A Gentle Introduction to Grid Computing

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Acknowledgements

- Food provided courtesy of Grid.org and the Department of Computer Science.

GRID.org

- Some slides borrowed from Ian Foster.

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- How does this work?
- More than just a “virtual supercomputer”
- Applications on the Grid
- Globus Toolkit 4
- I want to know more!

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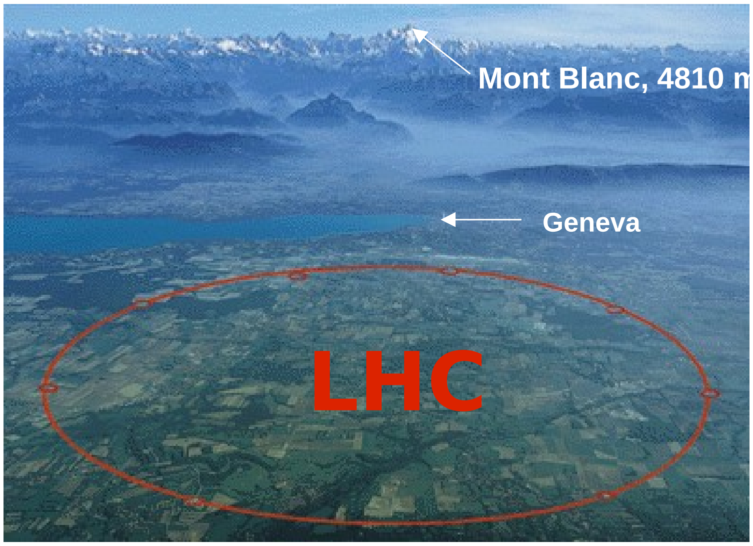
A problem... (I)

A problem... (II)

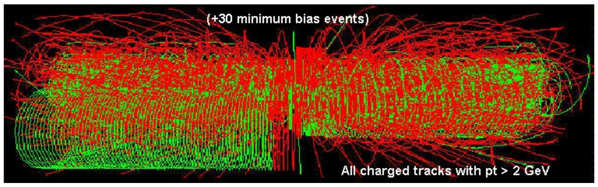


A problem... (III)

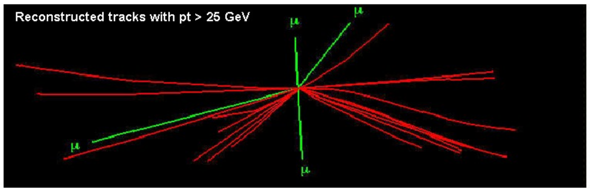
- The LHC (Large Hadron Collider), which is being built in CERN, is a particle accelerator/collider with a circumference of 27km (16.7mi).
- Will answer many interesting questions, specially: Does the Higgs boson exist?
- When it starts to work this year, it will produce *huge* amounts of information.

A problem... (IV)

From this event (1 event = 1 collision)...



We're searching for this characteristic signature:



1 in 10^{13}

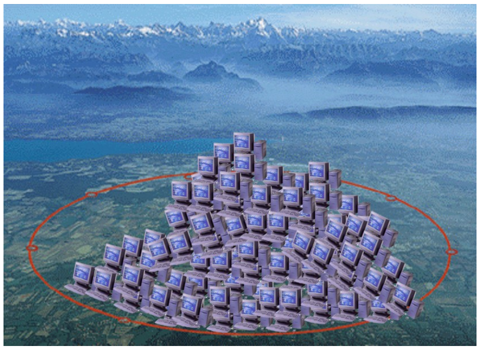
Like looking for one person in a thousand world populations.

A problem... (V)

- 40 million collisions per second (300 GB/s of data)
- These collisions are filtered, and only “interesting events” are kept.
  - ~300 MB/s (~25 TB/day!). This information requires a (non-trivial) processing, and must be stored for future reference and study.
- LHC will produce ~15 Petabytes of information per year.
  - 1000x of information published in books in a year.
  - 1% of all human-produced information in a year

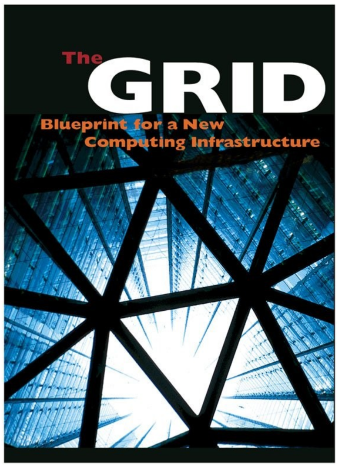
A problem... (VII)

- Using current technology, processing and storing all that data in a single site is impossible.
- An estimated 100,000 processors would be needed to deal with the LHC's computational needs.

