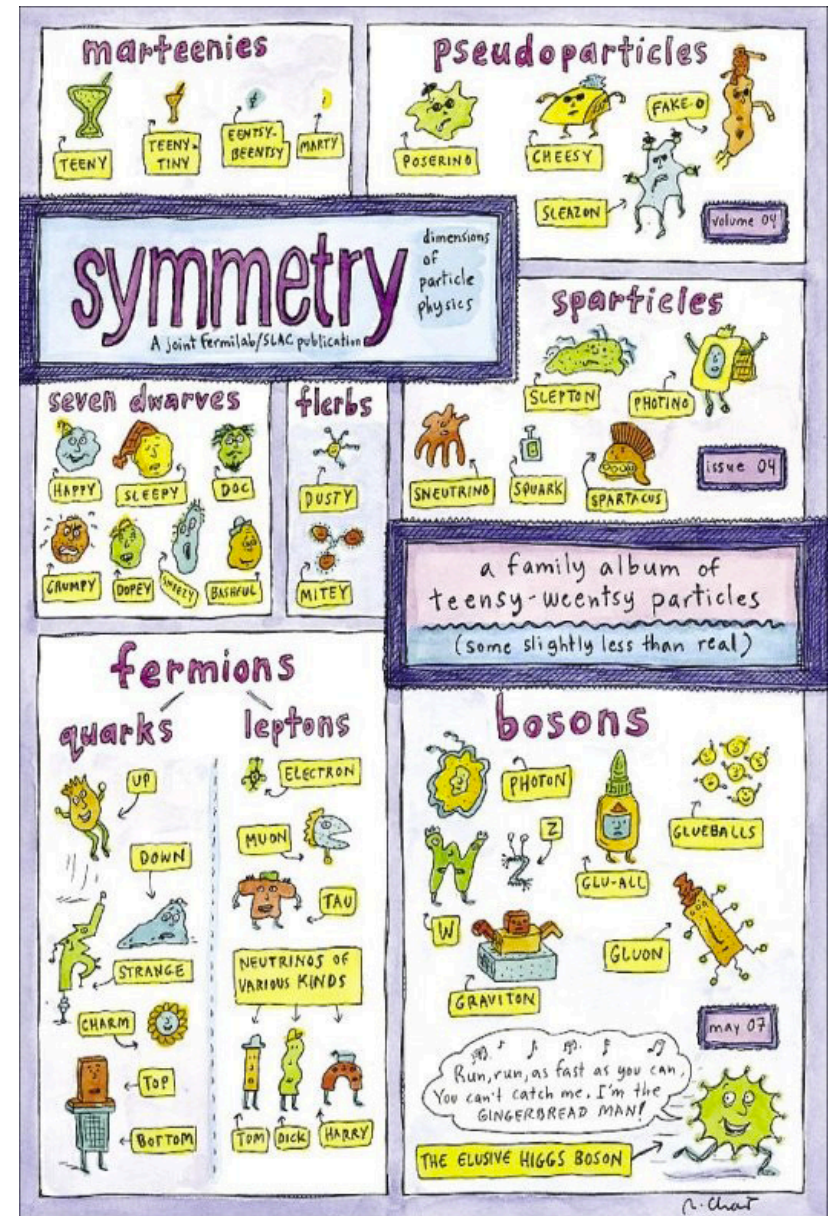
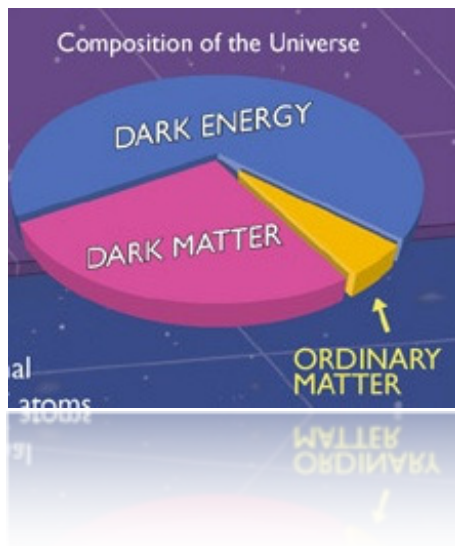
# Forefront Particle Physics

Origin of Mass (Higgs)

Supersymmetry

What is dark matter?

Do extra dimensions exist?





# Methodology

- Two modes: central production (simulation, reprocessing, pileup) and user analysis
- Both use the (pilot-based) Panda system which submits to “queues” at sites
- On OSG: Tier 1 at BNL, 5 (federated) Tier 2 centers (9 sites) - (17k slots, 15 PB disk)
- 2010 model: pre-placement of input datasets for analysis

# Outlook 2011-2012

- Expect constant production and analysis for the 2011-12 LHC run
- Tier 2 centers - have been operating within the US “cloud” - now going multi-Cloud
- Data pre-placement to (global) caching model
- ★ BIG change! 27 PB in old model reduced to 9 PB new model)
- ~26 Tier 3 sites will be ramping up
- Collaborating with OSG, CMS towards Xrootd federated data layer across all ATLAS storage facilities

# Belle II



<http://belle2.kek.jp>

Leo Piilonen, Virginia Tech

`piilonen@vt.edu`

*on behalf of the  
Belle II Computing Group*



OSG All Hands Meeting March 2011, Boston

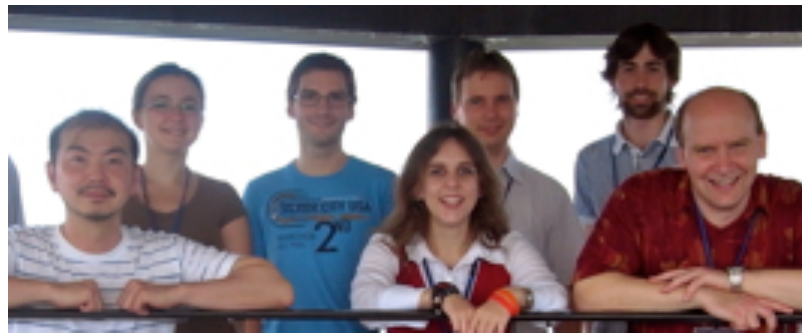
# The Team

- ✓ Computing team led by Thomas Kuhr and Takanori Hara [原隆宣]

*Kuhr*   *Fifield*



*Kuhr*



*Hara*

*Seviour*



*Hara*

- ✓ Distributed Computing and Data Management based in Australia (Tom Fifield, Martin Seviour) and Korea (Kihyeon Cho, JungHyun Kim, Soonwook Hwang, Sunhil Ahn, Taesang Huh)
- ✓ ... with support from China (Yan Liang Han [韩艳良]), Japan (Go Iwai [岩井剛]), Poland (Rafał Grzymkowski, Miłosz Zydbał), Slovenia (Marko Bračko) and all the people on the next slide
- ✓ Thanks to Ruth Pordes (OSG VO creation), Brian Bockelman and Burt Holzman (EGI interoperability, getting things running), and Douglas Olsen (OSG security).
- ✓ Thanks to the DIRAC team, without whom this would not be possible.



**... more of  
the team ...**

**APROC:**

Chen Yi Chien  
ShuTing Liao  
Eric Yen  
Jhen-Wei Huang  
Horng-Liang Shih  
Weijen Chang  
Felix Lee  
Syue-Yi Liaw  
Tz Ke Wu  
Albert Uang

**IJS:**

Marko Bracko  
Andrej Filipcic  
Borut Kersevan  
Dejan Lesjak  
Jan Jona Javorsek  
Jernej Porenta

**CESNET:**

Jan Kundrat  
Jan Svec  
Jiri Chudoba  
Milos Mulac  
Miroslav Ruda  
Tomas Kouba

**CYFRONET:**

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Lukasz Flis  
Maciej Pawlik  
Marek Magrys  
Patryk Lason  
Wojciech Ziajka

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Manabu Matsui  
Takashi Sasaki  
Yoshiyuki Watase

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Andreas Motzke  
Artem Trunov  
Bruno Hoeft  
Christopher Jung  
Dimitri Nilsen  
Doris Ressmann  
Foued Jrad  
Holger Marten  
Ingrid Schaeffner  
Jos van Wezel  
Manfred Alef  
Marian Zvada  
Silke Halstenberg  
Ursula Epting  
Xavier Mol

**Melbourne:**

Tom Fifield  
Tim Dyce

**KISTI:**

Cristophe Bonnaud  
Beob Kyun Kim  
Jae-Hyuk Kwak  
Jonghu Lee  
Soonwook Hwang  
Sunil Ahn

