Grid computing using

Open Science Grid

Alina Bejan
University of Chicago

Grid computing

- Aims to "*enable resource sharing and coordinated problem solving in dynamic, multi-institutional virtual organizations*"

  (Foster, Kesselman)

- Grids provide a distributed computing paradigm / infrastructure that spans VOs, with the goal of *enabling federated resource sharing in dynamic* distributed environments

How grids operate

- Use federated resources (commodity machines):
  - Compute
  - Storage
  - Network
- These resources are:
  - Heterogeneous
  - Dynamic
  - Geographically distributed

Different computational models

- Supercomputers
  - Tightly coupled massively parallel applications
  - Expensive, hard to get to
  - Use MPI, PVM
- Cluster computing
  - Involves homogenous machines interconnected by high speed network with locally accessible storage in one administrative domain
  - Also leverages cheaper commodity computing and storage hardware
- Grid computing
  - Integrating existing distributed resources, pertaining to different organizations, running different platforms
  - Suitable for loosely coupled applications

Open Science Grid (OSG)

- takes High Throughput Computing to the next level, to transform data-intensive science through a cross-domain, self-managed nationally distributed cyber-infrastructure.
- brings together campuses and communities, and facilitates the needs of Virtual Organizations at all scales.
- The OSG Consortium includes
  - universities
  - national laboratories
  - scientific collaborations
  - software developers

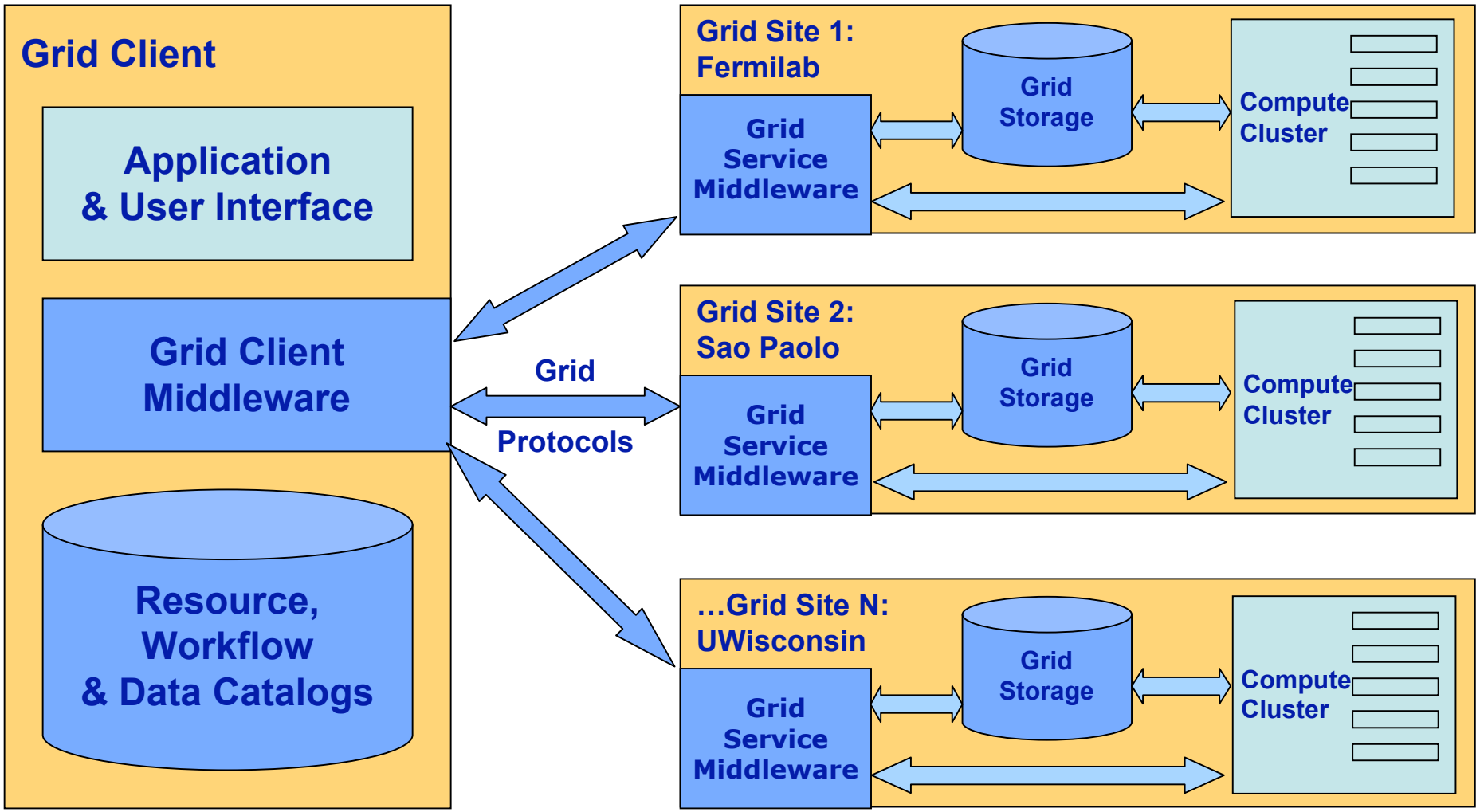
working together to meet these goals

What is a grid?