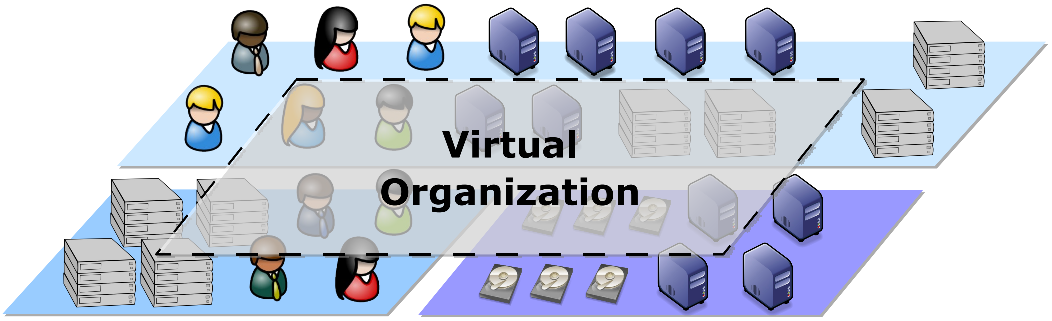


A solution

- Problem: A single node can't handle all that work.
    - But the combined power of *several* sites might be able to handle it.
- Solution: Achieving greater performance and throughput by pooling together resources from different organizations
    - Informally, this is what Grid Computing is all about (better definition coming up)



Virtual Organizations



- An organization can only use the resources it has under its control.
- Grid Computing involves multiple organizations.
- Resources from these organizations are dynamically pooled together, creating *virtual organizations*, to solve specific problems.

Easier said than done!

- How do we decide what resources are part of each virtual organization?
- Given a computational task, how do we decide what resources will be allocated to deal with that task? For how long?
- How do we get the resources to communicate amongst themselves? Take into account that these are *heterogeneous* resources from *different* organizations!
- If I want to "split up" a task so that it can be performed in parallel by several computers in different organization, how to I actually "split up" the program?
- A lot of security challenges. For example, how can an organization make sure its resources are only being used by trusted users and that they are not being abused by malicious users?

Why is this hard?

- No centralized control
  - We *cannot* and *do not* control the decisions of individual organizations. Grid Computing does not impose an all-powerful master that overrides local decisions.
  - We have to reconcile all the different policies in each site.
- Shared heterogeneous resources
  - We cannot assume that all resources are exactly alike (as we could assume in a computing cluster)
  - Resources appear and disappear on the grid.
- Communication and coordination
  - Different sysadmins, users, geo-political restrictions, etc.

A definition

- Ian Foster provides an (open) definition in the paper *What is the Grid? A Three Point Checklist.*
- A 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
- There is no “The Grid”, but there are many production “grids” around the world that support a wide variety of applications.

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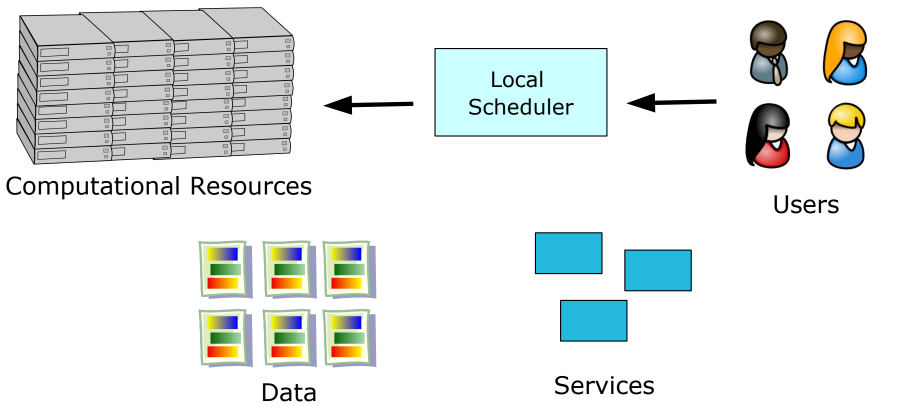
What a typical site could look like



