Diversity in Computing Technologies and Strategies for Dynamic Resource Allocation

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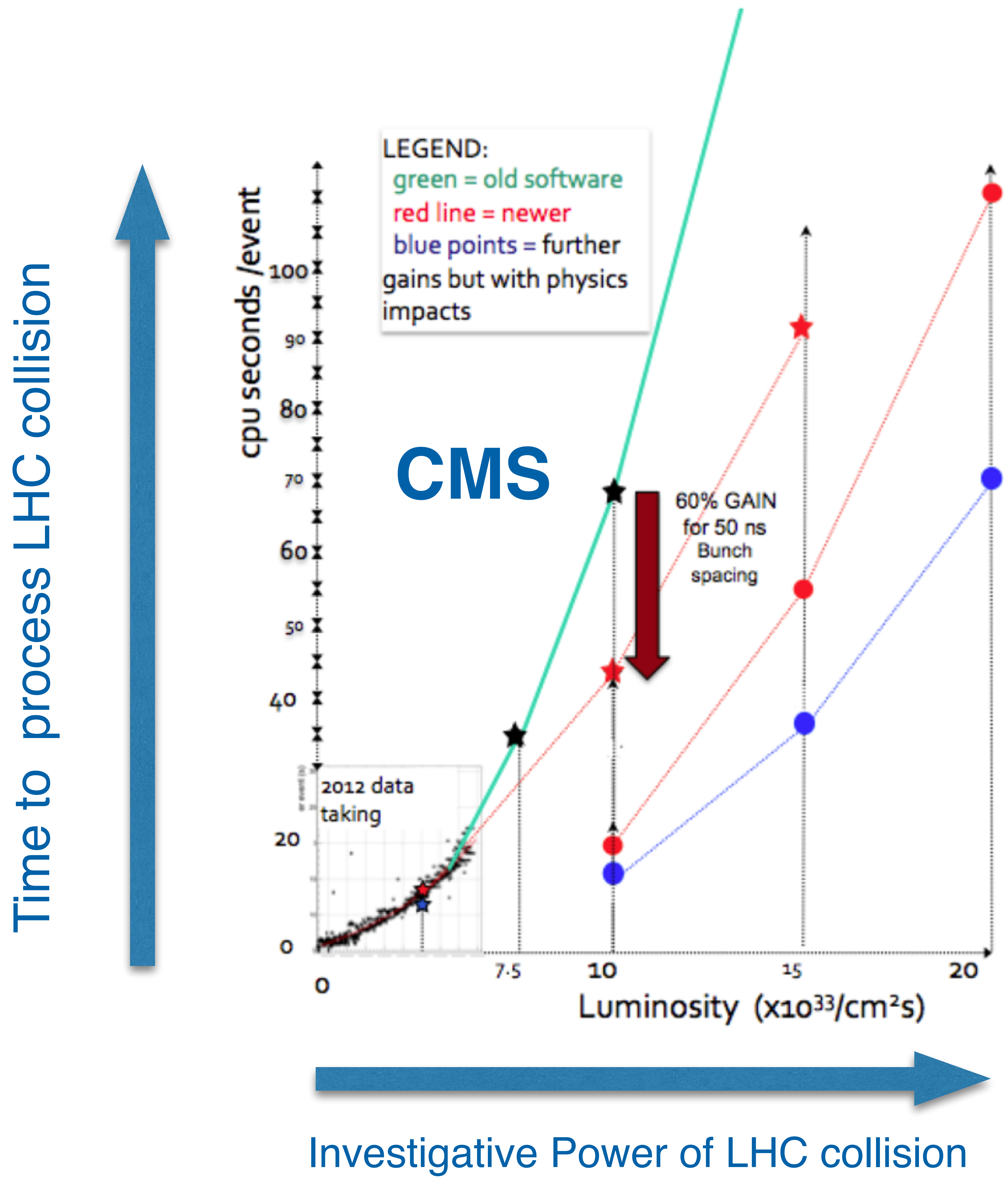
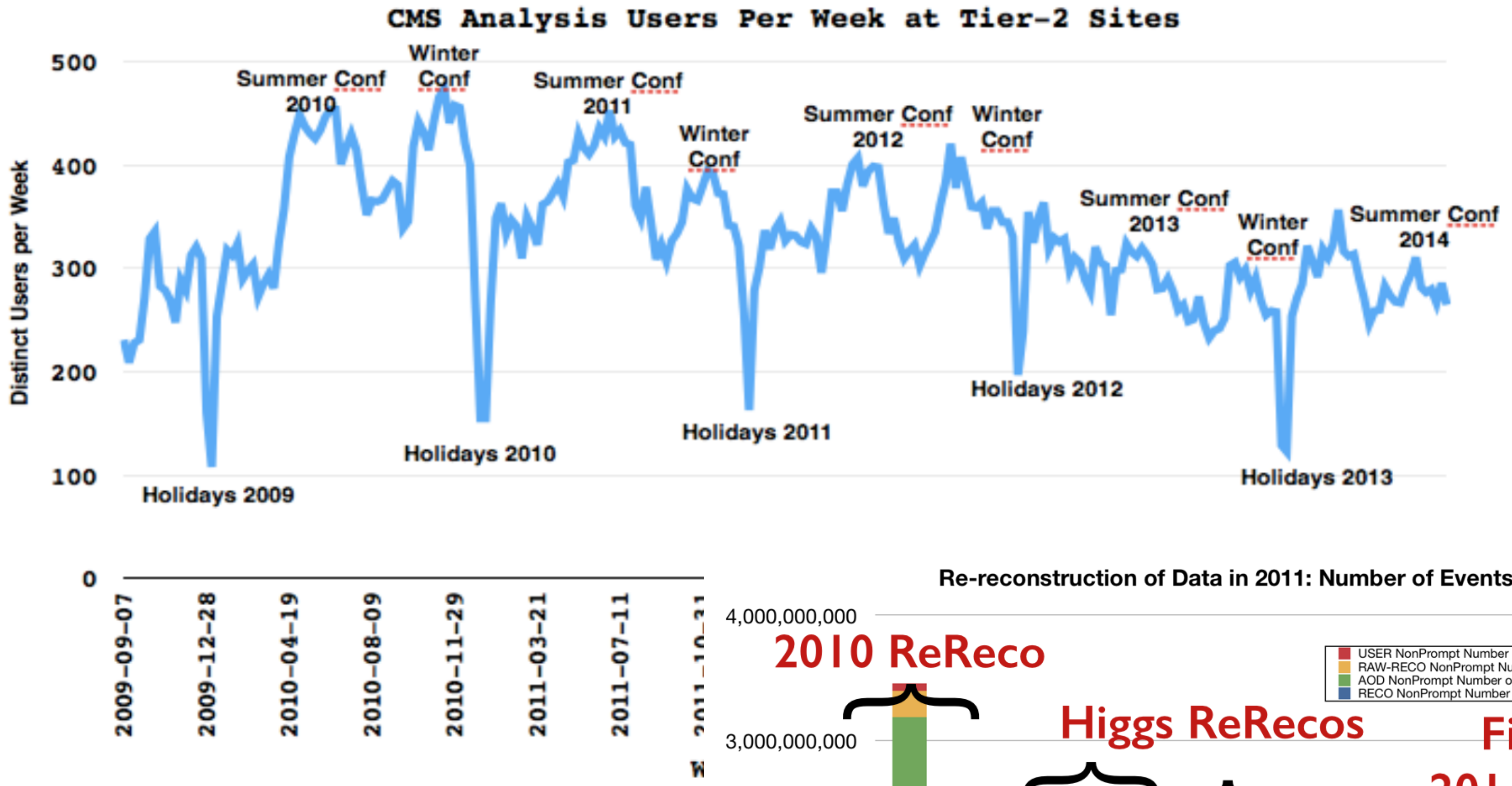
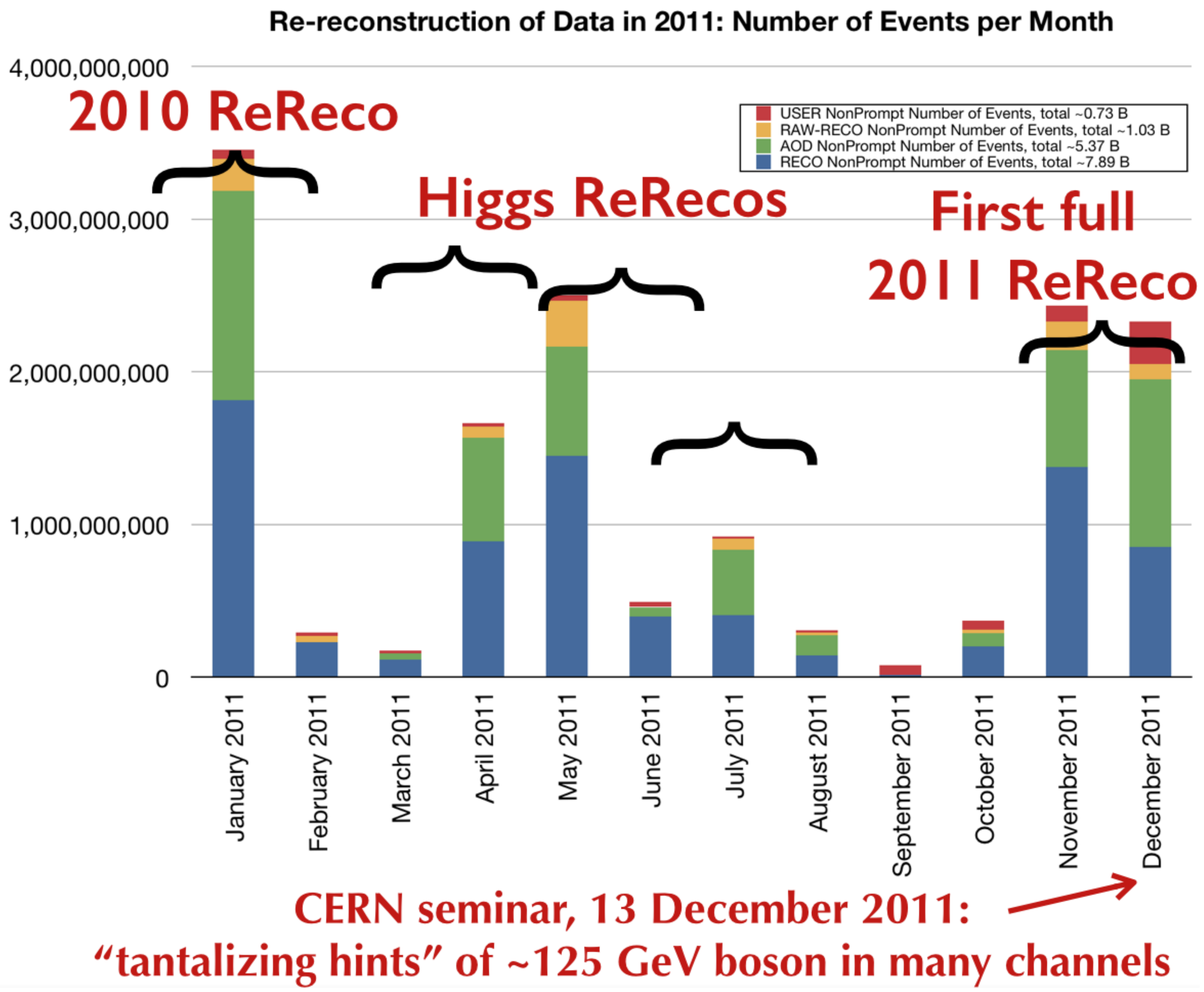
What keeps us up at night! (I)