**UNL:**

Brian Bockelman  
Carl Lundstedt  
Garhan Attebury

**VPI:**

Miles Gentry  
Roger Link

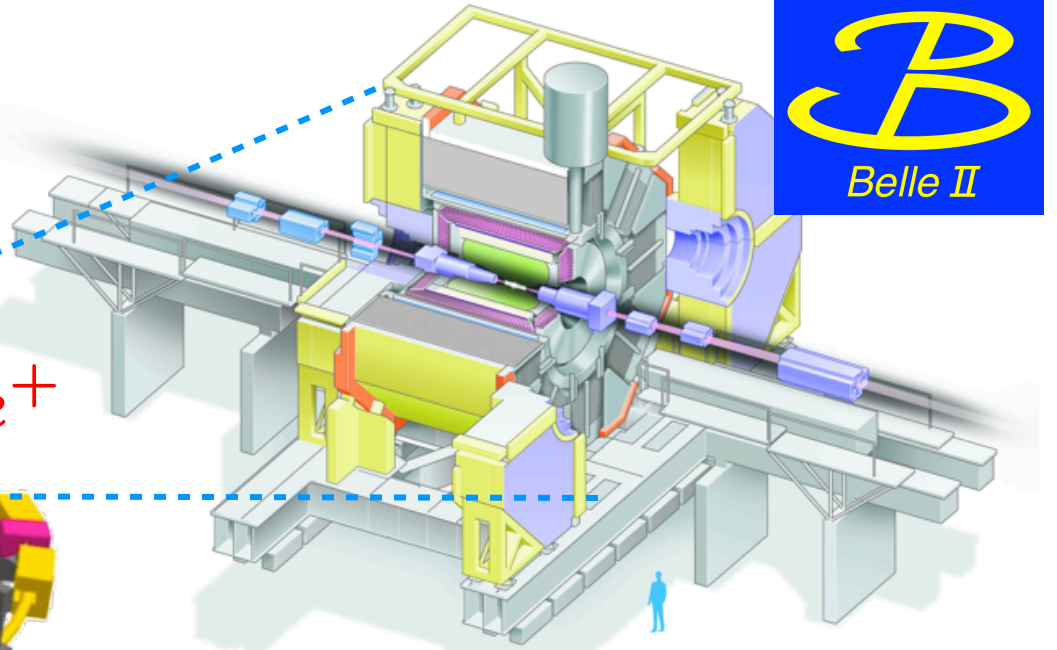
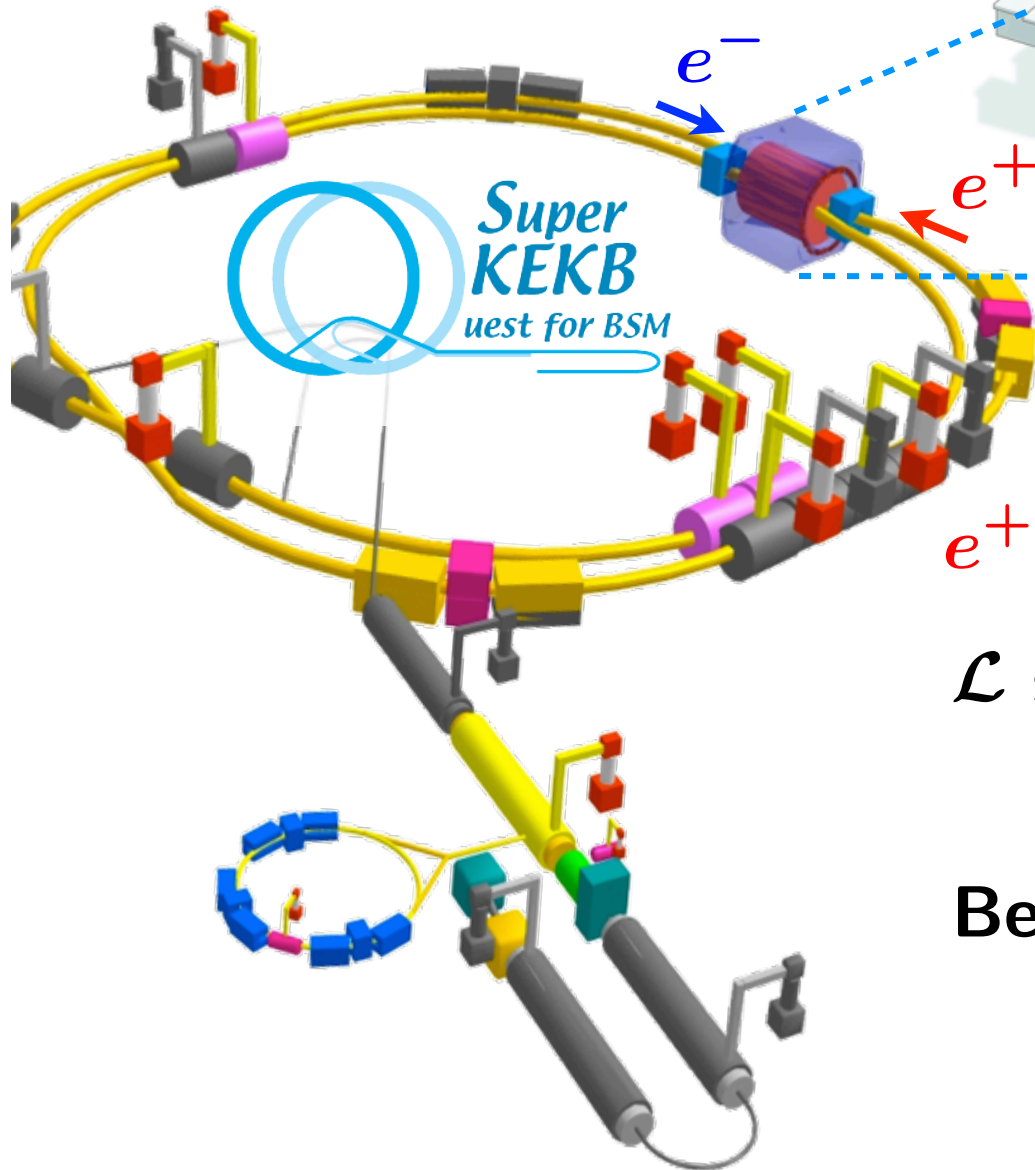
**Fermilab:**

Burt Holzman

**Versi:**

Ulrich Felzmann

# Belle II and SuperKEKB at KEK in Japan



$e^+e^-$  collisions at  $E_{\text{cm}} = M_{\Upsilon(4S)}$

$$\mathcal{L} \simeq 8 \times 10^{35} \text{ cm}^{-2} \text{ s}^{-1}$$

$$\rightarrow \int \mathcal{L} dt \approx 50 \text{ ab}^{-1} \text{ by 2021}$$

**Beyond the Standard Model :**

$$B \rightarrow \tau \nu, B \rightarrow K \pi,$$

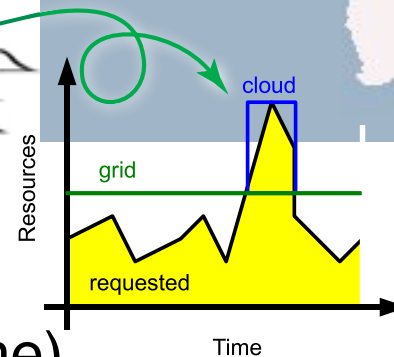
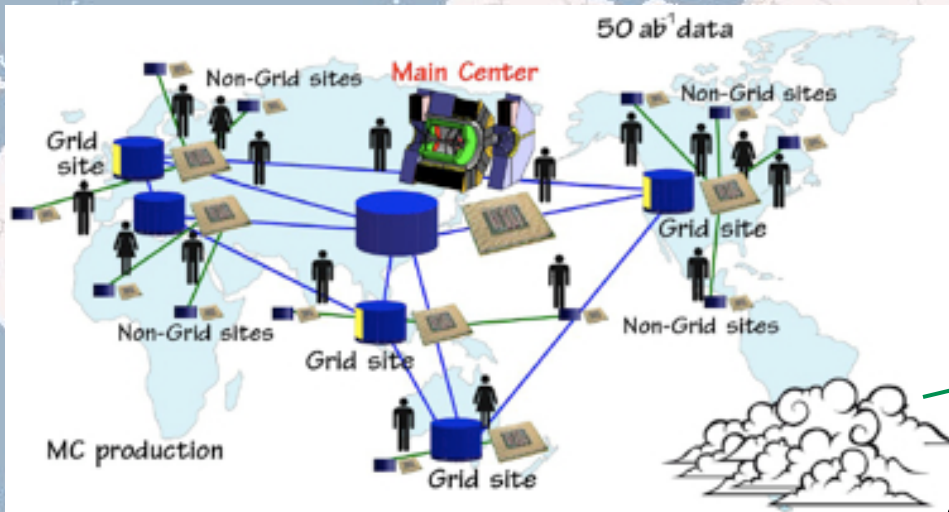
$$B \rightarrow X_s \gamma, B \rightarrow K^{(*)} \ell \ell, \dots$$

rare charm and  $\tau$  decays

# Belle II Collaboration: 13 countries/regions, 60 institutions, ~350 collaborators



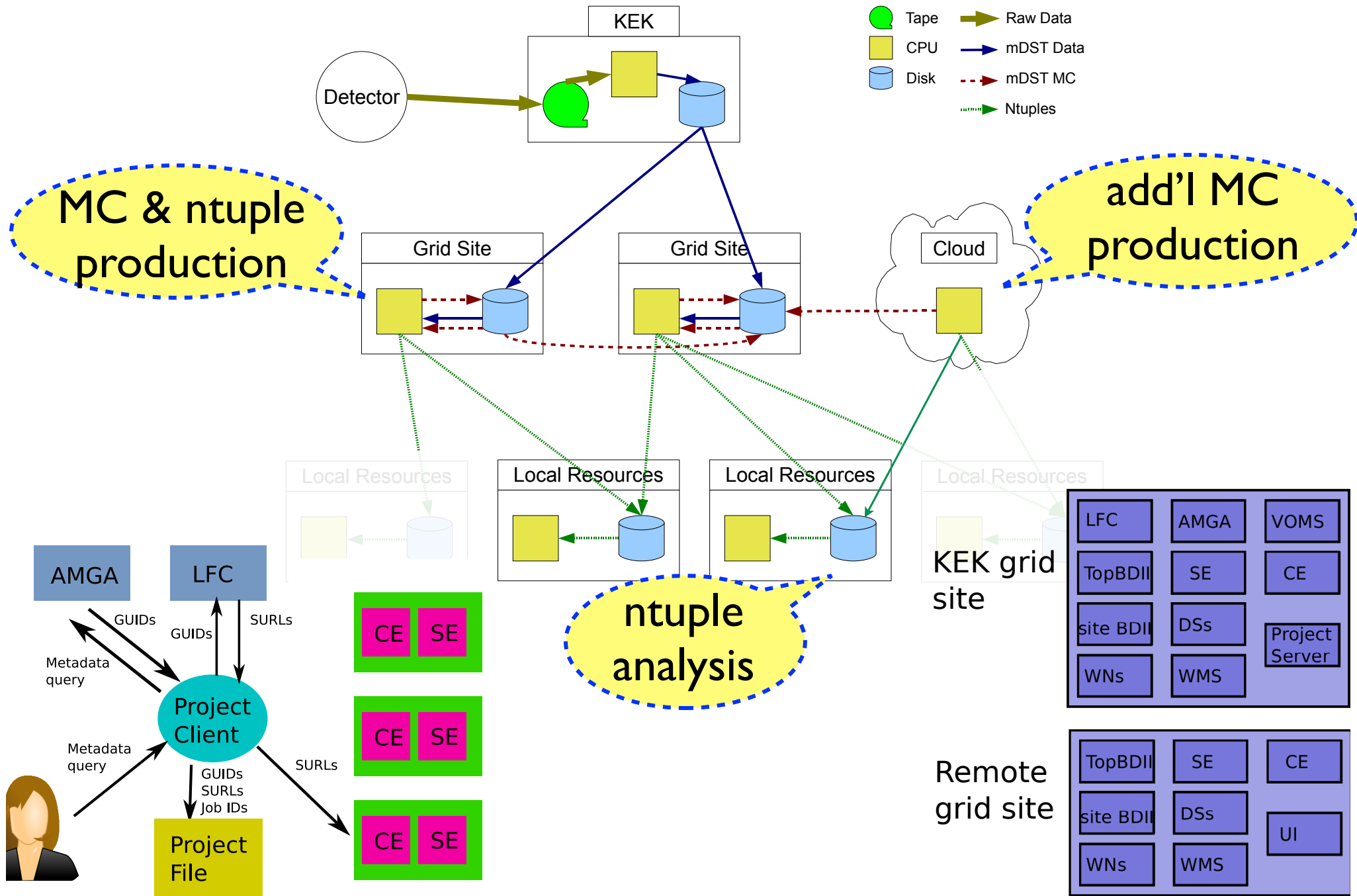
Belle II's U.S. grid site will be at  
Pacific Northwest National Laboratory