Computational Resources

Local Scheduler

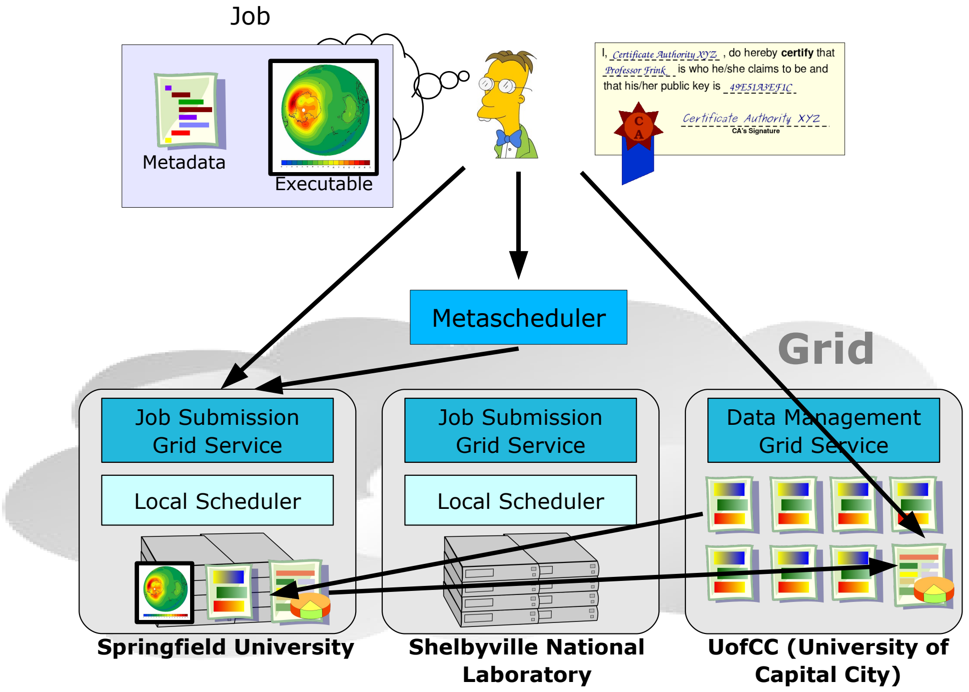
Users

Data

Services

- Example: UChicago has a cluster called Teraport (http://teraport.uchicago.edu/) that uses Torque/Maui as its local scheduler.

A typical interaction



I, Certificate Authority XYZ , do hereby **certify** that Professor Frink is who he/she claims to be and that his/her public key is 49E51A3EF1C

Certificate Authority XYZ
CA's Signature

Job
Metadata
Executable
CA
Metascheduler
Grid
Job Submission Grid Service
Local Scheduler
Job Submission Grid Service
Local Scheduler
Data Management Grid Service
Springfield University
Shelbyville National Laboratory
UofCC (University of Capital City)

The nuts and bolts

- The nuts and bolts of a grid system are mainly ***middleware***: networked services, protocols, sofware toolkits, etc.
- Standards for grid services:
  - Open Grid Services Architecture, developed by the Open Grid Forum (http://www.ogf.org/)
  - Standards from OASIS, W3C, IETF, ...
  - Many grid standards are still under development.
- ... and implementations:
  - Globus Toolkit (http://www.globus.org/)
  - gLite (http://cern.ch/glite)
  - UNICORE (http://www.unicore.eu/)