- Grid is a system that:
  - coordinates resources that are *not subject to centralized control*,
  - using standard, *open*, general-purpose protocols and interfaces,
  - to deliver nontrivial qualities of *service*

(based on Ian Foster's definition in http://www.gridtoday.com/02/0722/100136.html)

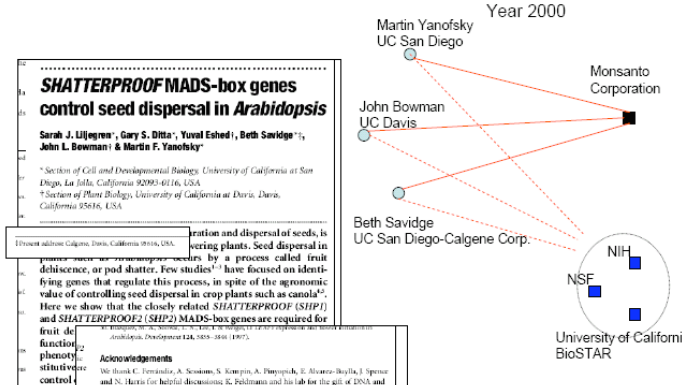
Grids consist of distributed clusters

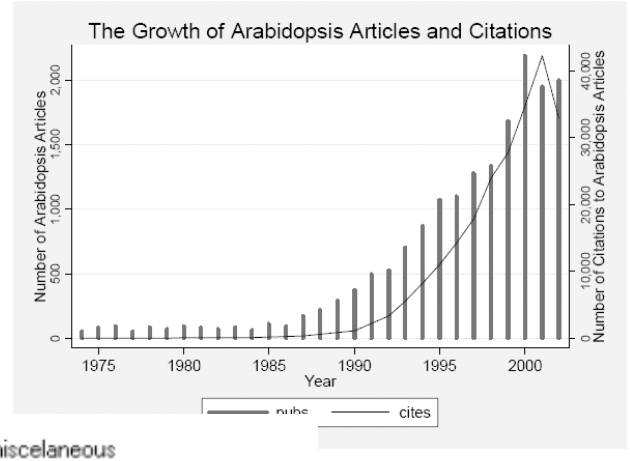


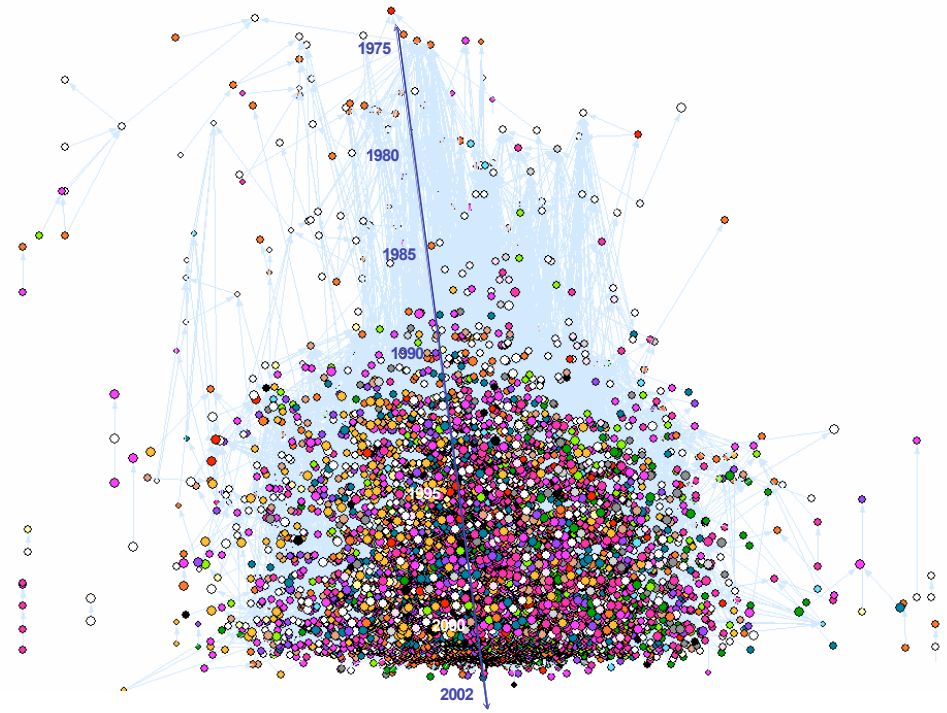
Why grids ?