- ✓ EGI–OSG interoperable VO: 13 countries
- ✓ Jobs submitted using DIRAC (of LHCb fame)
  - ❖ Input defined by Metadata queries (powered by AMGA)
  - ❖ Works on the idea of a “Project”
    - a collection of jobs
    - different data per job
    - same analysis code for each job
- ✓ Data source at KEK; distributed on demand
  - ❖ ~50 PB raw data and ~300 PB simulated/skimmed data by 2016
- ✓ MC production ramps up in 2012 in preparation for data in 2014



# The Belle II Computing Model



# CDF VO status and outlook

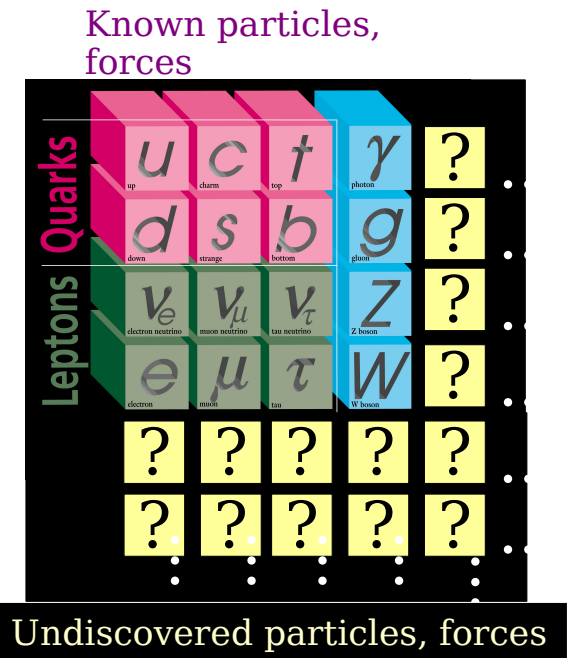
Rick Snider  
*for the CDF Offline Group*

OSG All Hands Meeting  
Harvard Medical School  
March 9, 2011

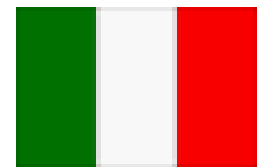
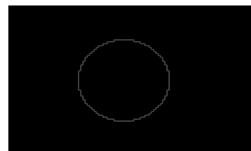
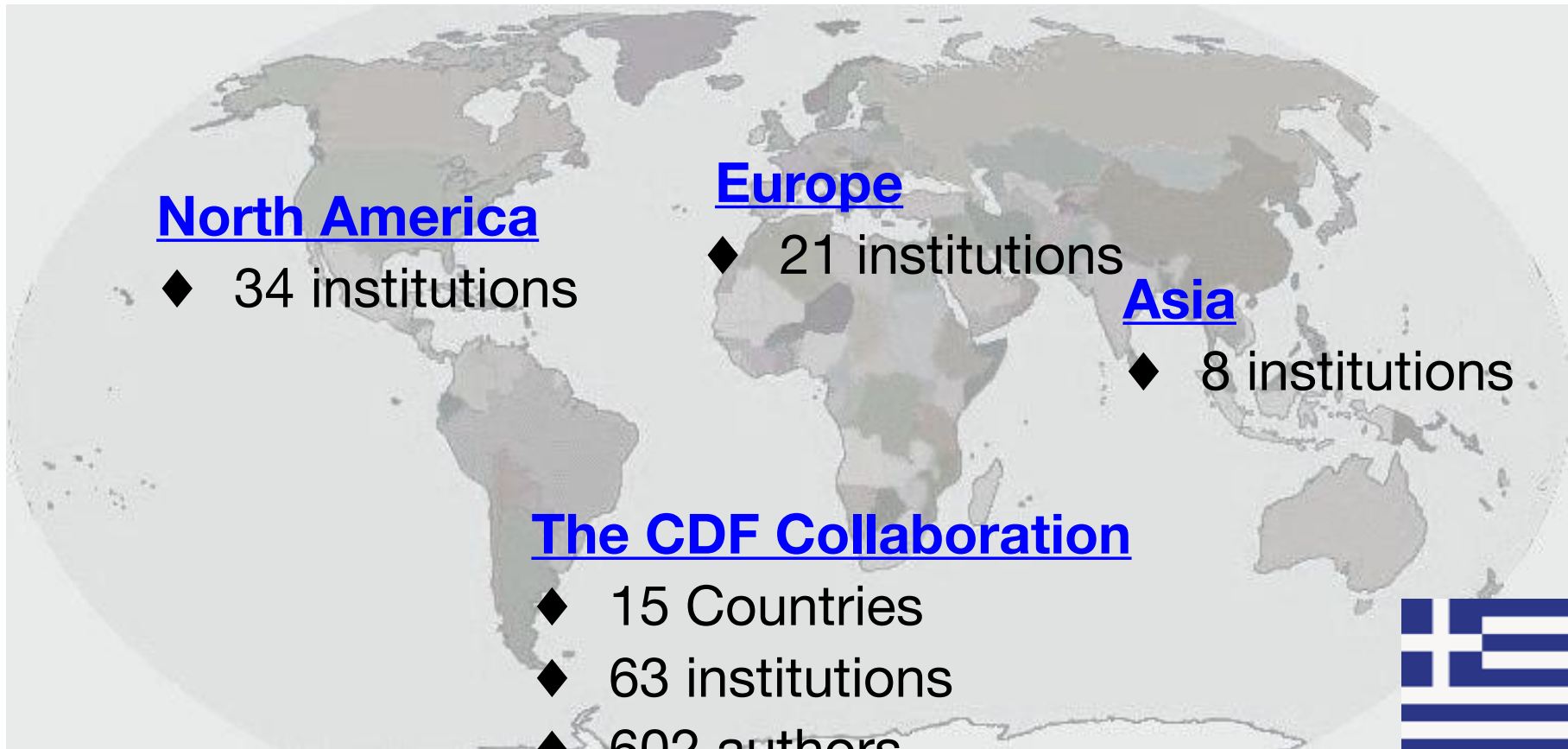
# The CDF experiment

- Fermilab Tevatron Collider

- ◆ Study the elementary structure of matter
  - ▶ Measure properties of know particles, forces
  - ▶ Search for new phenomena
- ◆ Collides 1 TeV beams of protons and antiprotons head-on at center of CDF experiment



# The CDF Collaboration

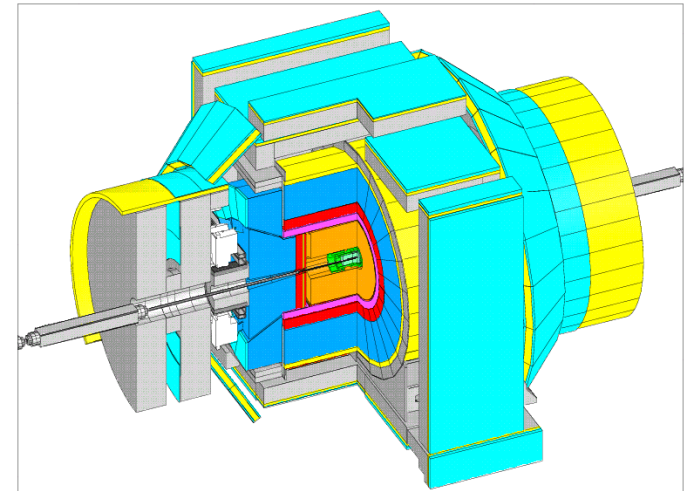




# Collider Detector at Fermilab experiment

- CDF detector

- ◆ Detector surrounds one of the collision points
  - ▶ Collisions every 400 ns
- ◆ Measures critical properties of each “event”
  - ▶ Where collision products go, energy and momentum, type of particle, whether some escape without being detected
- ◆ 750k channels of electronics
  - ▶ About 150 kB of data per event
- ◆ Record data at 20 MB/s
- ◆ Log data 100+ hrs per week, 40+ weeks per year since 2002
  - ▶  $13 \times 10^9$  events, 1.9 PB of raw data to date