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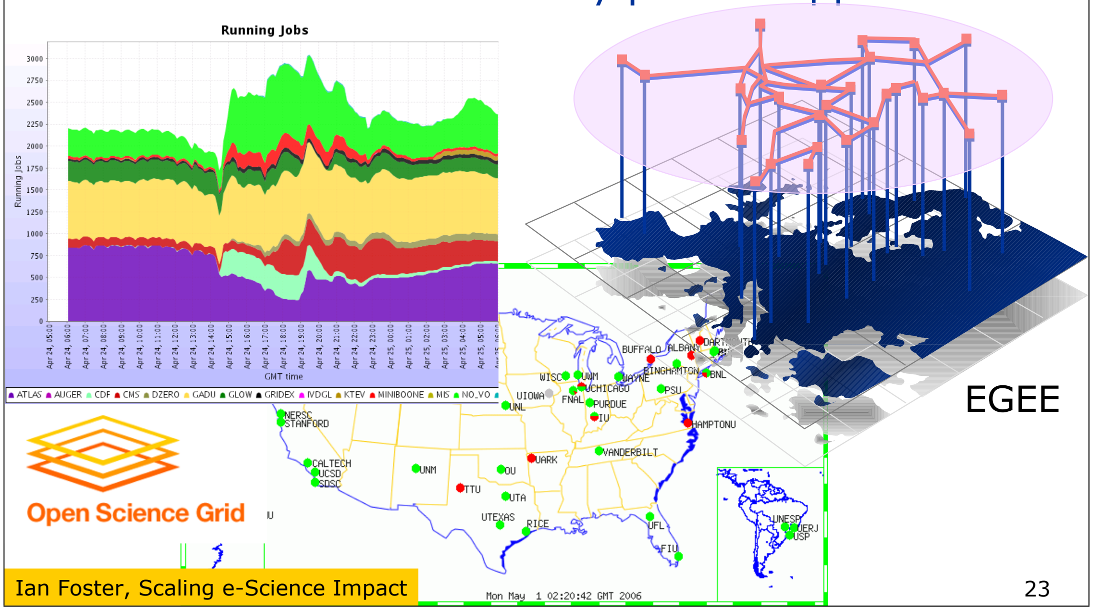
More than just a “virtual supercomputer”

- Grid Computing is sometimes characterized as creating a “virtual supercomputer”, capable of handling huge computations that cannot possibly be run on a single site (e.g., LHC)
- This is only one of the use cases for Grid Computing. There are many more.
- Grid Computing is not just about sharing computational power. A virtual organization also includes *services*, users, instruments, etc.
  - Service-Oriented Science (Ian Foster, Steve Tuecke, *The Many Faces of IT as Service;* Ian Foster, *Service-Oriented Science)*

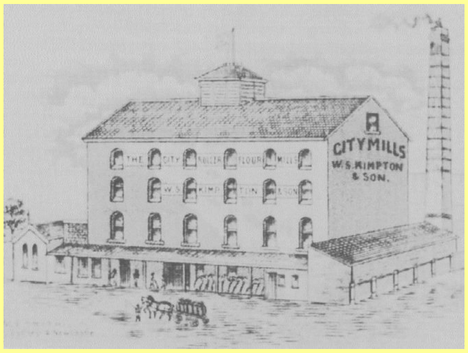
First Generation Grids

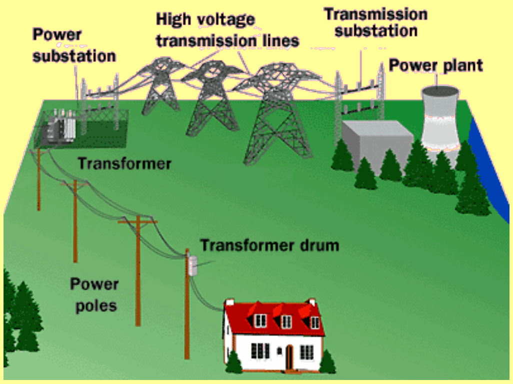
Focus on aggregating large amounts of resources for massively parallel applications



The original "electric grid" analogy

At first, we had to be close to electrical generators





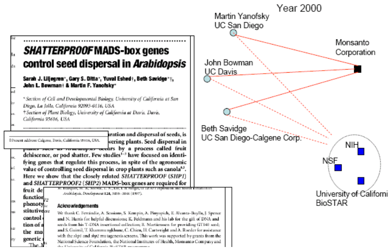
Now: the *electric grid* carries electricity from large producers to small consumers.

Can we do the same with computation?