- An example as motivation …

Scaling up Science: Citation Network Analysis in Sociology







- miscelaneous
- transcription factors / morphogens
- receptors
- phosphosphorylation cascades
- organogenesis
- terpines, synthesis
- physical defense
- commercial disease resistance
- innate immunology
- nutrient metabolism and movement
- nutrient uptake
- genomics
- photosynthesis
- functional enzymatics
- protein isolation & characterization
- targeting / splicing
- tropisms

Work of James Evans, University of Chicago, Department of Sociology

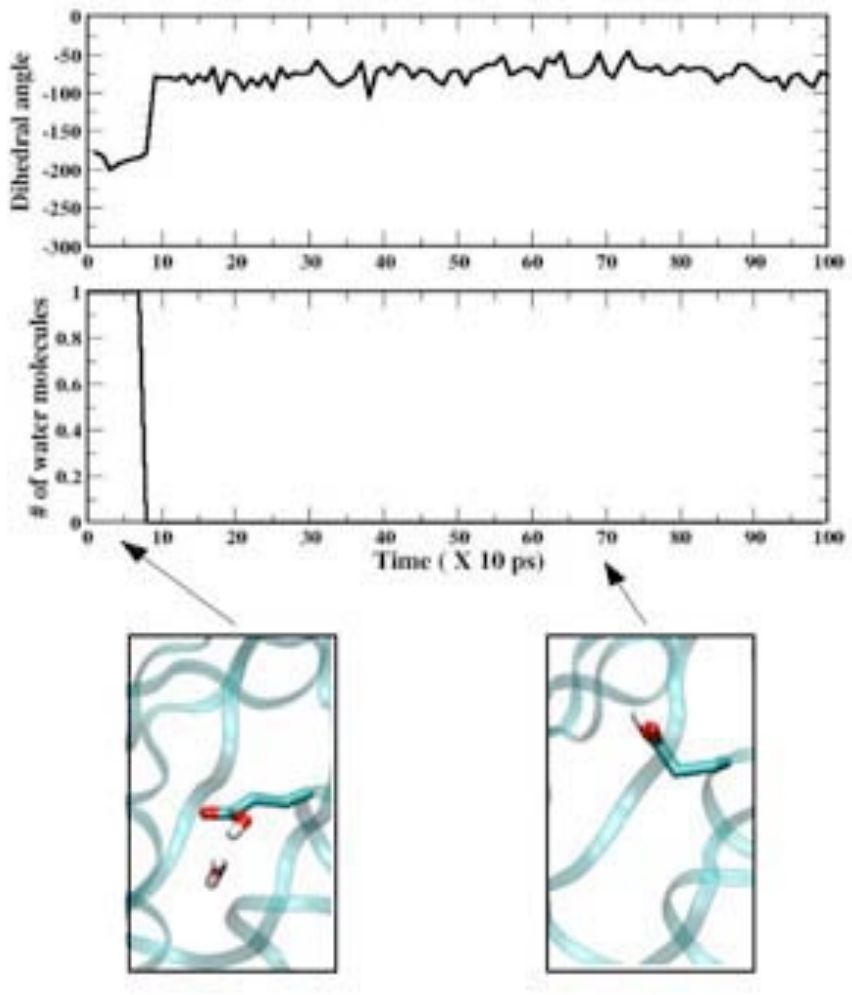
Scaling up the analysis

- Query and analysis of 25+ million citations
- Work started on desktop workstations
- Queries grew to month-long duration
- With data distributed across U of Chicago TeraPort **cluster**:
  - 50 (faster) CPUs gave 100 X speedup
  - Many more methods and hypotheses can be tested!
- Higher *throughput* and *capacity* enables *deeper analysis* and *broader community access*.