# CDF computing model

- Data analysis
  - ◆ Process raw data (1.3 times) to reconstruct particle trajectories, energy, momenta, particle ID, etc.
  - ◆ Process the results to refine the reconstruction, produce reduced datasets
  - ◆ Occasional perform large-scale re-processing of previous two steps
  - ◆ Monte Carlo simulation data produced in parallel following the same processing chain
  - ◆ Individual physicists:
    - ▶ Further process, analyze the reduced datasets, MC results
    - ▶ Run toy MC / pseudo-experiments / matrix element calculations

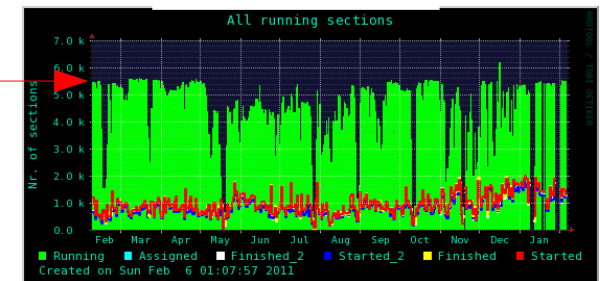
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Process on “CDF”  
OSG resources

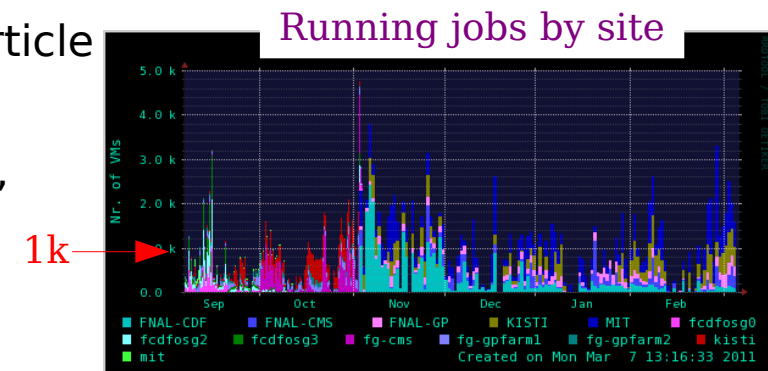
Running jobs



# CDF computing model

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Process primarily off-site and opportunistically on Fermigrid




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CDF site + Fermigrid  
+ CDF collaborating  
sites\*



\* New within the past  
year.

# Outlook for 2012

- OSG has been critical for success of CDF computing
  - ◆ Depend upon software infrastructure, operations support,...
  - ◆ Run ends in 2011, but large-scale computing will continue for several years
- A major task: re-processing
  - ◆ Several large re-processing tasks started last year, some still pending
  - ◆ Expect to re-process significant fraction of dataset after run ends
  - ◆ Re-processing model has been to tax general users
    - ▶ Costly to users who often have pressing short-term physics goals
  - ◆ Investigated running reconstruction on remote CDF + non-CDF resources
    - ▶ Have proof in principle that this works at some scale
    - ▶ Will consider using OSG more broadly for some re-processing

# Compact Muon Solenoid

- **2000 physicists** across 200 institutions in 40 countries, give or take a few.
- In 2010, we accumulated 35/pb of data.
  - => Led to ~ 30 publications so far.
- For 2012, we expect up to 2000/pb of data.
- 300Hz rate of 200kB events at 30% duty cycle of the accelerator =  $6e11$  kB/year ~ **PetaByte of user analysis data/year**
  - Not counting RAW, RECO, nor simulation.
  - Not counting same data processed using multiple different software releases.
- **A typical analysis processes more than 10% of the events.**

# Science Objectives of the LHC

- We study the fundamental constituents of matter and their interactions.
  - The Origin of Mass => Higgs Mechanism
  - Matter and Energy content of the Universe
    - Only ~4% is made of ordinary matter.
    - ~29% is “dark matter” and ~67% is “dark energy”, neither of which we have an explanation for.
  - Nature of space-time
    - Are there more than 4 dimensions in nature as “desired” by some theories ?

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  - Nature of space-time
    - Are there more than 4 dimensions in nature as “desired” by string theories?

**Guaranteed**

**Well Motivated**

**Speculative**



# CMS Outlook

- 2011: full year of data taking
- 2012: full year of data taking
- 2013/14: LHC accelerator shutdown
- Beyond that, fkw can't read the tea leaves.



# The DØ Collaboration

DØ is an international collaboration of 487 physicists from 20 nations who have designed, built and operate the DØ detector at the Tevatron and perform data analysis

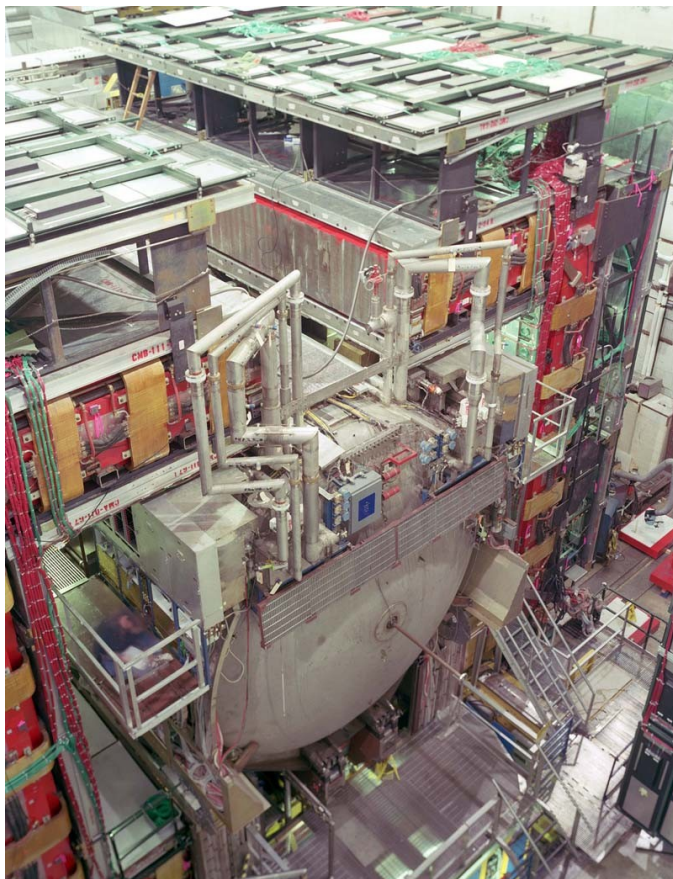


Institutions: 80 total, 36 US, 44 non-US





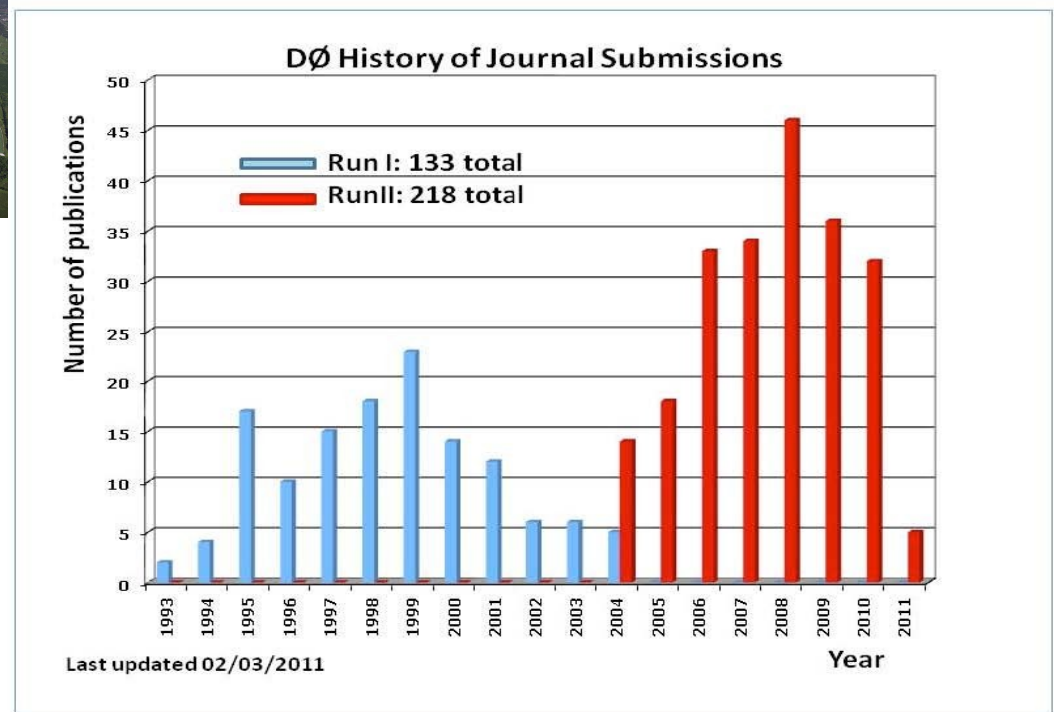
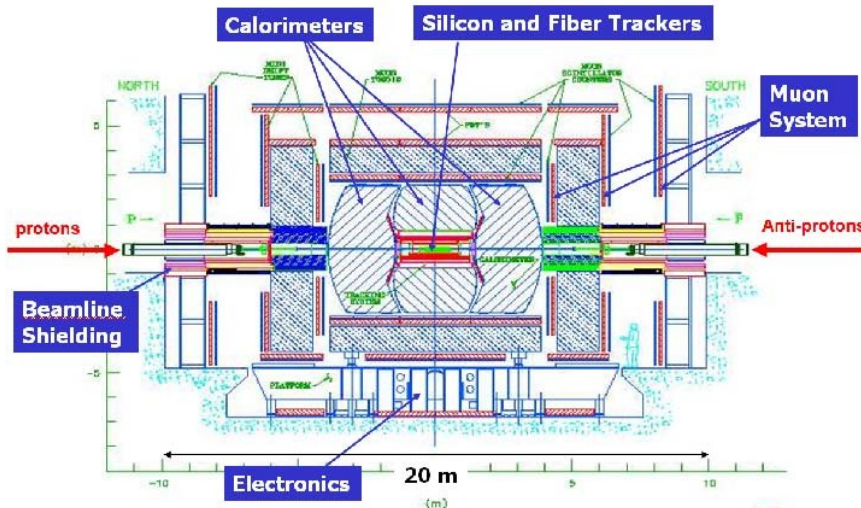
# The DØ Experiment