- The nature of science:
  - Probe nature in more and more detail
  - Instruments get more powerful
  - Processing and analyzing data gets more resource intensive
- Software development is making continuously big strides
  - Improving software efficiency significantly
- But increased complexity of data is driving ever increasing resource demand
- Question: How can we provide access to sufficient resources? ➜ **CAPACITY**

What keeps us up at night! (II)





- Activity of experiments is not constant
  - It varies significantly with external triggers
    - Operation schedule
    - Conference schedule
    - Holidays, vacation time, etc.
- Question: How can we provision resources efficiently? ➜ **ELASTICITY**

Fermilab

This talk

- In the recent past, HEP resources were firmly based on **Grid** technologies
  - HEP applications == HTC
    - High Throughput Computing applications
- The need for more **capacity** and **elasticity** makes us look at other resource providers:
  - **Cloud**
  - **HPC** = High Performance Computing

GRID

Cloud

HPC

10,000 feet overview

Grid

- Virtual Organizations (VOs) of users trusted by Grid sites
- VOs get allocations ➜ **Pledges**
  - Unused allocations: opportunistic resources

Trust Federation

10,000 feet overview

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Trust Federation

Cloud

- Community Clouds - Similar trust federation to Grids
- Commercial Clouds - **Pay-As-You-Go** model
  - Strongly accounted
  - Near-infinite capacity ➜ **Elasticity**
  - Spot price market

Economic Model

10,000 feet overview

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Economic Model

HPC

- Researchers granted access to HPC installations
- Peer review committees award **Allocations**
  - Awards model designed for individual PIs rather than large collaborations

Grant Allocation

Challenges

GRID

Cloud

HPC

- How can we use Clouds and HPC installations with HEP HTC applications?
- How can we transparently integrate them into our Grid-based setups?
- How can we marry the different allocation models (static, economic, grant)?

Grid

GRID

The Grid

- The Grid is many things
  - Allows transparent access to a vast amount of resources
  - Solved the authentication problem
  - Established a trust model
- ➡ Federation of resources

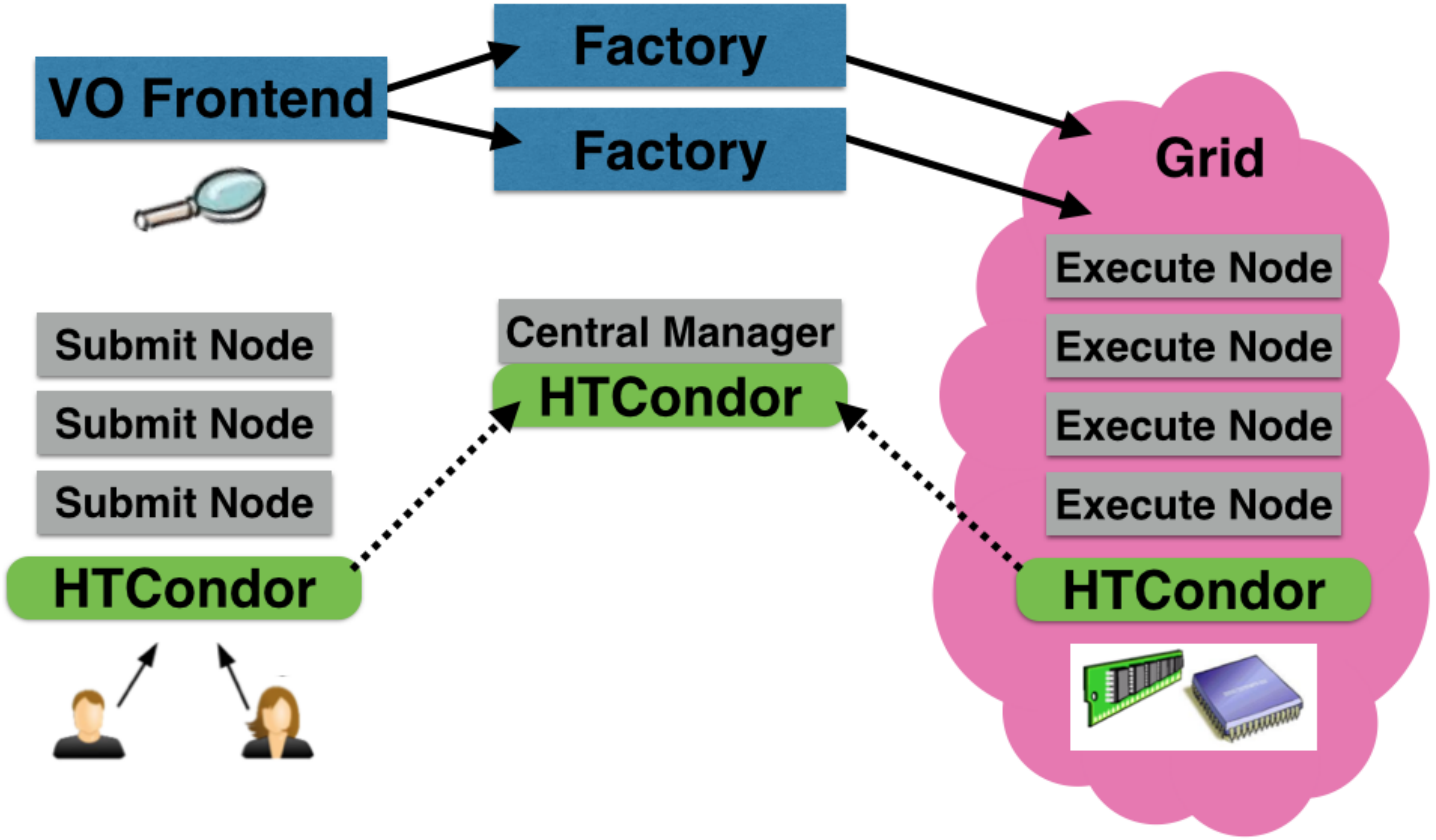
- The Grid is successful
  - The LHC experiments were amongst the first to rely on the Grid ➜ Worldwide LHC Computing Grid (WLCG)
  - National Grids are successful to bring large scale computing to “smaller” science communities

Grid submission today: Pull Era of the Grid

- Submission evolved from earlier days of the GRID ➜ **pilot-based submission infrastructures**