Grids work like a CHARMM for molecular dynamics

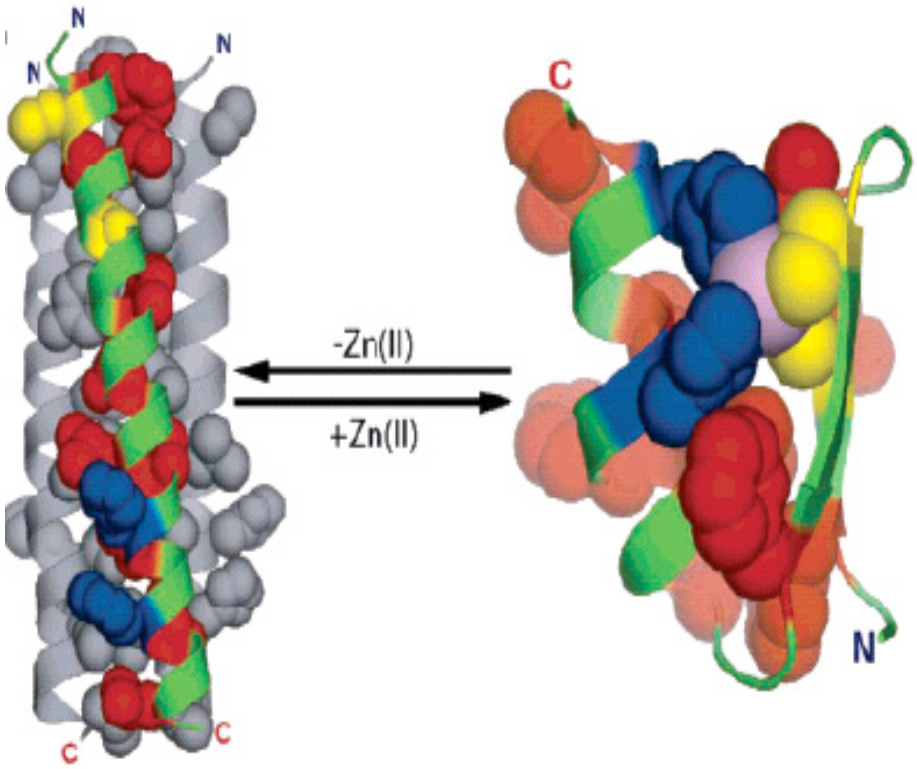
- Understanding the mathematics of molecular movement helps researchers simulate slices of the atomic world

- But when accurate nanosecond simulations pose a serious challenge, how can you simulate full microseconds of complex molecular dynamics?



Designing Proteins from Scratch

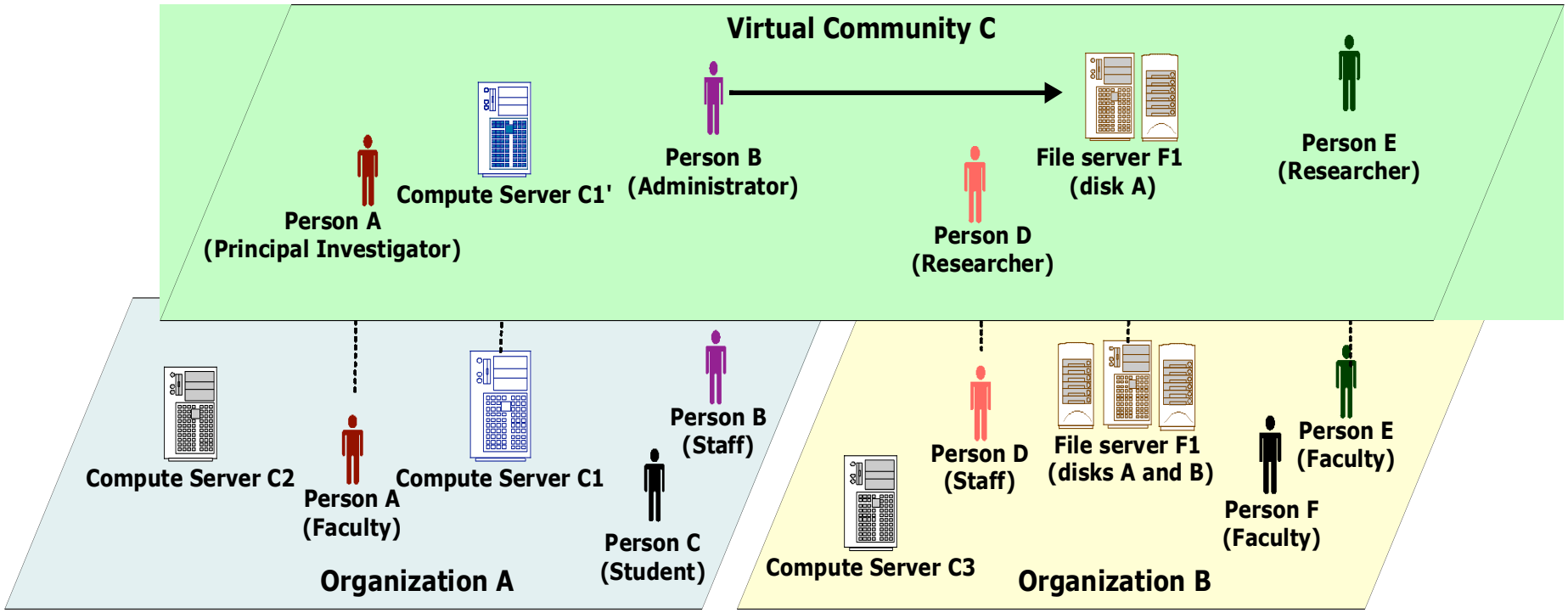
- Scientists use OSG to design proteins that adopt specific 3D structures and more ambitiously bind and regulate target proteins important in cell biology and pathogenesis



Which sciences can benefit ?