Studies fundamental physical constituents and their interactions by colliding 1 TeV protons with 1 TeV anti-protons

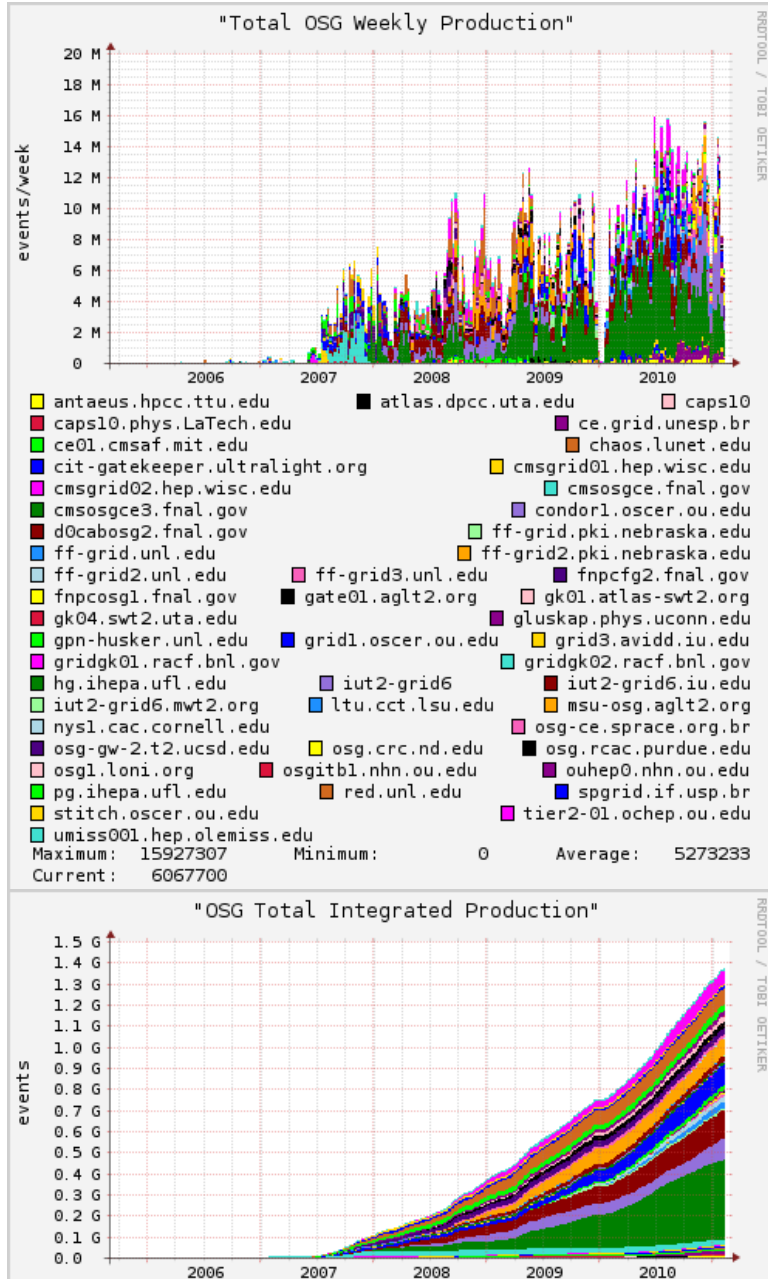
## Topics of inquiry include:

- Bottom quark physics
- Top quark physics
- Higgs boson physics
- Electroweak physics
- Quantum Chromodynamics
- New phenomena beyond SM



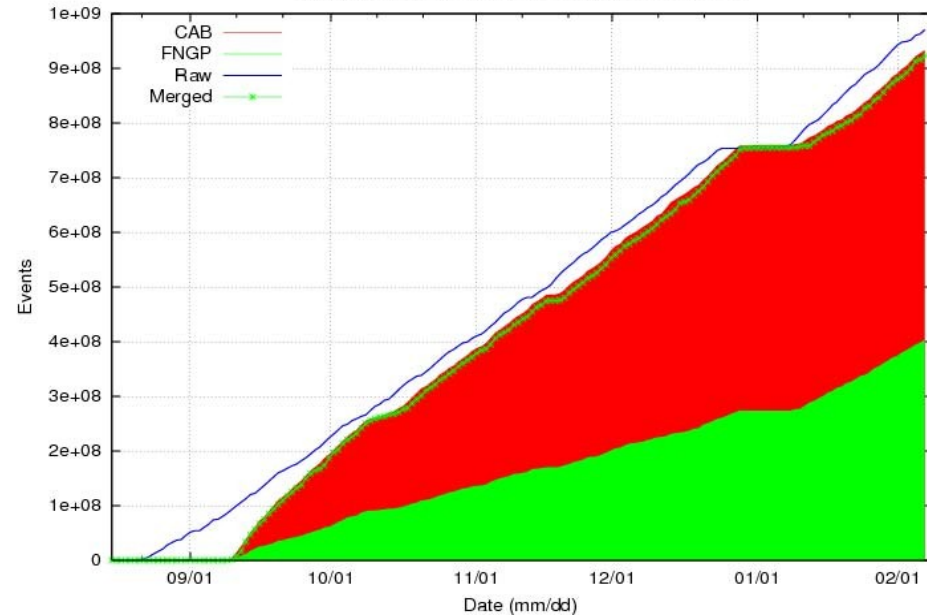
# Monte Carlo Production

# DØ OSG Use



## Data Production

Cumulative p20 Production (2b-4 Only) to 08-Feb-2011



- DØ integrates legacy grid and data handling systems with the OSG. Job submission is all done at FNAL.
- Data production only uses a few CE's located at FNAL with dedicated workers.
- MC jobs are submitted from a work queue by a daemon to a scheduler. MC is almost completely opportunistic and currently uses 30 CE's & 8 SE's.
- There are also some CPU intensive analysis jobs done on the OSG.

1.4 billion MC events represents about 5000 CPU-years



# DØ 2012 Outlook

- Tevatron program ends in September 2011
  - Data production use of the OSG will end
  - MC production and analysis will continue for several years
- DØ use of the OSG in 2012 is crucial to provide adequate and timely simulated data for physics analyses that produce publications.
- The DØ collaboration thanks the DOE, NSF, and the various international funding agencies that support this work

Joel Snow, Langston University/FNAL, on behalf of the DØ collaboration

# **OSG Engage VO**

## **Status and Outlook**

**John McGee, Steve Cox, Mats Rynge**

OSG AHM 2011



# OSG Engage

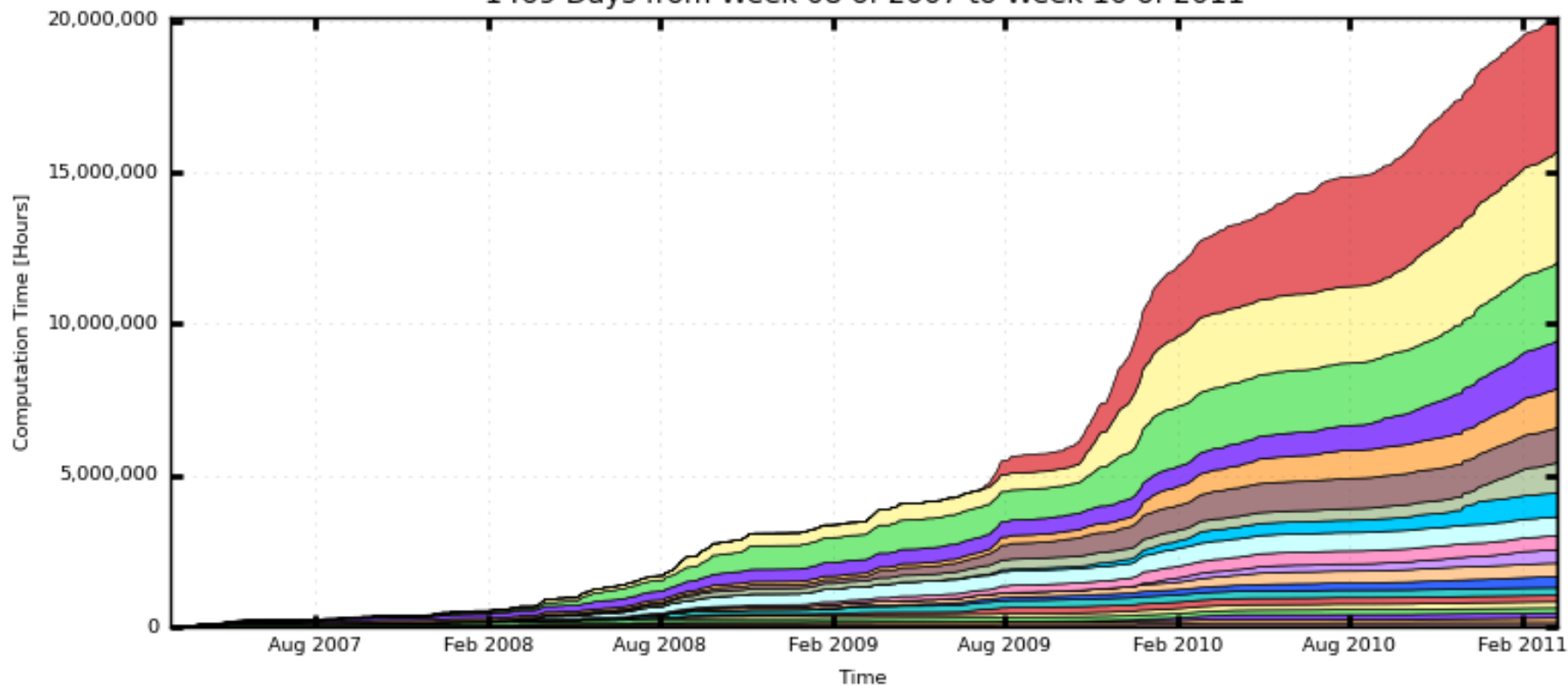
- Infrastructure, Services, and human expertise to help new users and communities ramp up to national CI
- A broad set of science domains have been engaged over the years
  - Biochemistry, genomics, mechanical engineering, mathematics, Systems biology, coastal modeling, electrical engineering, etc
  - '09/10 project year: 10 publications citing OSG usage due to Engage effort
- Detailed independent analysis of Engage program conducted by Howison et al of CMU via VOSS award