Enabling e-Science

- Grid Computing can provide a “cyberinfrastructure” to projects that require...
  - ... analysis of large quantities of data, but are currently confined to running on a single site (or even a single computer!)
  - ... interdisciplinary and/or interorganizational collaboration.
  - ... dynamic reorganization of resources (possibly including instrumentation) to explore new experiment configurations.
- Allowing...
  - ... composition of new applications based on existing services.
  - ... existing systems to scale and test new hypothesis, explore more experiment configurations, etc.
  - ... users to focus on their applications, while grid software takes care of planning execution on remote sites (e.g., Swift: http://www.ci.uchicago.edu/swift/)

Scaling up Social Science: Citation Network Analysis



SHATTERPROOF MADS-box genes control seed dispersal in Arabidopsis

Sarah J. Liljegren*, Gary S. Ditta*, Yuval Eshed†, Beth Savidge*‡, John L. Bowman† & Martin F. Yanofsky*

* Section of Cell and Developmental Biology, University of California at San Diego, La Jolla, California 92093-0116, USA
† Section of Plant Biology, University of California at Davis, Davis, California 95616, USA

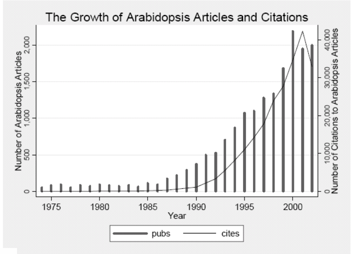
‡ Present address: Calgene, Davis, California 95616, USA.

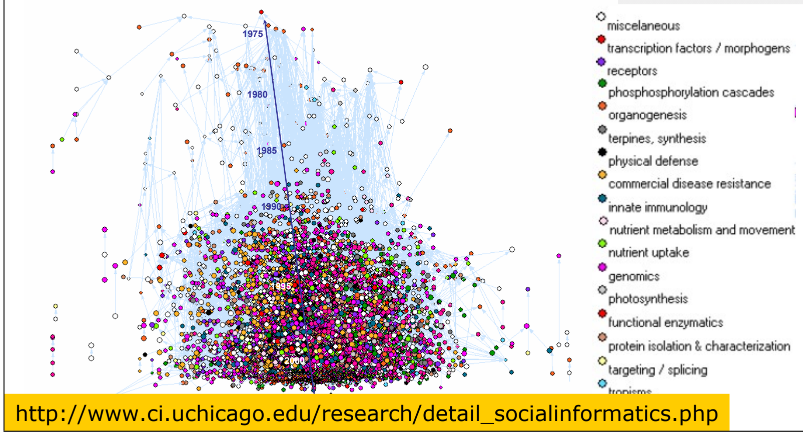
...ration and dispersal of seeds, is ...wering plants. Seed dispersal in ... occurs by a process called fruit dehiscence, or pod shatter. Few studies[1-3] have focused on identifying genes that regulate this process, in spite of the agronomic value of controlling seed dispersal in crop plants such as canola[4,5]. Here we show that the closely related SHATTERPROOF (SHP1) and SHATTERPROOF2 (SHP2) MADS-box genes are required for fruit de... function... phenoty... stitutive... control... tion of... the mo... genetic...

Arabidopsis. Development 124, 3835–3844 (1997).

Acknowledgements

We thank C. Ferrándiz, A. Sessions, S. Kempin, A. Pinyopich, E. Alvarez-Buylla, J. Spencer and N. Harris for helpful discussions; K. Feldmann and his lab for the gift of DNA and seeds from his T-DNA insertional collection; R. Martienssen for providing GT140 seed; and S. Guimil, T. Khammungkhune, C. Chien, H. Cartwright and A. Roeder for assistance with the shp1 and shp2 mutagenesis screens. This work was supported by grants from the National Science Foundation, the National Institutes of Health, Monsanto Company and the University of California BioSTAR programme.





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

http://www.ci.uchicago.edu/research/detail_socialinformatics.php

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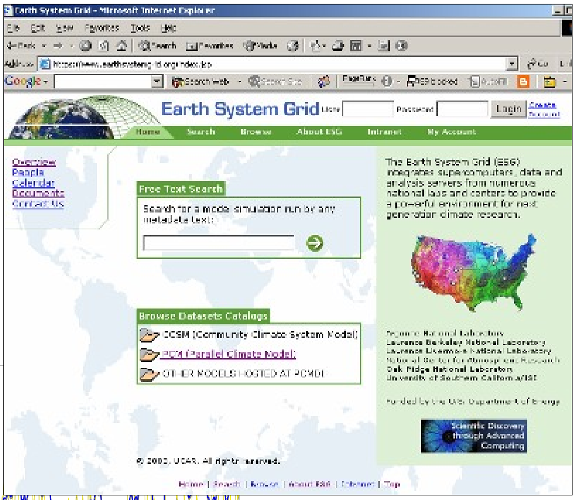
Earth System Grid