- particle and nuclear physics
- astrophysics
- bioinformatics
- gravitational-wave science
- computer science
- mathematics
- medical imaging
- nanotechnology
- *potentially any other science …*

Virtual Organization (VO) Concept



- Logical entity
- Members share the resources as if they belong to same organization

- Research Participation
  - Majority from physics : Tevatron, LHC, STAR, LIGO.
  - Used by 10 other (small) research groups.
  - 90 members, 30 VOs,
- Contributors:
  - 80 sites / 50 organizations
  - 5 DOE Labs : BNL, Fermilab, NERSC, ORNL, SLAC.
  - 65 Universities.
  - 5 partner campus/regional grids.
- Accessible resources:
  - 43,000+ cores
  - 6 Petabytes disk cache
  - 10 Petabytes tape stores
  - 14 internetwork partnership
- Usage
  - 15,000 CPU WallClock days/day
  - 1 Petabyte data distributed/month.
  - 100,000 application jobs/day.
  - 20% cycles through resource sharing, opportunistic usage.

The OSG project research

Has two components:

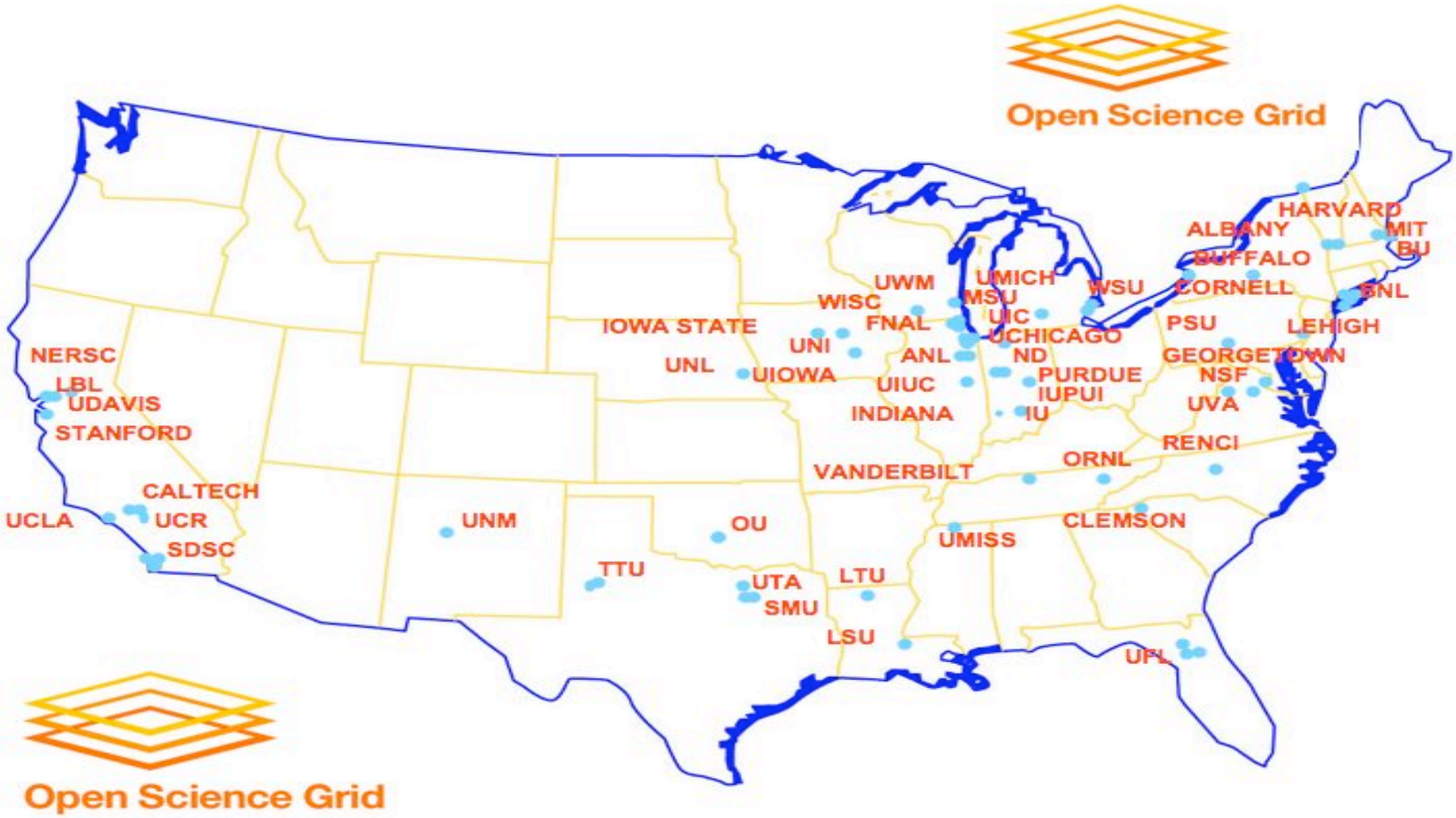
- To enable scientific discovery by providing a state of the art production distributed infrastructure for *science*