  - Create overlay batch system ➜ Essentially a virtual pool spanning multiple sites
    - Use lightweight pilots to claim resource
    - Pilot pulls work and executes it

  - Advantages
    - Late binding ➜ control scheduling on global scale
    - Reduction of failure rate ➜ job execution only starts after resource was successfully claimed
    - Integration of new kinds of resources ➜ simply enable resource to run pilot and pull work
  - Disadvantages
    - Debugging problems is more complex



- Example: glideinWMS
  - What I like about the concepts implemented in glideinWMS:
    - Provisioning systems can be shared amongst many different communities
    - Separate pools of resources can be provisioned per community
    - Community has control over policies/priorities within its pool

Fermilab

HPC

HPC

HTC on HPC installations

- HTC: High Throughput Computing
  - Independent, sequential jobs that can be individually scheduled on many different computing resources across multiple administrative boundaries(*)
- HPC: High Performance Computing
  - Tightly coupled parallel jobs, must execute within a particular site with low-latency interconnects(*)

- Long history in HEP in using HPC installations
  - Lattice QCD and Accelerator Modeling exploit the low latency interconnects successfully for a long time

- Traditional HEP framework applications are starting to get allocations awarded
  - unmodified if HPC is intel-based
  - cross-compiled if HPC is non-Intel-based

- In all cases, allocation is proposal-driven and awarded through peer review committees
  - Examples are separate committees for all HPC installations funded by either the National Science Foundation (NSF) or the Department of Energy (DOE); or by committees specific to individual installations
  - Differ in proposal requirements from demonstrating technical capabilities to relevance of scientific research

(*): adapted from Wikipedia: http://en.wikipedia.org/wiki/High-throughput_computing

San Diego Supercomputer Center (SDSC)

- Example for intel-based HPC installation
  - SDSC operates wide range of HPC clusters ranging from ~10k to ~50k cores
- Allocation award procedure
  - Individual Principal Investigators (PIs) submit proposals
  - Committee meets every 3 months to award allocations
  - Successful proposals have one year to use their allocations
    - Follow-up proposals need to demonstrate scientific impact
- CMS was awarded first grant in 2013 to re-process specific primary datasets (HTMHT & VBF)
  - Used pilots submitted through ssh login node
  - Follow up grants and proposals are progressing well, other experiments are equally successful
  - New: CE access to SDSC clusters simplifying access

SDSC's Gordon Supercomputer Assists in Crunching Large Hadron Collider Data

UC San Diego/Open Science Grid Collaboration Speeds Quest for Dark Matter Discovery

Gordon, the unique supercomputer launched last year by the San Diego Supercomputer Center (SDSC) at the University of California, San Diego, recently completed its most data-intensive task so far: rapidly processing raw data from almost one billion particle collisions as part of a project to help define the future research agenda for the Large Hadron Collider (LHC).

UC San Diego Physics Professor Frank Wuerthwein.
Photo: Ben Tolo/SDSC

Under a partnership between a team of UC San Diego physicists and the Open Science Grid (OSG), a multi-disciplinary research partnership funded by the U.S. Department of Energy and the National Science Foundation, *Gordon* has been providing auxiliary computing capacity by processing massive data sets generated by the Compact Muon Solenoid, or CMS, one of two large general-purpose particle detectors at the LHC used by researchers to find the elusive Higgs particle.

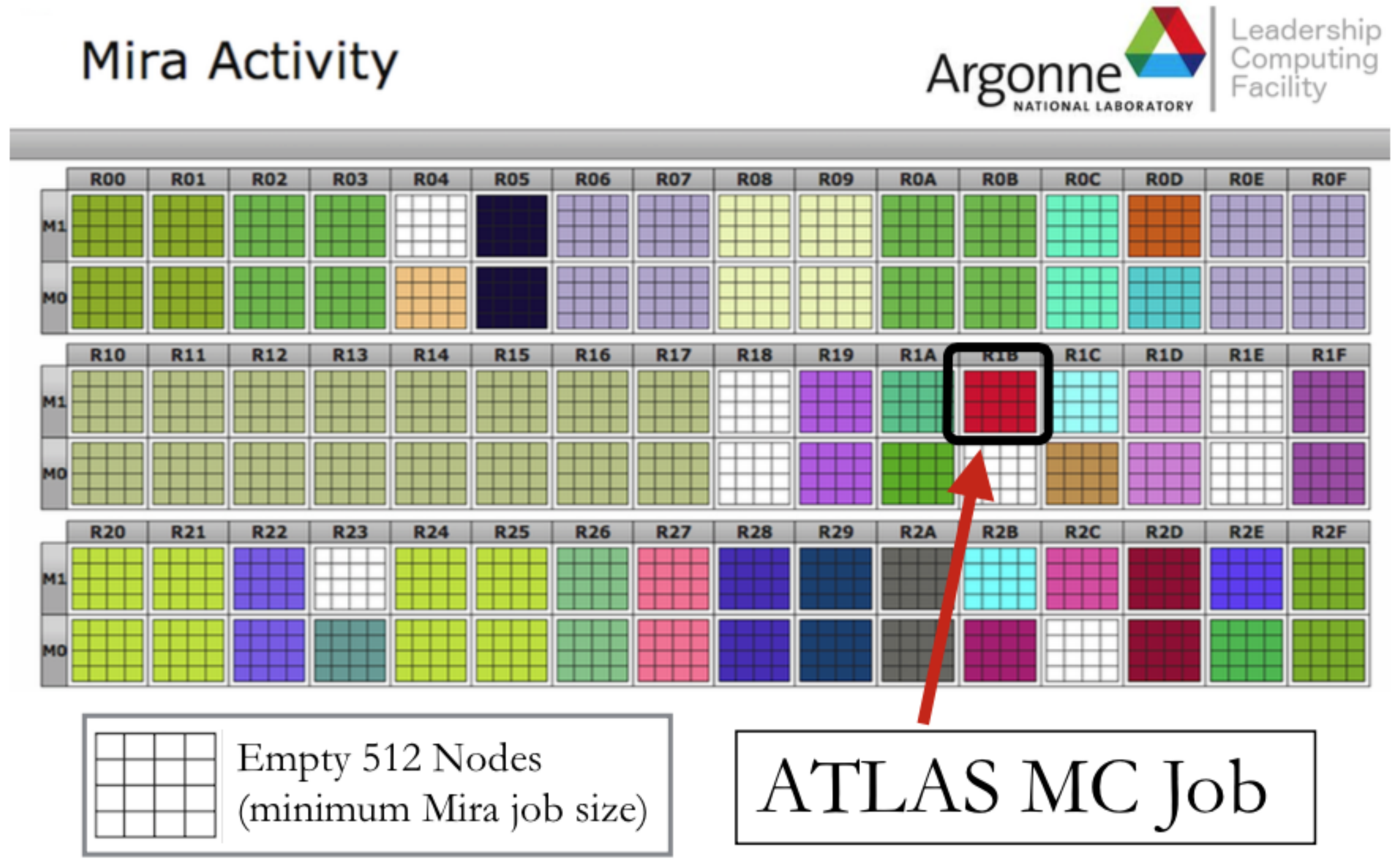
"This exciting project has been the single most data-intensive exercise yet for *Gordon* since we completed large-scale acceptance testing back in early 2012," said SDSC Director Michael Norman, who is also an astrophysicist involved in research studying the origins of the universe. "I'm pleased that we were able to make *Gordon's* capabilities available under this partnership between UC San Diego, the OSG, and the CMS project."

from: http://ucsdnews.ucsd.edu/pressrelease/sdscs_gordon_supercomputer_assists_in_crunching_large_hadron_collider_data

Mira at Argonne National Laboratory

- Example for non-Intel-based HPC installation
  - Mira (PowerPC, ~49k nodes each 16 cores, almost 800k cores)
- Similar Allocation Award procedure
  - Proposals need to demonstrate enabling new science through using Mira
- Generating Atlas LHC Events on Argonne
  - Necessary: Alpgen (Fortran-based HEP event generator) recompiled using IBM XL compilers
    - (Effectively using MPI to run N-instances of Alpgen in parallel)
- Mira has minimum partition size (512 nodes)
  - Opens ability to effectively use ‘backfill’ queues which can yield ‘free’ computing time.
  - Jobs are submitted by a custom workflow system with the goal of integrating Mira into the Atlas production workflow system.