# Classes of Engage Users

- Individual researcher
  - many examples
- PI/Lab with steady stream of students
  - Steffen Bass at Duke University, theoretical physics
- Systems Integration
  - Andreas Prlic, RCSB Protein Data Bank

# Cumulative Hours Spent on Jobs By Facility

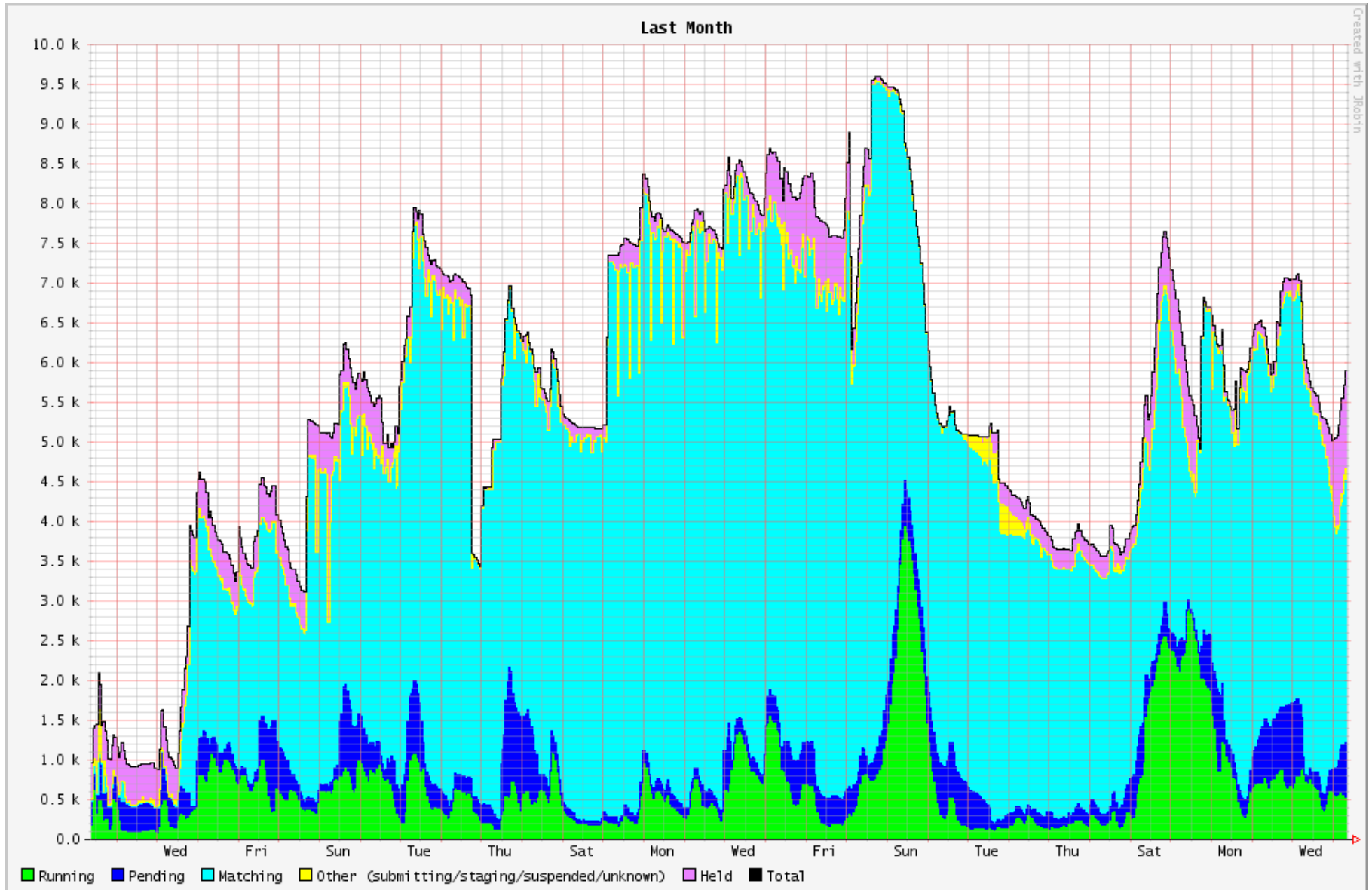
1469 Days from Week 08 of 2007 to Week 10 of 2011



Firefly (4,462,412)	USCMS-FNAL-WC1 (3,672,708)	FNAL_FERMIGRID (2,576,694)	Other (1,564,796)
Nebraska (1,292,597)	UFlorida-HPC (1,156,412)	UCSDT2 (996,956)	Clemson-Palmetto (787,443)
MIT_CMS (623,853)	Purdue-RCAC (459,315)	prairiefire (440,683)	FNAL_GPGRID_1 (439,132)
RENCI-Engagement (367,954)	NYSGRID_CORNELL_NYS1 (256,288)	SMU_PHY (210,671)	UCR-HEP (204,133)
TTU-ANTAEUS (165,097)	IU_OSG (164,287)	BNL-ATLAS (148,358)	CIT_CMS_T2 (139,889)

Total: 20,129,686 Hours, Average Rate: 0.16 Hours/s

# Migrating to a GlideinWMS FE using SDSC Factory by April 2011



# OSG Engage Outlook 1 of 2

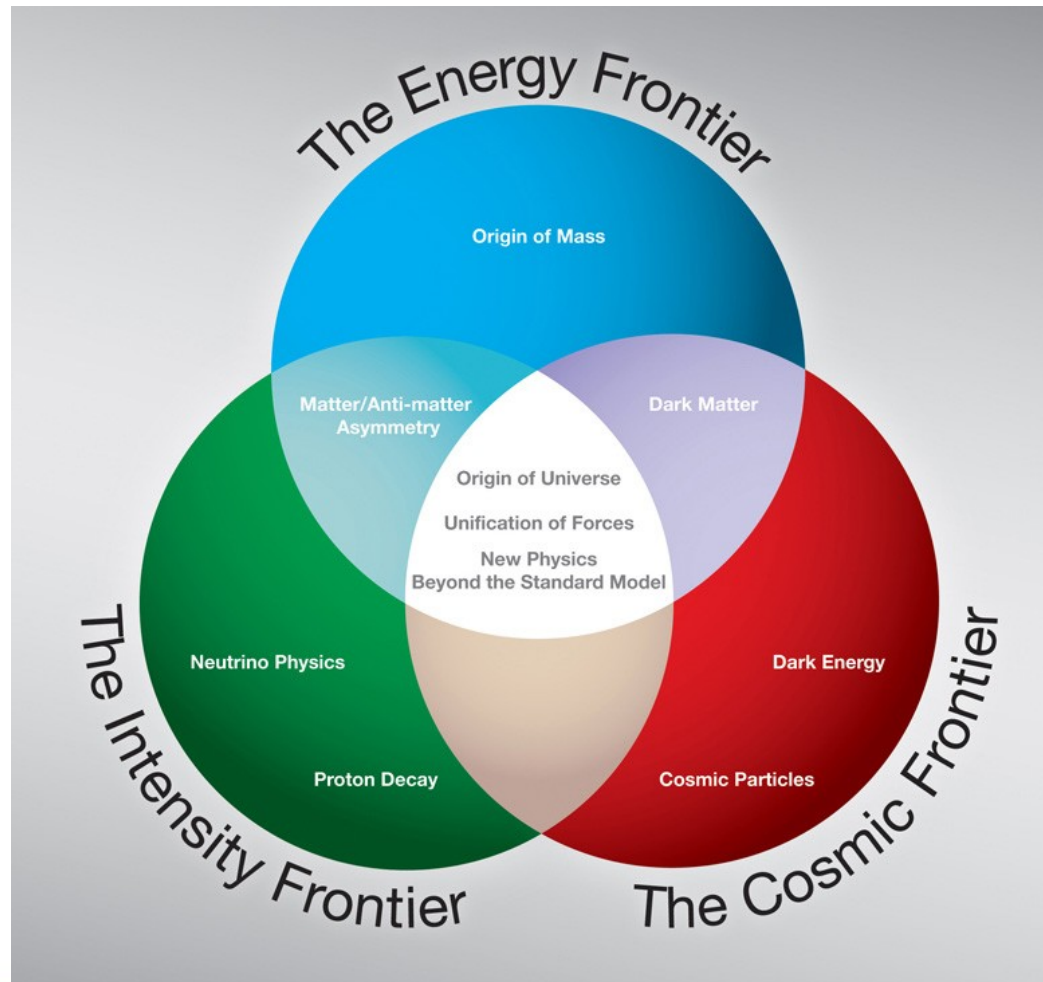
- Satellite effort funded through 3/31/2011
- No cost extension available through 3/2012
- Continued support of the Engage infrastructure and submission mechanisms at RENCI
- VO management services may be migrated to the GOC
- It is not clear that funding agencies are interested in individual level researcher support, focus appears to be on large VO/science efforts and campus integration

# OSG Engage Outlook 2 of 2

- A lot of interest in opportunistic HTPC from: environmental sciences, molecular dynamics, computational chemistry
- GPGPU
- Focus on PI groups and campus integration



# Fermilab VO (Intensity Frontier)



# Fermilab VO projects

- All Fermilab employees and users part of Fermilab VO
- Only certain subgroups exported to OSG
- Intensity frontier experiments
  - Running: MINOS, MiniBooNE, MINERvA, NOvA, ArgoNeuT
  - Building/Planning: MicroBooNE, Mu2e, LBNE (soon to be own VO).
- Accelerator and beamline simulation
- Theoretical simulation
- Cosmic frontier—Cryogenic Dark Matter Search
- ALL publications of Intensity Frontier make use of OSG.