- To advance the state of the art in distributed computing through *experimental computer science* through a large scale production quality distributed system

OSG's grids

- *Grids can be*
  - *Campus, Community, Regional, National, International*
- *OSG scope includes bridging, and interfacing between them*

OSG sites

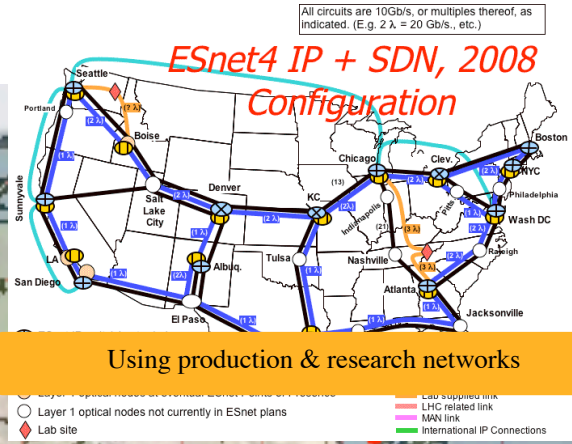

Open Science Grid
HARVARD
ALBANY
MIT
BU
BUFFALO
CORNELL
BNL
UWM
UMICH
WSU
MSU
WISC
UIC
FNAL
IOWA STATE
UCHICAGO
PSU
LEHIGH
UNI
ANL
ND
GEORGETOWN
NERSC
UNL
UIOWA
PURDUE
NSF
LBL
UIUC
IUPUI
UDAVIS
INDIANA
IU
UVA
STANFORD
RENCI
ORNL
VANDERBILT
CALTECH
UCLA
UCR
UNM
OU
CLEMSON
UMISS
SDSC
TTU
LTU
UTA
SMU
LSU
UFL
Open Science Grid

OSG Snapshot

96 Resources across
production & integration infrastructures

Sustaining through OSG submissions:
3,000-4,000 simultaneous jobs .
~100K jobs/day
~50K CPUhours/day.
Peak test jobs of 15K a day.

~30,000 CPUs (from 30 to 4000)
~6 PB Tapes
~4 PB Shared Disk



Using production & research networks

Snapshot of Jobs on OSGs

Farm	Last value	Min	Avg	Max
ATLAS	259	0	338.8	1516
CDF	1278	0	336.6	2086
CMS	579	0	439	3733
DES	39	0	0.385	40
DOSAR	25	0	9.93	192
FERMILAB	4	0	21.38	192
GADU	0	0	23.84	730
GLOW	0	0	35.44	541
GRIDEX	29	0	20.36	268
GROW	41	0	1.434	111
IVDGL	0	0	0.852	73
KTEV	35	0	15.52	260
LIGO	13	0	2.539	88
MINIBOONE	1053	0	128.7	1254
MIPP	2	0	15.32	206
MIS	0	0	0.269	20
NANOHUB	99	0	26.83	187
OPS	2	0	0.017	3
OSG	0	0	0.226	11
SDSS	33	0	3.941	199
STAR	38	0	12.77	150
Total	**3529**		**1434**	

30 Virtual Organizations +6 operations
Includes 25% non-physics.

Globus and Condor play key roles

- Globus Toolkit provides the base middleware
  - Client tools
  - APIs (scripting languages, C, C++, Java, …) to build your own tools, or use direct from applications
  - Web service interfaces
  - Higher level tools built from these basic components, e.g. Reliable File Transfer (RFT)
- Condor provides both client & server scheduling
  - In grids, Condor provides an agent to queue, schedule and manage work submission

To efficiently use a Grid, you must locate and monitor its resources.