- Provides access to all IPCC data
- >150 TB data downloaded
- >300 scientific papers written


Earth System Grid - Microsoft Internet Explorer
File Edit View Favorites Tools Help
Back Search Favorites Media
Address https://www.earthsystemgrid.org/index.jsp
Google Search Web PageRank
Earth System Grid
User
Password
Login
Create Account
Home
Search
Browse
About ESG
Intranet
My Account
Overview
People
Calendar
Documents
Contact Us
Scientific Discovery through Advanced Computing

Free Text Search

Search for a model simulation run by any metadata text:

Browse Datasets Catalogs

CCSM (Community Climate System Model)

PCM (Parallel Climate Model)

OTHER MODELS HOSTED AT PCMDI

The Earth System Grid (ESG) integrates supercomputers, data and analysis servers from numerous national labs and centers to provide a powerful environment for next generation climate research.

Argonne National Laboratory
Lawrence Berkeley National Laboratory
Lawrence Livermore National Laboratory
National Center for Atmospheric Research
Oak Ridge National Laboratory
University of Southern California/ISI

Funded by the U.S. Department of Energy

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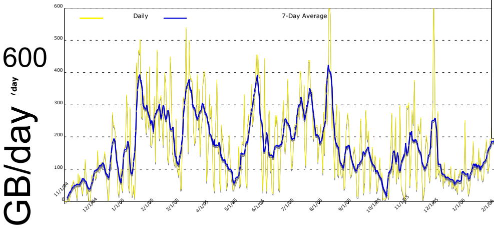
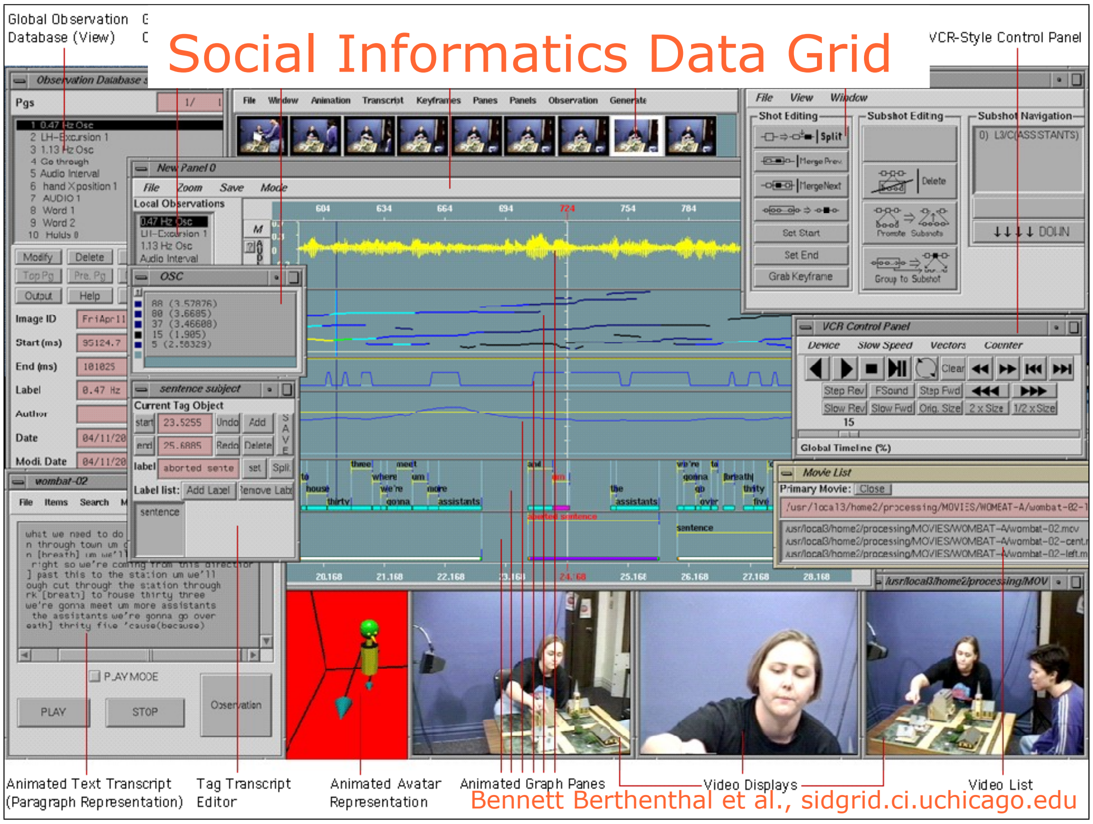