# Intensity Frontier Hardware Architecture

End User

Developer/  
Debugger

Administrator



Framework  
Job Submission  
Analysis Tools  
Application Wrapping & Staging  
Monitoring and Reporting

“ART”, “GAUDI”, “LOON”  
“jobsub”  
ROOT  
ups/upd  
CAFMon, MCAS

## Applications

Workload Management  
Workflow Management  
Storage Management  
Data Management – Event and  
Conditions/Calibrations

CONDOR, *Glidein-WMS*  
*DAGMAN*  
*SRM*  
*SAM,*  
*NuConDB, DBI, others*

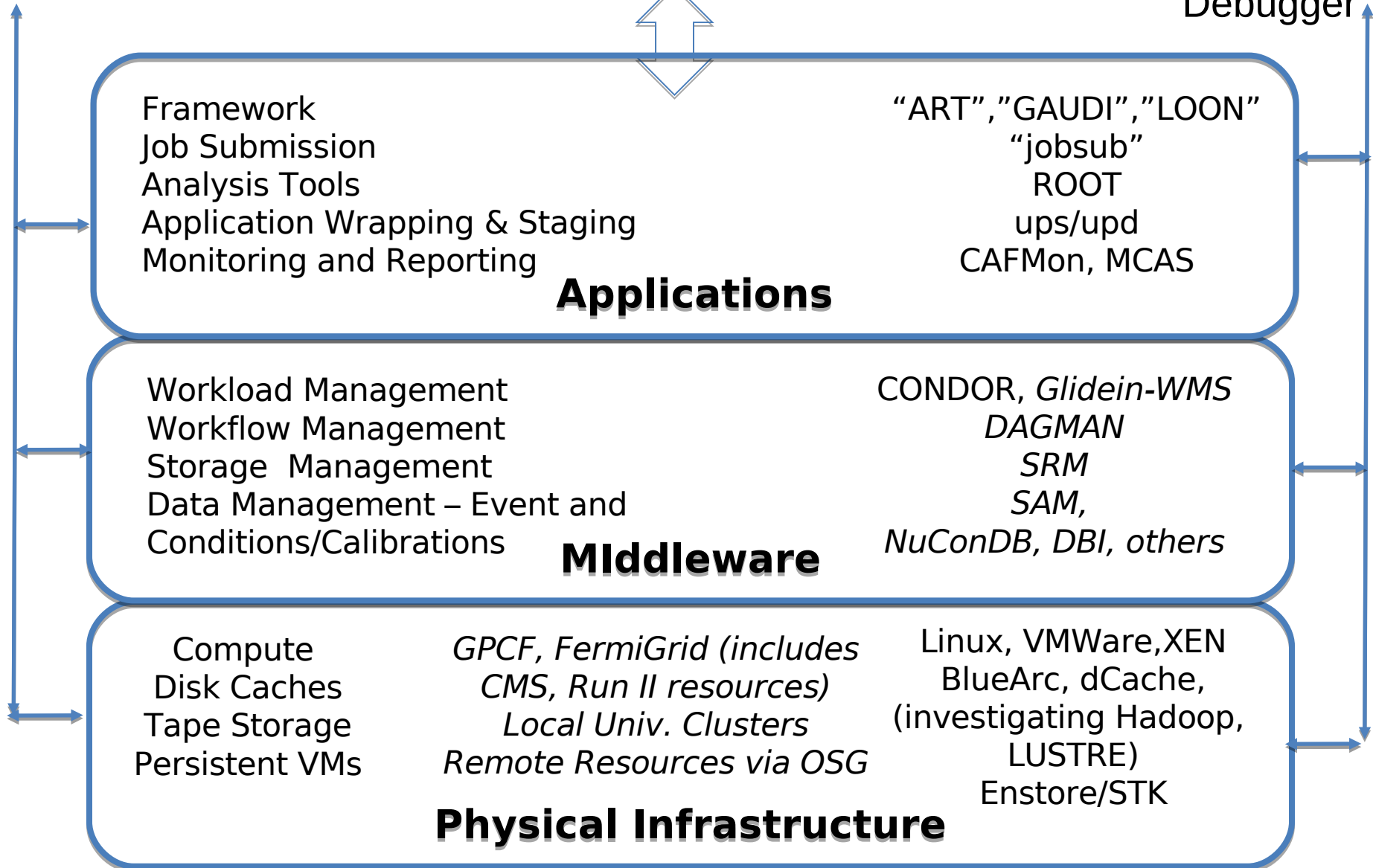
## Middleware

Compute  
Disk Caches  
Tape Storage  
Persistent VMs

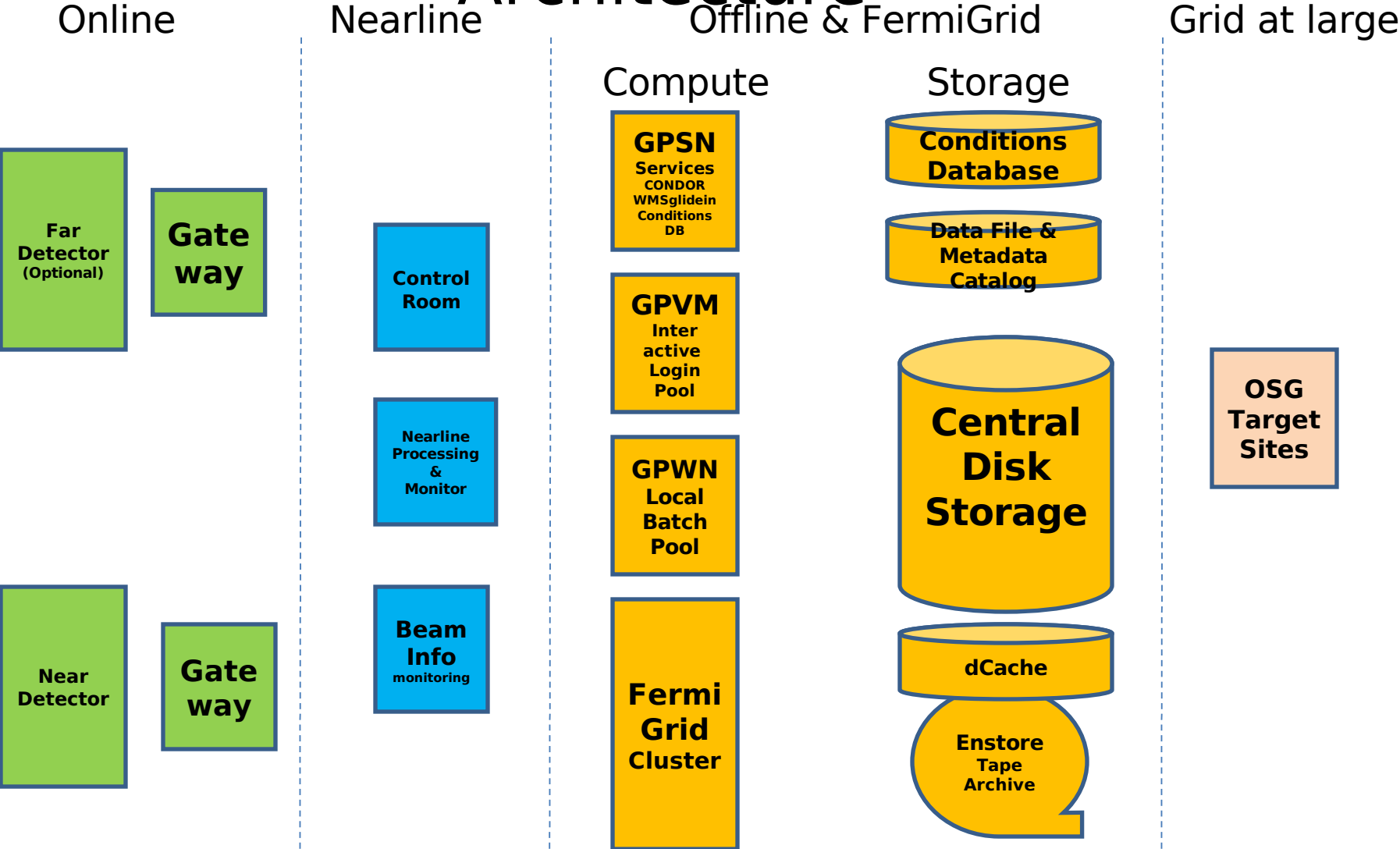
*GPCF, FermiGrid (includes  
CMS, Run II resources)  
Local Univ. Clusters  
Remote Resources via OSG*

Linux, VMWare, XEN  
BlueArc, dCache,  
(investigating Hadoop,  
LUSTRE)  
Enstore/STK