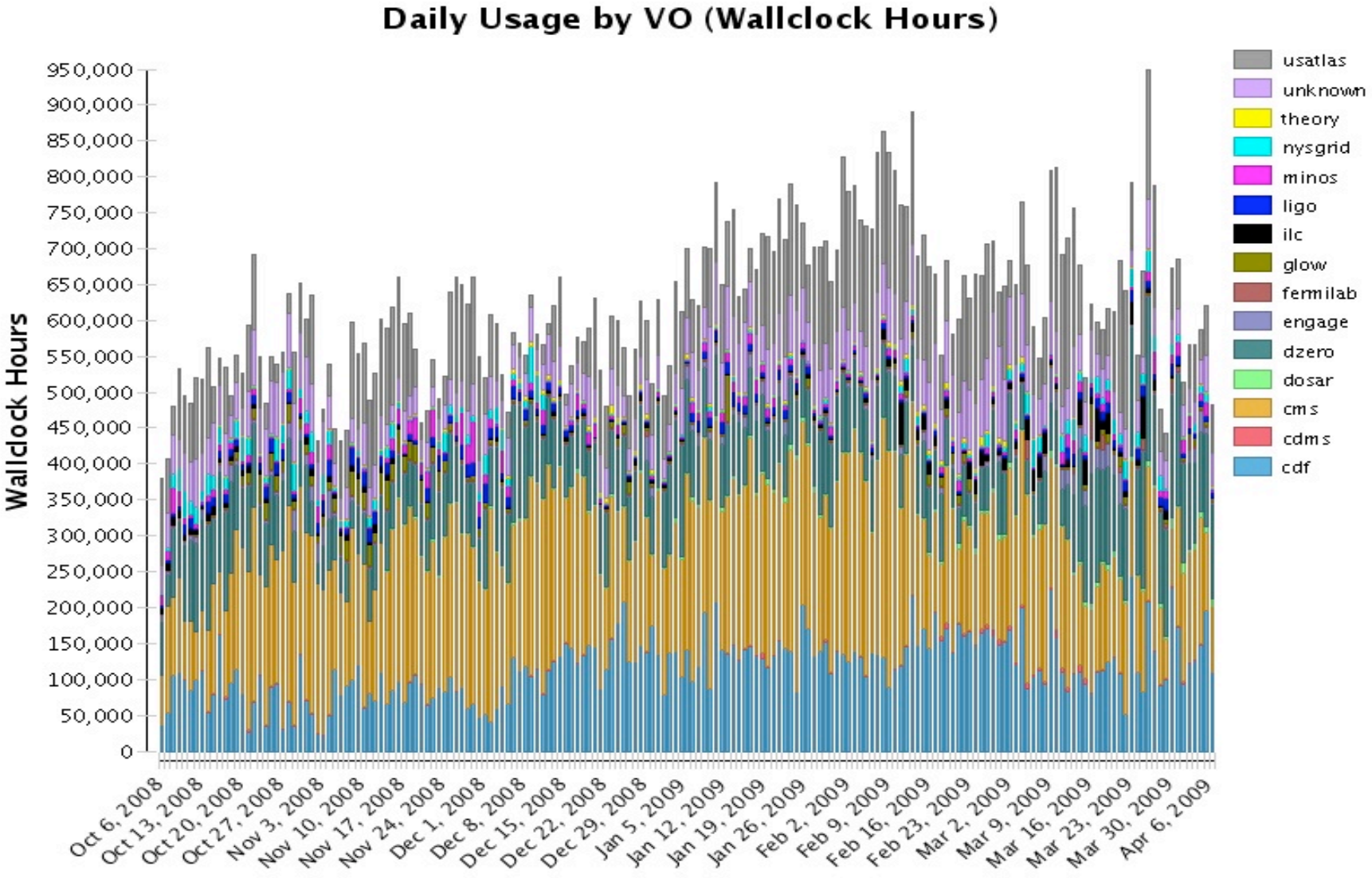
- Check the availability of different grid sites
- Discover different grid services
- Check the status of “jobs”
- Make better scheduling decisions with information maintained on the “health” of sites
- GIS: VORS -> myOSG

Example:
Virtual Organization Resource Selector - VORS
http://vors.grid.iu.edu/

- Custom web interface to a grid scanner that checks services and resources on:
  - Each Compute Element
  - Each Storage Element
- Very handy for checking:
  - Paths of installed tools on Worker Nodes.
  - Location & amount of disk space for planning a workflow.
  - Troubleshooting when an error occurs.

Gratia -- job accounting system

http://gratia-osg.fnal.gov:8880/gratia-reporting/



Conclusion: Why Grids?