www.earthsystemgrid.org

Social Informatics Data Grid



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what we need to do
n through town um
n [breath] um we'll
 right so we're coming from this direction
] past this to the station um we'll
ough cut through the station through
rk [breath] to house thirty three
we're gonna meet um more assistants
 the assistants we're gonna go over
eath] thrity five 'cause(because)
```

```
/usr/local3/home2/processing/MOVIES/WOMBAT-A/wombat-02-1
/usr/local3/home2/processing/MOVIES/WOMBAT-A/wombat-02.mov
/usr/local3/home2/processing/MOVIES/WOMBAT-A/wombat-02-cent.
/usr/local3/home2/processing/MOVIES/WOMBAT-A/wombat-02-left.m
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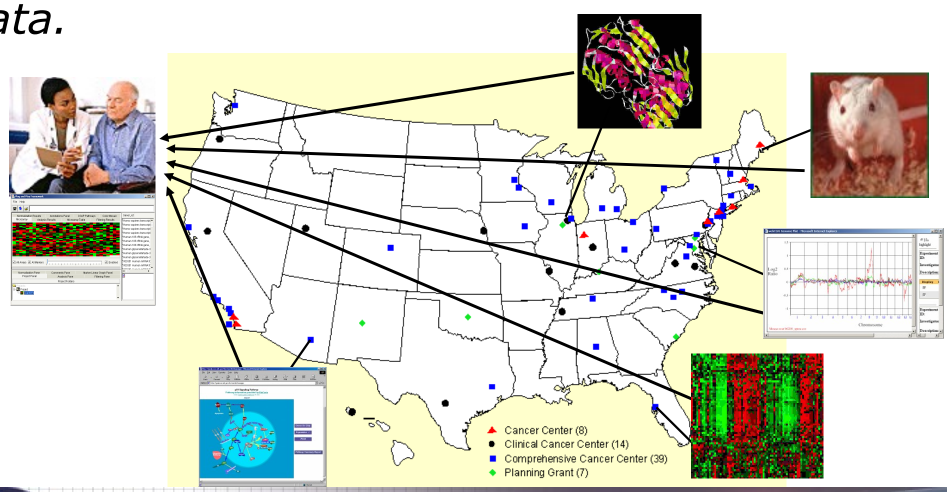
Bennett Berthenthal et al., sidgrid.ci.uchicago.edu

NIH's
Cancer Biomedical Informatics Grid

caBIG: sharing of infrastructure, applications, and data.


▲ Cancer Center (8)
● Clinical Cancer Center (14)
■ Comprehensive Cancer Center (39)
◆ Planning Grant (7)

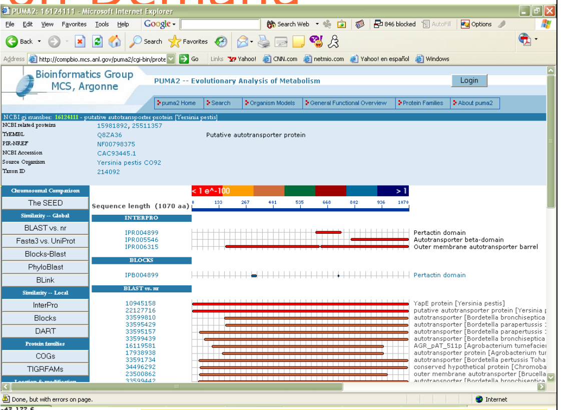
caBIG cancer Biomedical Informatics Grid

https://cabig.nci.nih.gov/

Integrating Data and Computing, on Demand

Public PUMA Knowledge Base

Information about proteins analyzed against ~2 million gene sequences


PUMA2: 16124111 - Microsoft Internet Explorer

File Edit View Favorites Tools Help Google Search Web 846 blocked AutoFill Options