Argonne NATIONAL LABORATORY | Leadership Computing Facility



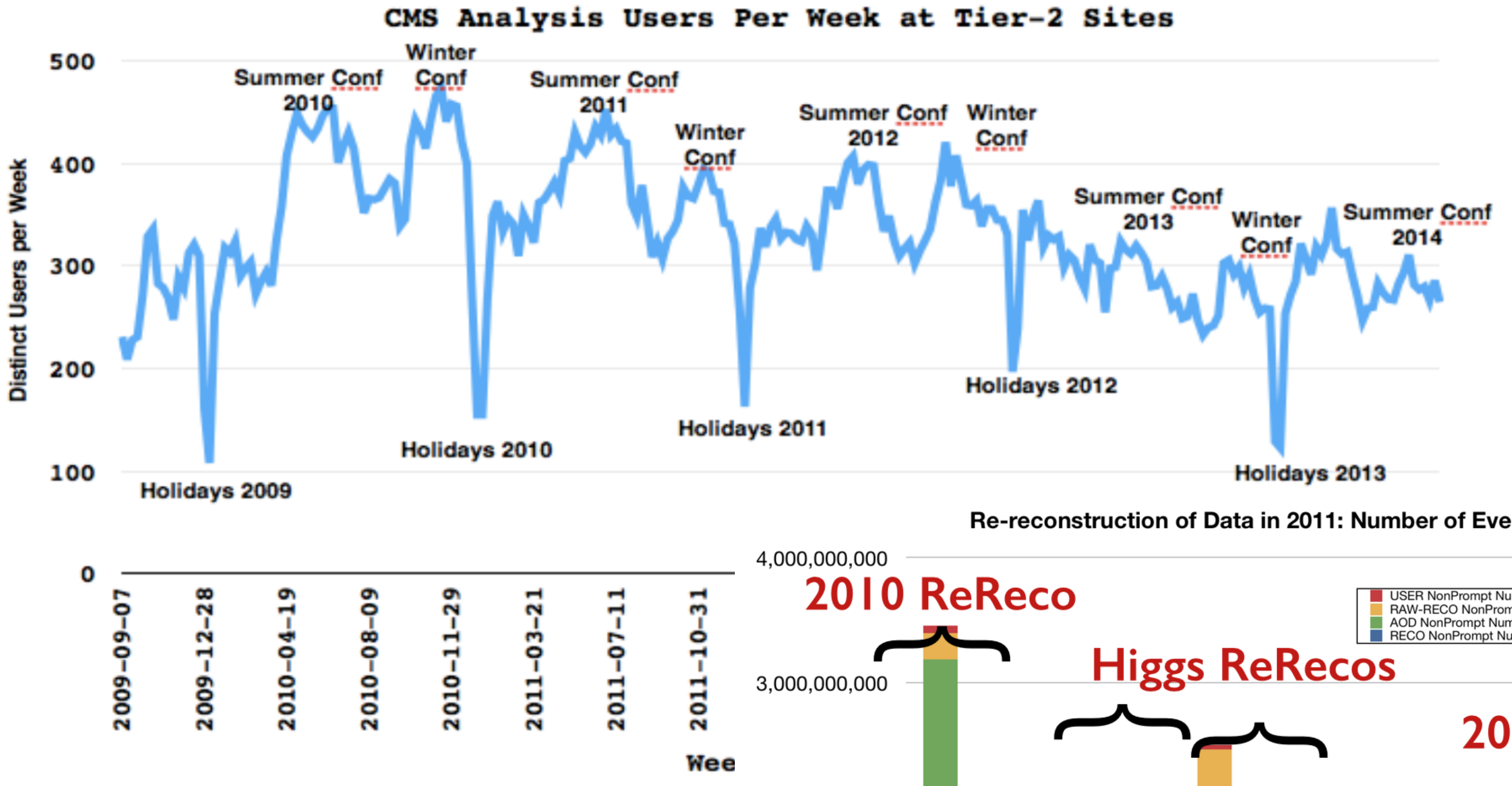
For more information, see Taylor Childers Track 8 parallel session contribution on Thursday afternoon: “Simulation of LHC events on a million threads”

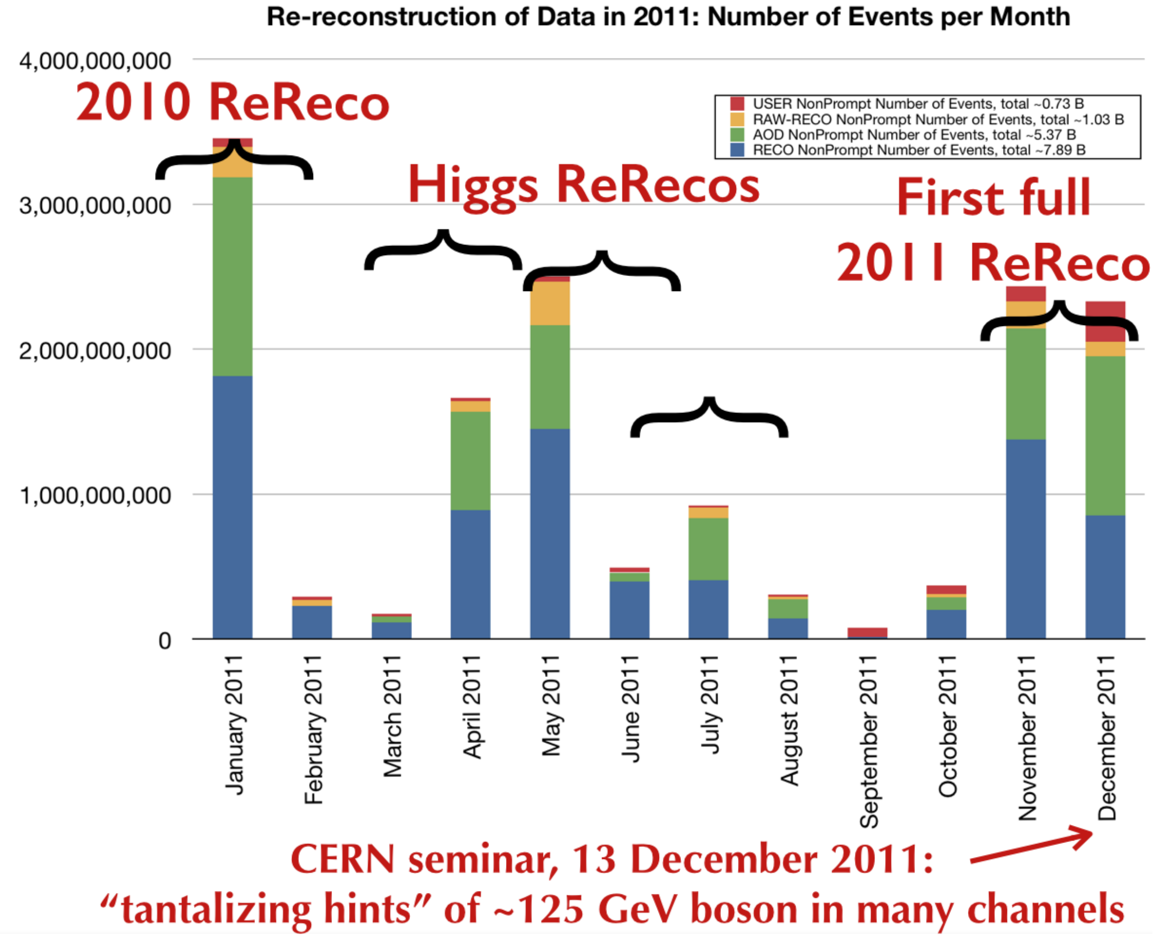
Cloud

Cloud

Cloud Allocation Model - The peaks...

- The activity of the experiments is not constant!
  - It varies significantly with external triggers
    - Instrument operation schedule
    - Conference schedule
    - Holiday festivities, vacation time, etc.





- There might be a solution on the horizon:
  - Commercial Clouds
- Commercial Clouds offer “Pay-As-You-Go”
  - Offer scaling to infinite (...very large...) capacity on short time scales ➜ **Elasticity**
    - “There is no difference in price at AWS when using 1 CPU for 1000 hours or 1000 CPUs for 1 hour” (Jamie Kinney, Sr. Manager, AWS Scientific Computing)
- Can we use commercial clouds competitively to fulfill our peak demands?

Cloud Allocation Model - … and the solution?