- New approaches to inquiry based on
  - Deep analysis of huge quantities of data
  - Interdisciplinary collaboration
  - Large-scale simulation and analysis
  - Smart instrumentation
  - ***Dynamically assemble the resources to tackle a new scale of problem***
- Enabled by access to resources & services without regard for location & other barriers

Grids:
Because Science needs community …

- Teams organized around common goals
  - People, resource, software, data, instruments…
- With diverse membership & capabilities
  - Expertise in multiple areas required
- And geographic and political distribution
  - No location/organization possesses all required skills and resources
- Must adapt as a function of the situation
  - Adjust membership, reallocate responsibilities, renegotiate resources

Getting Started with OSG

- I want to use OSG resources
- I want to get my application running on OSG
- I want information about adapting my campus IT facility to form a campus grid
- I want to federate or partner my grid with OSG
- I want to make resources available to OSG
- I want to help build OSG

I want to use OSG resources

- Must join a VO:
  - Individual/small for independent research
    - Join OSG VO
  - Join an existing member VO (see the list of current OSG VOs)
  - Form new VO for your research community
- Run VO specific applications

Want to get my app running on OSG

- Engagement team
  - Dedicated effort
  - Genetics, library science, earthquake simulation, video processing, physics; Examples:
    - Production running using 20,000+ CPU hours of the CHARMM molecular dynamic simulation to the problem of water penetration in staphylococcal nuclease using opportunistically available resources across 10+ OSG sites (see Grids work like a CHARMM for molecular dynamics)
    - Improvement of the performance of the nanoWire application from the nanoHub project on OSG/TeraGrid, such that stable running of batches of 500 jobs across more than 5 sites is routine; (see Keeping up with Moore's Law)
    - Adaptation and production running opportunistically using 100,000+ CPU hours of the Rosetta application from the Kuhlman Laboratory in North Carolina across more than 13 OSG sites (see Designing proteins from scratch)
    - Production runs of the Weather Research and Forecast (WRF) application using more 150,000 CPUhours on the NERSC OSG site at Lawrence Berkeley National Laboratory (LBNL)

Want to form a campus grid

- You have a campus IT facility
  - Want to make it a campus grid
  - And federate it with OSG
- OSG is committed to including US universities in the national cyberinfrastructure.
  - *The OSG middleware and operational framework enables any site to participate as an OSG resource, provided it is a well maintained resource that users can count on*
- Technically there are no hurdles in having every US university and college contribute resources to OSG and use OSG resources in return.
  - *See module on Thursday*
- Several campuses have done so very well: Purdue University, University of Wisconsin- Madison, and Clemson University
- Several other universities participate in OSG through individual research groups.

I want to federate or partner my grid with OSG

- OSG Consortium envisions a world-wide grid formed of a number of different federations of grids (analogous to the Internet as a network of networks)
- Federation, therefore, is a natural concept within OSG
- We are interested in *partnerships* with other grids trying to develop richer methods and tools for federation.

I want to make resources accessible to OSG

- Recommended that you join a VO
- Minimal requirements
  - sufficient to assure interoperability, stability
  - set of "standard" services which define the requirements on interfaces and capabilities.
- Register resource with GOC
  - *See module on Thursday*

I want to learn more about grids

- Join the Education VO
  - www.opensciencegrid.org/Education
  - eot@opensciencegrid.org
  - Account, cert
  - Online course
  - Experiment with job submissions

Thank you !

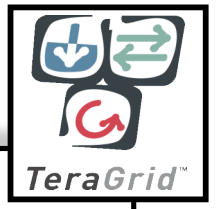
Questions ?

Grid Resources in the US

OSG

- Research Participation
  - Majority from physics : Tevatron, LHC, STAR, LIGO.
  - Used by 10 other (small) research groups.
  - 90 members, 30 VOs,
- Contributors:
  - 5 DOE Labs
    - BNL, Fermilab, NERSC, ORNL, SLAC.
  - 65 Universities.
  - 5 partner campus/regional grids.
- Accessible resources:
  - 43,000+ cores
  - 6 Petabytes disk cache
  - 10 Petabytes tape stores
  - 14 internetwork partnership
- Usage
  - 15,000 CPU WallClock days/day
  - 1 Petabyte data distributed/month.
  - 100,000 application jobs/day.
  - 20% cycles through resource sharing, opportunistic use.

TeraGrid



- Research Participation
  - Support for Science Gateways
  - over 100 scientific data collections (discipline specific databases)
- Contributors:
  - 11 Supercomputing centers

    Indiana, LONI, NCAR, NCSA, NICS, ORNL, PSC, Purdue, SDSC, TACC and UC/ANL
- Computational resources:
  - > 1 Petaflop computing capability
  - 30 Petabytes of storage (disk and tape)
  - Dedicated high performance internet connections (10G)
  - 750 TFLOPS (161K-cores) in parallel computing systems and growing