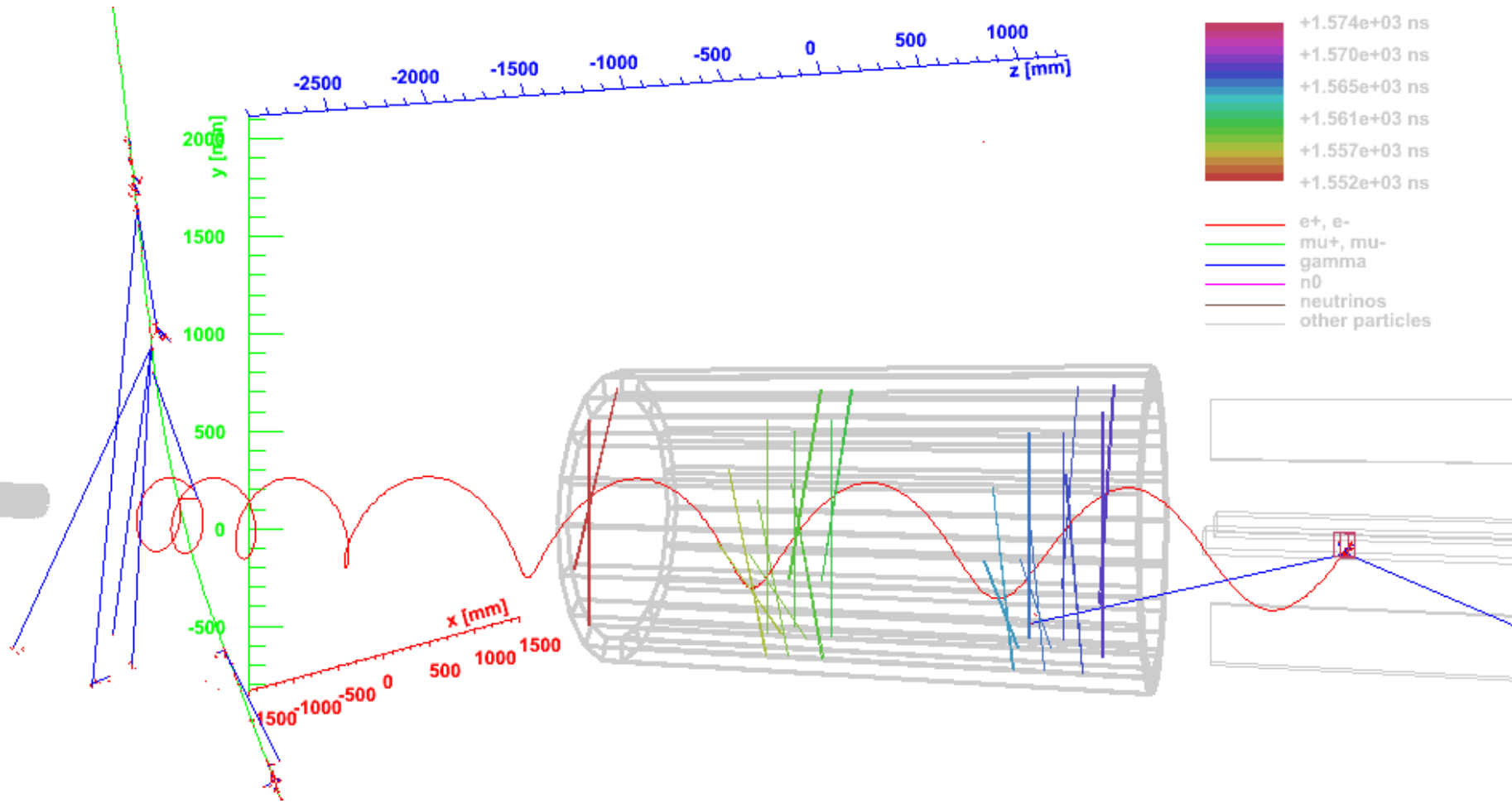
## Physical Infrastructure



# Intensity Frontier Hardware Architecture



# Mu2E High-statistics Background Simulation



# HCC TEAM

- CMS: Brian Bockelman, Carl Lundstedt, Garhan Attebury (Ken Bloom, Aaron Dominguez)
- OSG: Derek Weitzel, Adam Caprez, Ashu Guru
- HCC: Chris Cox, Ryan Lim, Tom Harvill

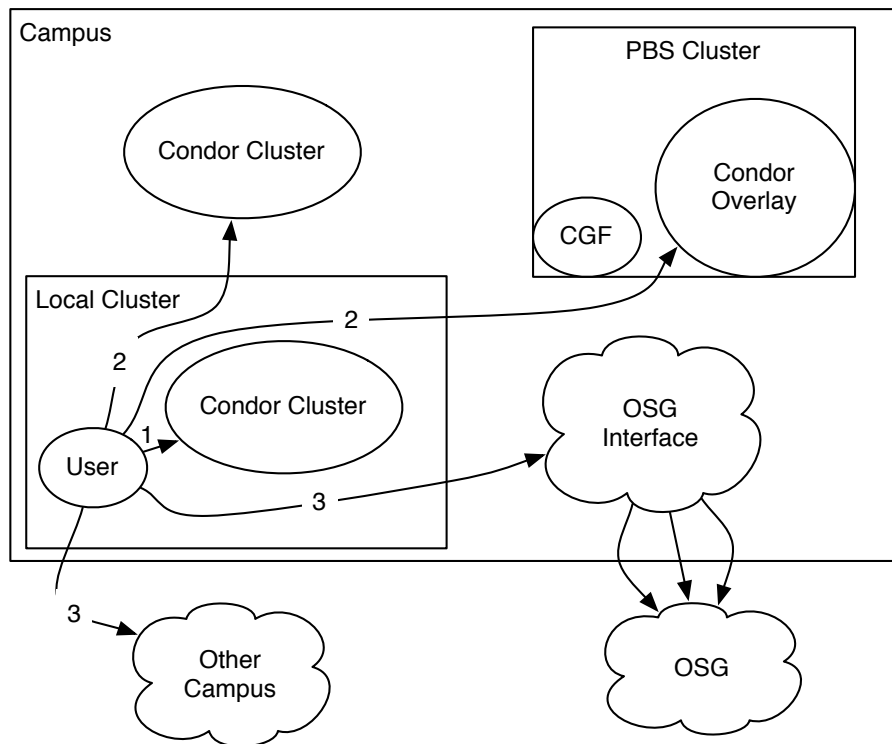




# HCC SCIENCE

- CMS [8.8M cpu hr last yr] and other friends [30.2M]
  - Non-HCC engagement: TotalJobs: 472675 TotalWallTime: 1.2M]
- Dr. Bob Powers, UNL Chemistry (CPASS -Comparison of Protein Active Site Structures) [TotalJobs: 126880 TotalWallDuration: 68k]
- Derrick Stolee, UNL Mathematics (Graph Theory Existence Studies) [7.4M]
- Dr. Ding, UNMC (OMSSA - Nuclear Matrix Proteomics) [170,000 cpu hr one weekend]

# HCC METHODOLOGY



- Campus Grid approach

# 2011 - 2012

- Collaborative award with Puerto Rico (HubZero)
- Campus grids, HTPC, Xrootd
- DYNES
- 20 gbps between HCC sites in Omaha and Lincoln
- New hires (3)
- OSG AHM (!)



Vitali Vashkevich

Michelle Ottaviano

Per Eisenbraun

SBGrid Consortium

sbgrid.org/coe

Ian Leveeque

Piotr Sliz, PI

Stephen Jahl

## Structural Biology & SBGrid

NSF RCN

Open Science Grid

Laboratory

Ian Stokes-Rees

Daniel O'Donovan

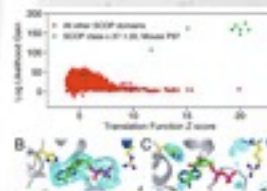
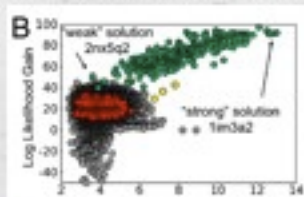
Peter Doherty

## Science: Structural Biology



### X-ray Crystallography: Wide Search Molecular Replacement

- Stokes-Rees I, Sliz P Protein Structure Determination by exhaustive search of Protein Data Bank derived databases. PNAS (2010).
- Stokes-Rees I, Sliz P, Compute and data management strategies for grid deployment of high throughput protein structure studies. 3rd IEEE workshop on Many-Task Computing on Grids and Supercomputers. (2010).



### Molecular Dynamics:



Lazarus MB, Nam Y, Jiang J, Sliz P, Walker S. Structure of human O-GlcNAc transferase and its complex with a peptide substrate. Nature (2011).

2011:

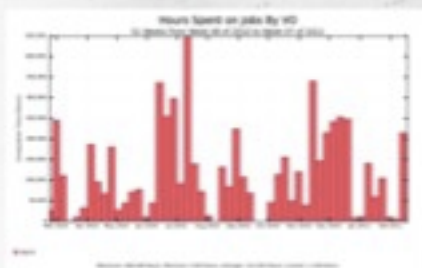
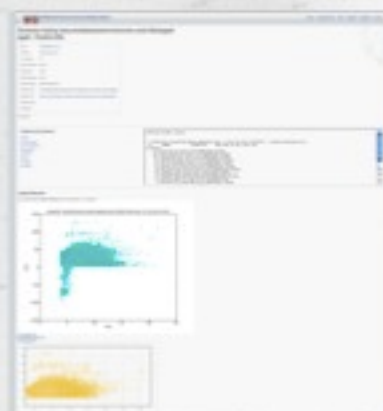
### X-ray Crystallography: Low Resolution Refinement (DEN)

### NMR: Fragment Approach



## SBGrid - General Methodology

- New workflows to support experimental structure determination
- Reuse existing applications
- GlideinWMS for job submission (OSG-gfactory at UCSD)
- Web portal for WSMR workflow submission
- Extensive data analysis
- Typically 2000-7000 job slots
- Used 6 million hours in last 12 months
- 4th largest non-HEP VO



## SBGrid 2011/12 Outlook

- 2-3 new workflows (NMR, X-ray crystallography)
- New resources
- Integrated user environment with LDAP, Kerberos, KX.509 and possibly SLCS
- Improved end-user data management facilities (exploring Globus Online)