- It's all about scale!
  - What are the challenges we face to run at scale on commercial clouds?
  - As an example: concentrate on Amazon Web Services (AWS)

- Many HEP experiments and facilities are working with AWS
- Goal: Improve integration with HEP workflows
  - Examples: Atlas, CMS, STAR, NOvA*, etc. / BNL**, FNAL, etc.
  - It's all about understanding how most efficiently to use AWS capabilities

- Several areas of work
  - Provisioning
  - Economic model
  - Networking
  - Storage
  - On-demand Services

* Parag Mhashlikar: "Cloud services for the Fermilab scientific stakeholders", parallel talk in track 7 on Thursday

* Andrew Norman: "Large Scale Monte Carlo Simulation of neutrino interactions using the Open Science Grid and Commercial Clouds", poster session A

** John Hover at HEPiX Spring 2015: "Running ATLAS at scale on Amazon"

Provisioning

- Provisioning straight forward
  - Use cloud interfaces to include resources in pilot-based submission infrastructures
- We can provision resources on AWS by …
  - … paying for regular instances and design the instances to our needs
    - Our instances need: enough memory and local disk for our jobs and ability to run long enough to complete our jobs
  - … by using the spot price market
    - AWS spot pricing: bid your top price and pay the market price until it goes above your bid ➜ disadvantage, instance might go away when market changes
    - Works well as long as spot price is stable on time scales >> than typical runtimes and/or workflows can deal with pre-emptable Grid cycles
- Integration challenges:
  - Develop mechanisms to expand and contract provisioned resources while job queue is full
  - Important to provision sufficient resource on the spot price market: integration with AWS availability zone management

Economic model

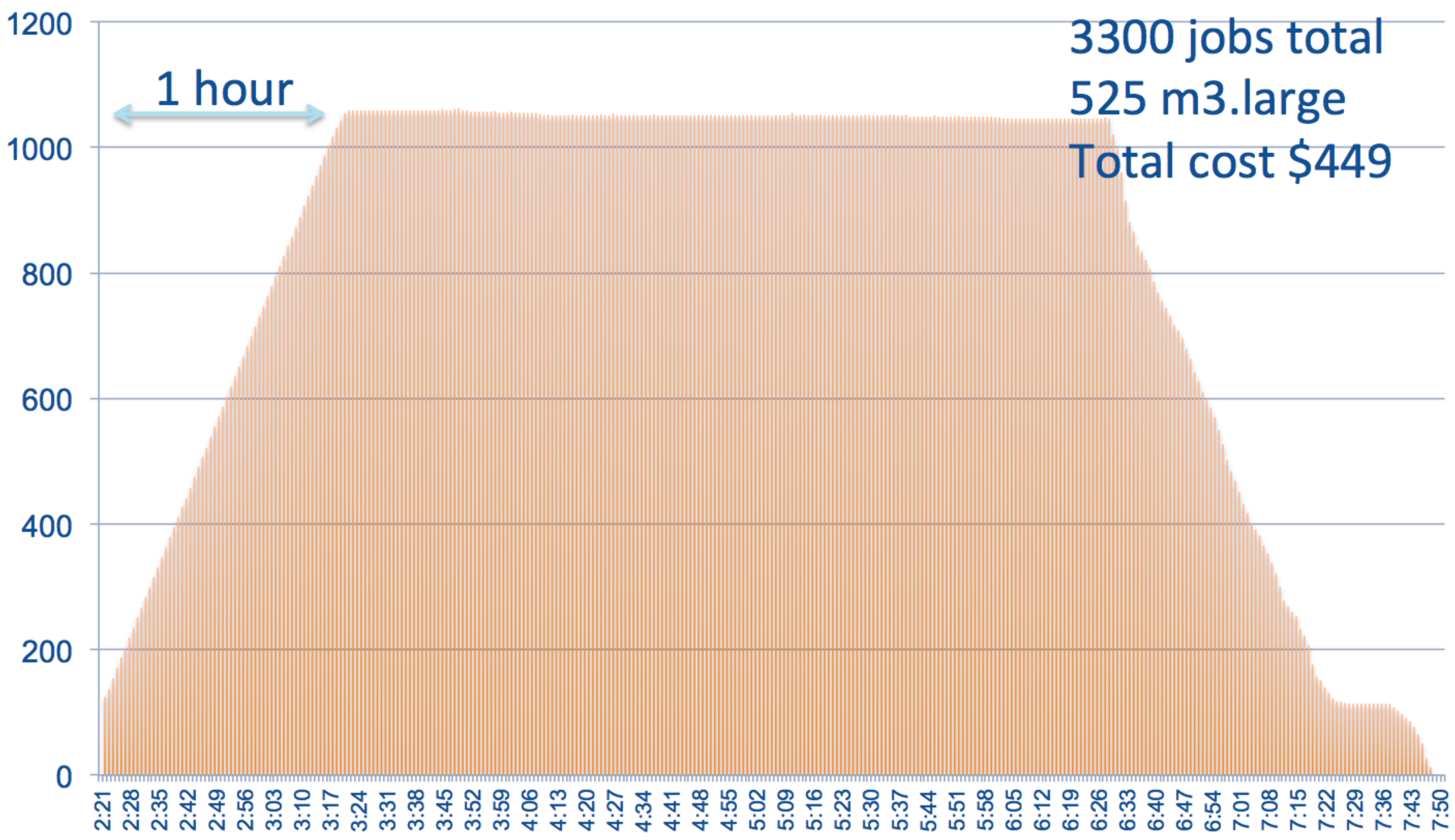
- Cost of 1 CPU h at AWS compared to to our facility costs (order of magnitude):
  - AWS 1 vCPU regular instance (m3.medium) per core ➜ ~ $0.07
  - BNL 2013 estimate at RACF* per core ➜ ~ $0.04
  - Fermilab 2011 estimate at FermiCloud per core ➜ ~ $0.03
  - AWS 1 vCPU spot pricing (m3.medium) per core ➜ ~ $0.01

T. Wong at HEPiX Fall 2013: "Operating Dedicated Data Centers - Is it cost-effective?"

- To exploit elasticity need detailed understanding of cost model
  - Benchmarks of our workflows very important
  - Detailed understanding of characteristics of our workflows helps optimizing costs
    - Example: HEP applications can deal with arbitrary number of cores if memory and local disk is large enough ➜ industry prefers resources with fewer cores
- Integration challenges:
  - Reliable comparison of provider's unit computation core (e.g. AWS ECU) and "standard" Grid equivalent (e.g. HS06)
  - Determine metrics for cost model, for example: I/O characteristics, service needs, data volumes, etc.

Scale test example

- Test to run at scale on both owned and rented resources
  - Results obtained through a 3-years collaboration with the Korean Institute of Science and Technology Information (KISTI)
- Up to 1000 jobs run simultaneously on each AWS and FermiCloud at Fermilab
  - Compute charges $398 ($0.14 per machine/hr), 525 VM's
  - $51 of data transfer charges.
- Lessons learned
  - Commercial clouds charge for outgoing data transfers!
    - Needed to optimize jobs to reduce data transfer charges
  - Jobs need services to run!
    - Naive model using services provided externally has its limit
    - First trial overloaded the CVMFS stratum 1 infrastructure at Fermilab



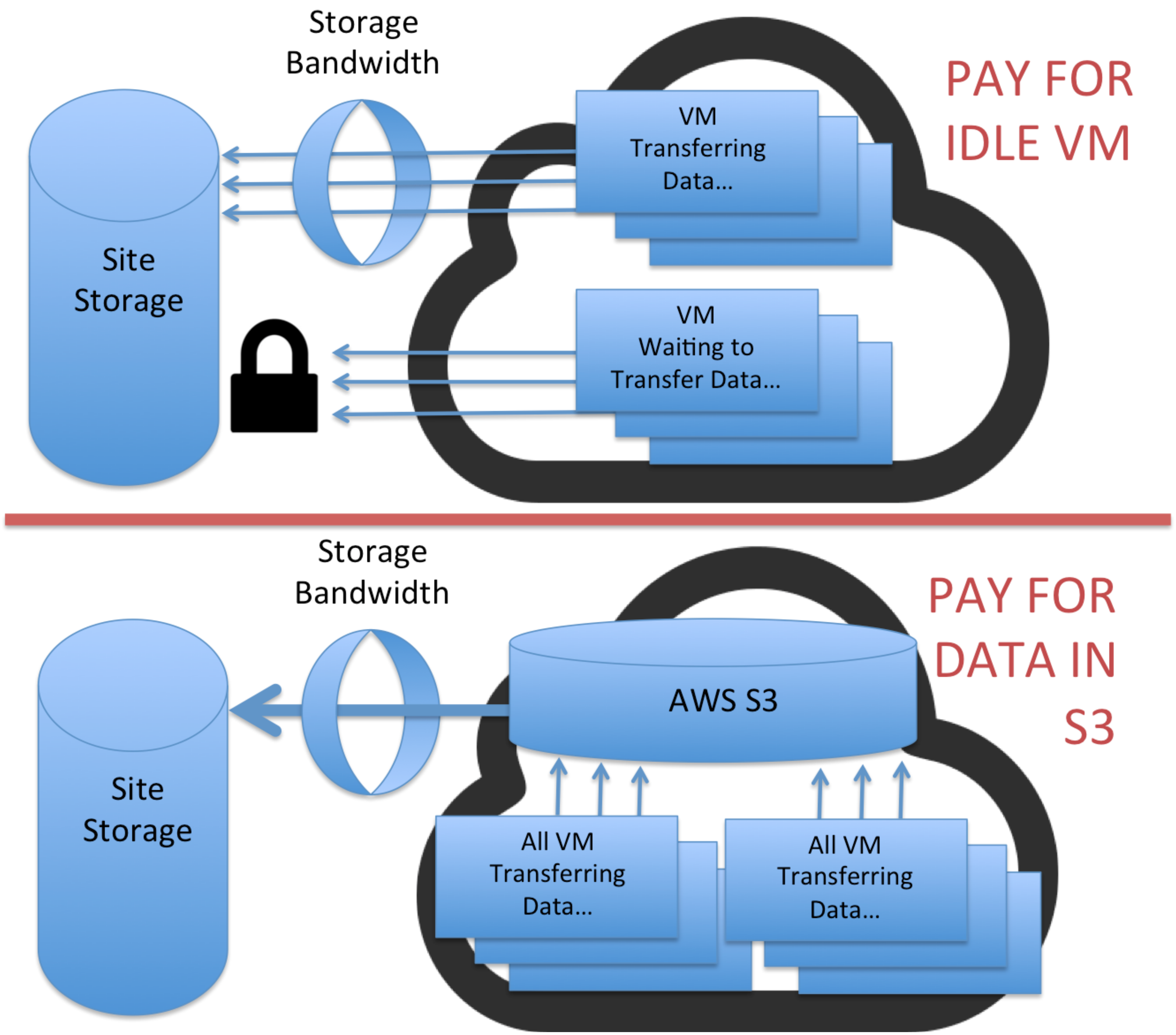
NOvA use case:

* Parag Mhashlikar: "Cloud services for the Fermilab scientific stakeholders", parallel talk in track 7 on Thursday

* Andrew Norman: "Large Scale Monte Carlo Simulation of neutrino interactions using the Open Science Grid and Commercial Clouds", poster session A

Storage

- Optimization of storage interaction of our workflows is crucial
  - Outgoing network bandwidth capacity is limited and needs to be payed for
- 2 main strategies for data transfers
  - Fill the available network transfer by having some jobs wait ➜ **Pay for idle resources**
  - Store data inside cloud (AWS: S3) and transfer data back asynchronously ➜ **Pay for data in S3**
- R&D will be necessary to optimize storage interaction
  - The cheapest strategy depends on the storage bandwidth, number of jobs, etc.

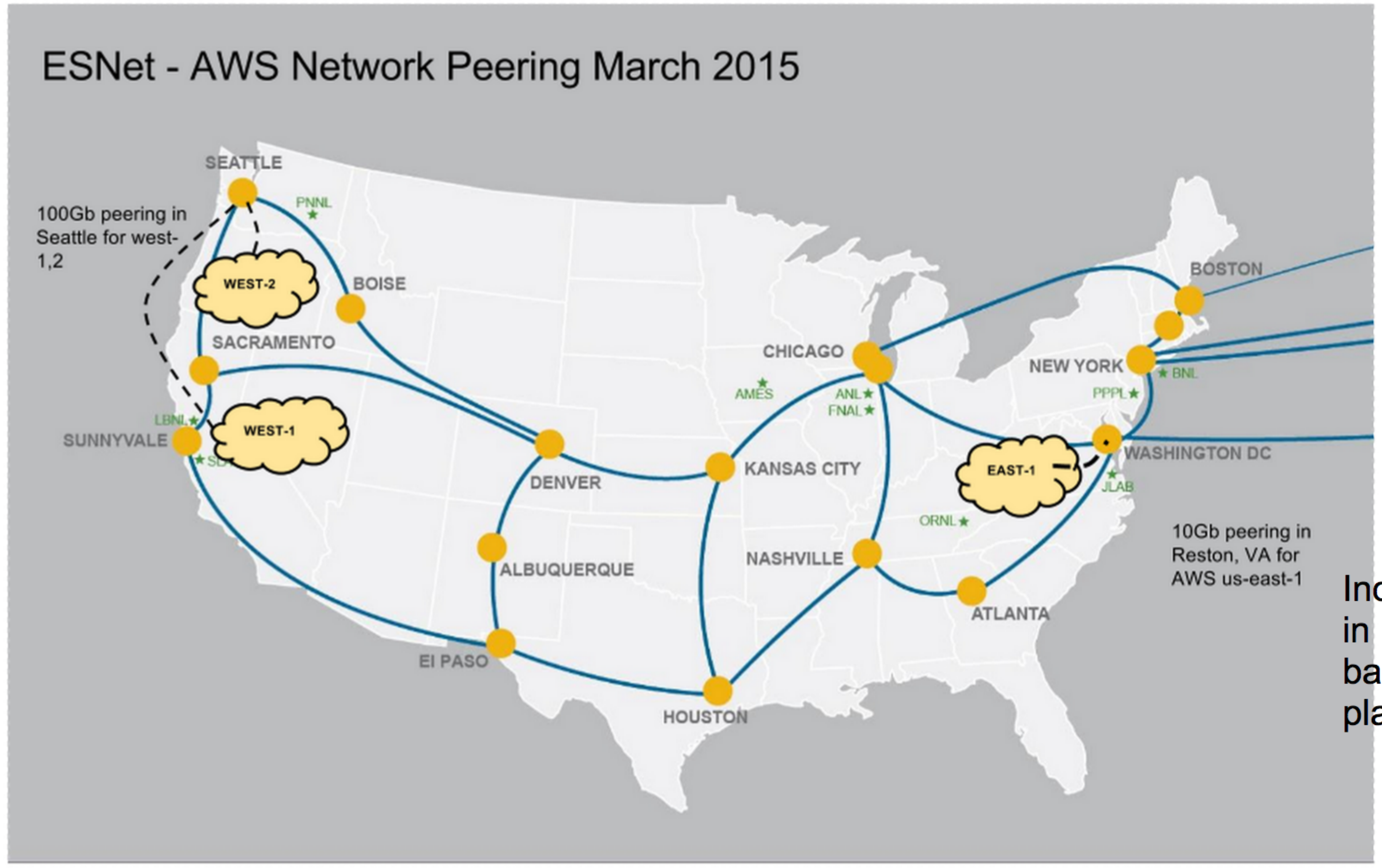


Networking

- Attack data transfer costs from a different angle

- Implement peering of our scientific networks directly with AWS infrastructure
  - Utilize upfront investments in scientific networks
  - Example: ESNet peering with AWS availability zones in the US

- AWS / ESNet data egress cost waiver
  - Transfer charges are waived for data costs up to 15% of the total bill - if network transfer goes exclusively through ESNet



European GEANT peering on the way.

Increases in East bandwidth planned.

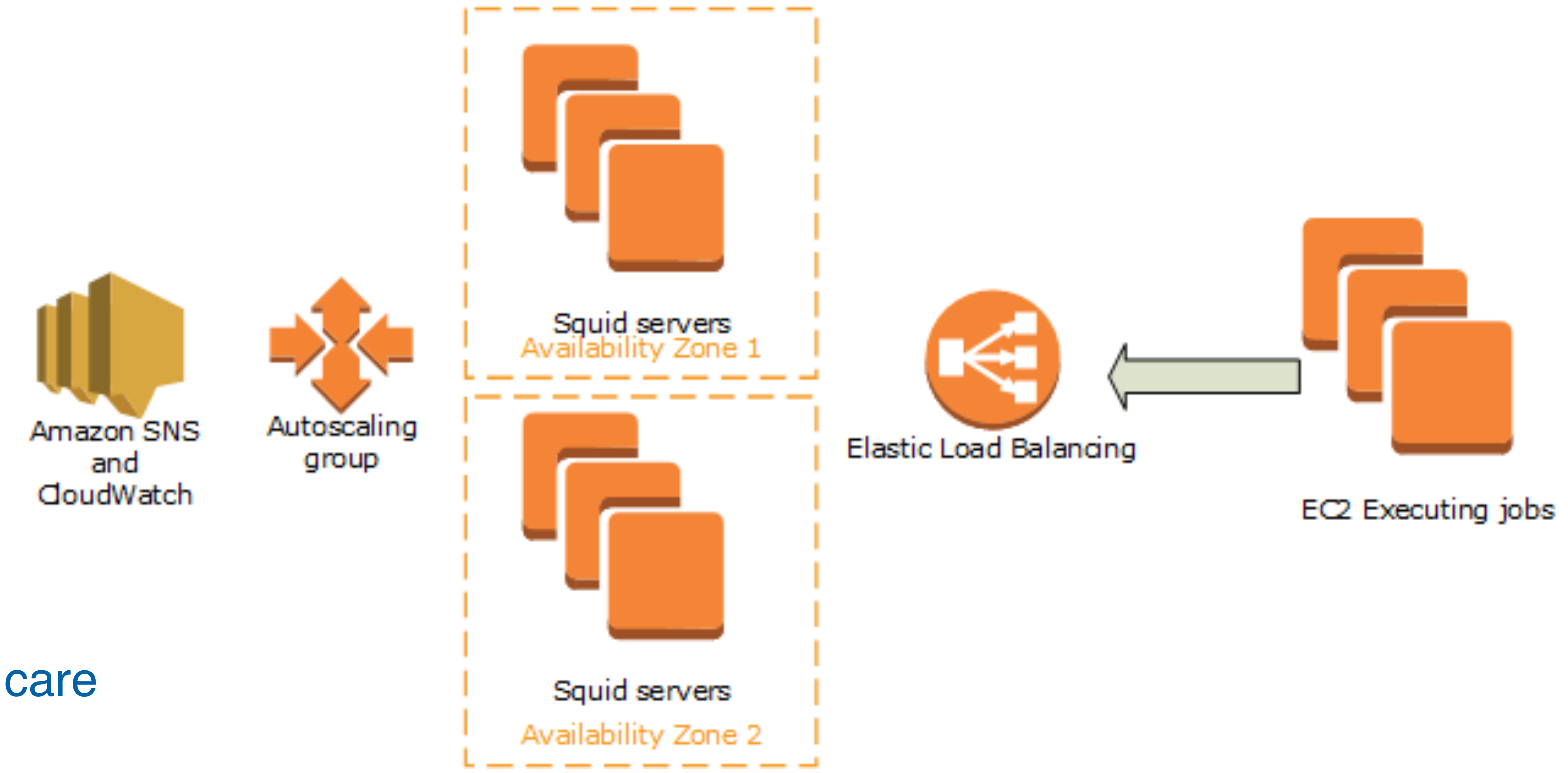
John Hover at HEPiX Spring 2015: "Running ATLAS at scale on Amazon"

On-demand Services

- Jobs depend on services to run, they can be deployed
  - at sites outside the clouds
  - inside the cloud

- In both cases, they have to be dimensioned correctly to scale sufficiently
  - Services include data caching (e.g. Squid) WMS , submission service, data transfer, software delivery (e.g. CVMFS stratum 1), etc.

- Automating the deployment of these services on-demand in clouds enables scalability and cost savings ➜ active area of R&D
  - Use classical scaling techniques using service discovery, central name service, centrally controlled additions/removal
  - Clouds provide their own orchestration layers (for example AWS CloudFormation) which take care of on-demand scaling even more efficiently



Next Step: Educational Grants from Amazon

- Amazon currently works with different experiments/institutes to bring HEP use of Cloud resources to reliable, production use
  - Atlas is currently leading this area, CMS and Intensity Frontier are utilizing own grants
- Example grant for Intensity Frontier experiments at Fermilab:
  - Run data-intensive NOvA applications and Neutrino Beam Simulations on AWS
  - Considering adding other use cases from Intensity frontier experiments
- To put this test into context
  - FermiGrid (without CMS resources) has capacity of 145 million hours/year
    - NOvA alone ran 10.2 million hours in 2014
  - Total expected AWS usage for this test: 2.1 million hours (100x 2014 test)
- Tests are continuously being increased in scale
  - Explore limits of elasticity and overcome them

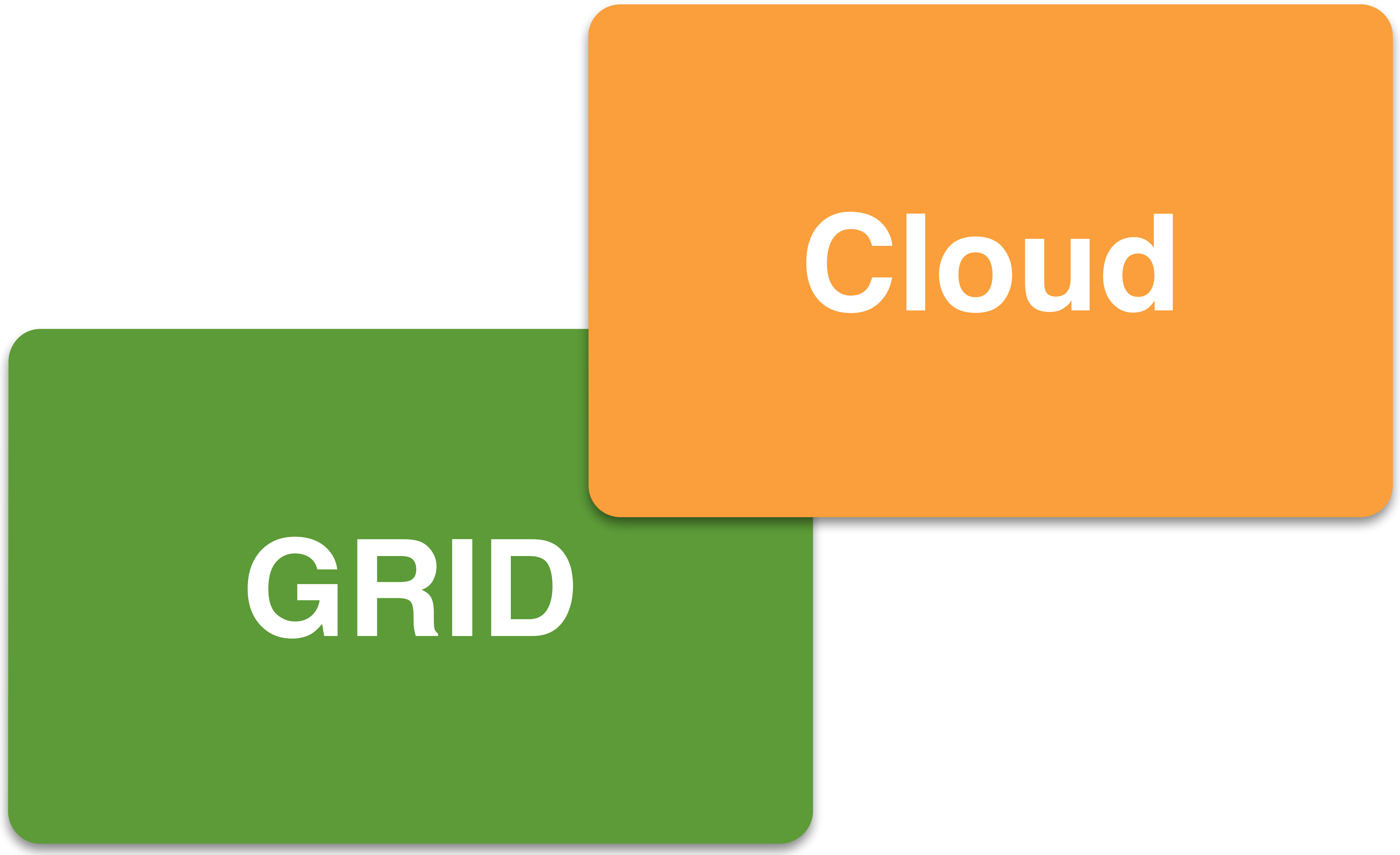
AWS Spot Price Market

- To be able to use the spot market efficiently, applications need to be "preempt-able" in one way or another
  - spot price market instances are being shut down within X minutes when market price goes above bid ➜ goal is to minimize loss of work and maximize efficiency

- Solutions are being worked on
  - Simplest solution is to shorten the processing time of jobs, accept efficiency losses and resubmit jobs
  - Atlas accelerated their work on the Atlas Event Service:
    - This service permits a pilot job to perform units of work smaller than a full ATLAS job, e.g. about 10 minutes.
      - Intermediate results are stored in an object store.
      - These are later merged to create final output (identical to what would have resulted from a full-length job).
      - Intermediate objects can be discarded.

John Hover at HEPiX Spring 2015:
"Running ATLAS at scale on Amazon"

Evolution of the Grid site



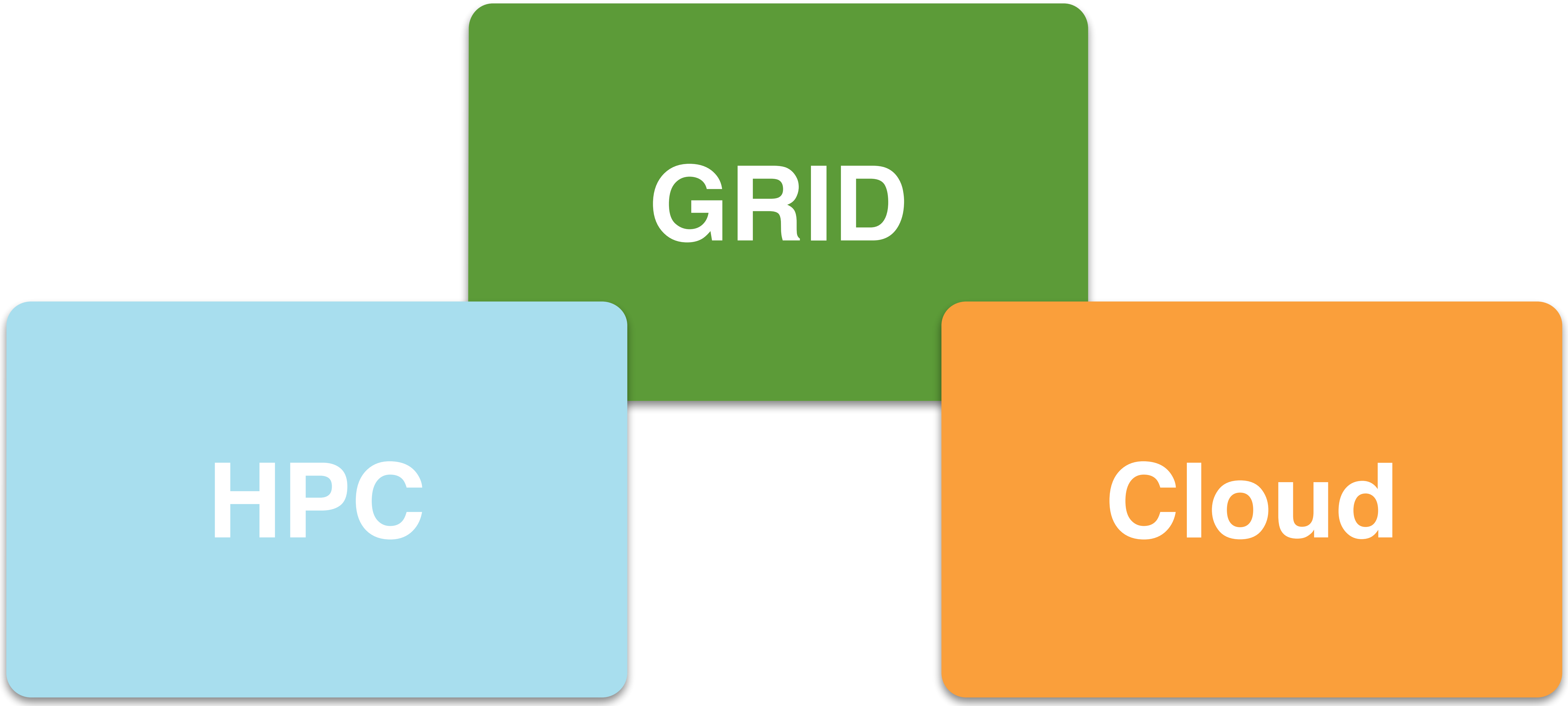
Virtual Facility

- Not only experiments can benefit from the elasticity promise of commercial clouds

- Grid sites are starting to rethink their current setup
  - Instead of only static allocations, provide ability to dynamically expand resources depending on resource needs of users
  - Provide needed resources for users without provisioning owned resources for peak
    - Optimize balance between owned resources and “rented” resources
  - This will be an intense area of R&D in the near-term future

- Sites could start providing “complete solutions” for their users
  - CPU capacity with guaranteed level of service
    - Users would not have to care about wether their jobs are running on “owned” or “rented” resources
    - Sites could make the economic decision themselves and optimize their cost structure
  - Storage services that adapt to where the jobs are running
  - On-demand auto-scaling services

Transparent access for the Science Community



Open Science Grid

- Created out of the goal to share the LHC experiments' Grid infrastructures and other Experiment/University/Lab infrastructures in the US amongst all HEP sciences and beyond

- Major clusters at Universities & National Labs connected to the
  - Sharing policy is locally controlled.
  - All owners want to share to maximize the benefit to all.

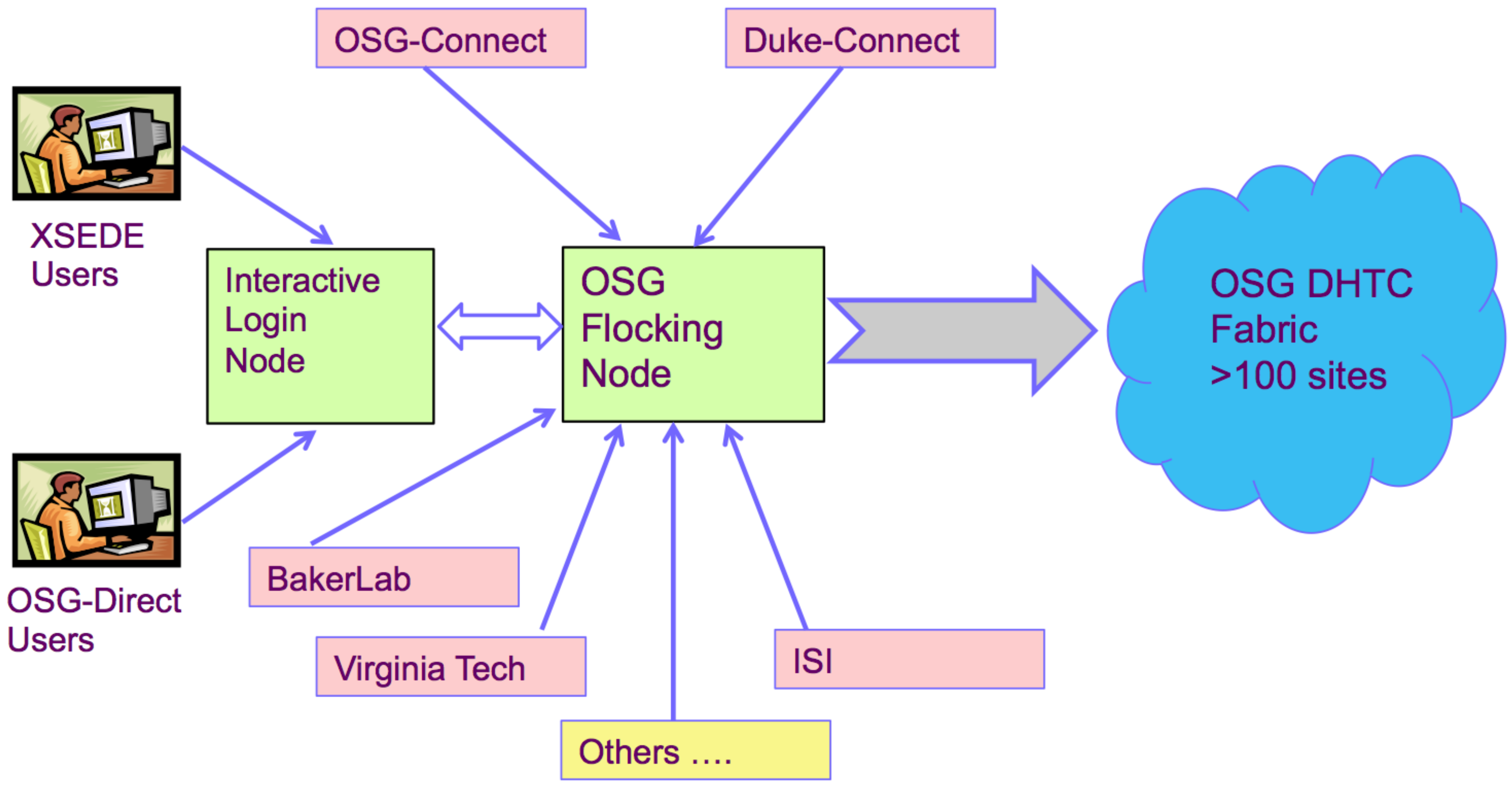
- Researcher use a single interface to use resources …
  - ... they own
  - ... others are willing to share
  - ... they have an allocation on
  - ... they buy from a commercial (cloud) provider

- OSG focuses on making this technically possible for Distributed High Throughput Computing
  - Operate a shared Production Infrastructure ➜ Open Facility (glideinWMS)
  - Advance a shared Software Infrastructure ➜ Open Software Stack
  - Spread knowledge across Researchers, IT professionals & Software developers ➜ Open Ecosystem

from: OSG All-Hands Meeting March 2015: Executive Director's Update

How the Open Science Grid is used

- Single PI Perspective
  - OSG-Connect:
    - OSG operates login node, disk space, application software repo, and provisions resources across the facility for single PIs and small groups
  - OSG-XD
    - ~same functionality, but users are being redirected to OSG from HPC allocation committees (XSEDE)
- IT Organization Perspective
  - Universities/Labs use OSG technologies to “flock” local work to the OSG
- Large Scale Research Community Perspective
  - LHC experiments and other large VOs use the OSG directly



from: OSG Annual Report to DOE & NSF (March 2015)

Summary & Outlook

- Resource landscape for HEP is changing
  - GRID is augmented by
    - Cloud
    - HPC
- Cloud
  - Integration challenges are being worked on by many and it is exciting to see the progress
  - What we should look out for:
    - When are the regular commercial Cloud resources becoming competitive?
    - How will we be able to benefit from the spot price markets?
- HPC
  - Interesting solution for specific problems in HEP computing
    - Or maybe for more?
- Future of the Virtual Facility?
- How will other sciences continue to benefit from HEP's large scale computing experience?

Questions

Grid	Cloud	HPC
▪ **Pledges** ◉ **opportunistic resources**	▪ **Pay-As-You-Go**	▪ **Allocations**
Trust Federation	**Economic Model**	**Grant Allocation**

- Grid, Cloud and HPC have different resource allocation models
- The question:
  - How can we integrate these three different models?
  - Do we have to evolve the static allocation model we are used to?

Acknowledgements

- Many thanks for the invitation to the CHEP organizing committee.
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  - Stuart Fuess, Burt Holzman, John Hover, Bo Jayatilaka, Jim Kowalkowski, Ruth Pordes, Panagiotis Spentzouris, Steve Timm, Margaret Votava, Frank Würthwein