Back Search Favorites

Address http://compbio.mcs.anl.gov/puma2/cgi-bin/prote Go Links Yahoo! CNN.com netmio.com Yahoo! en español Windows

Bioinformatics Group
MCS, Argonne

PUMA2 -- Evolutionary Analysis of Metabolism

Login

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NCBI gi number: 16124111 - putative autotransporter protein [Yersinia pestis]

NCBI related proteins	15981892, 25511357	
TrEMBL	Q8ZA36	Putative autotransporter protein
PIR-NREF	NF00798375	
NCBI Accession	CAC93445.1	
Source Organism	Yersinia pestis CO92	
Taxon ID	214092	

Chromosomal Comparison
The SEED
Similarity -- Global
BLAST vs. nr
Fasta3 vs. UniProt
Blocks-Blast
PhyloBlast
BLink
Similarity -- Local
InterPro
Blocks
DART
Protein families
COGs
TIGRFAMs

Sequence length (1070 aa)

INTERPRO

IPR004899	Pertactin domain
IPR005546	Autotransporter beta-domain
IPR006315	Outer membrane autotransporter barrel

BLOCKS

IPB004899	Pertactin domain

BLAST vs. nr

10945158	YapE protein [Yersinia pestis]
22127716	putative autotransporter protein [Yersinia p
33599810	autotransporter [Bordetella bronchiseptica
33595429	autotransporter [Bordetella parapertussis 1
33595157	autotransporter [Bordetella parapertussis 1
33599439	autotransporter [Bordetella bronchiseptica
16119581	AGR_pAT_511p [Agrobacterium tumefacie
17938938	autotransporter protein [Agrobacterium tu
33591734	autotransporter [Bordetella pertussis Toha
34496292	conserved hypothetical protein [Chromoba
23500862	outer membrane autotransporter [Brucella
33599442	autotransporter [Bordetella bronchiseptica

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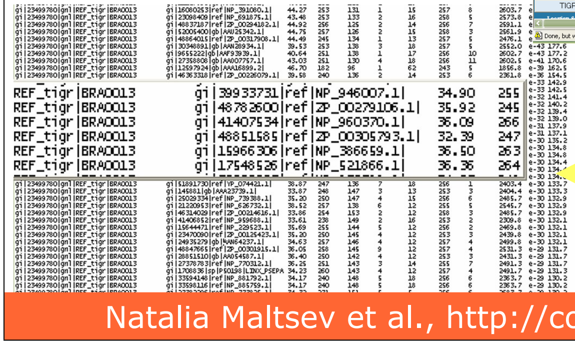
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e-33 142.9
e-33 142.5
e-32 141.4
e-32 140.2
e-32 139.4
e-32 139.0
e-31 137.9
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```

Back Office Analysis on Grid

Millions of BLAST, BLOCKS, etc., on OSG and TeraGrid

Natalia Maltsev et al., http://compbio.mcs.anl.gov/puma2

Global Communities

TERAGRID
Grid.it project
Grid-Ireland
PPDG
iVDgL
Open Science Grid
INFN GRID
EUROGRID
K*GRID
D-GRID
Communities
Arbeit
DataGRID
National Grid NG SINGAPORE
Grid3 2003
ACCESS GRID
grangenet
GRIDPP UK Particle Physics
DataTAG
NEESgrid Building the National Virtual Collaboratory for Earthquake Engineering
GriPhyN Data Intensive Science
CERN openlab for DataGrid applications
Developing Solutions for the Data-Intensive Science of the Large Hadron Collider
LCG
WestGrid
NORDUGRID Grid Solution for Wide Area Computing and Data Handling
eGee Enabling Grids for E-science in Europe
GridCat
tota la informació sobre el projecte
presentació
descripció tècnica
els serveis oferts
participants
documentació pública
com puc participar?
accés al Portal
Intranet per a investigadors
estat dels serveis actius
dintre del grid
grid grid grid grid
Versió en Català
English Version
Versión en Castellano
APEC APGrid Asia-Pacific Grid Implementation Project
NAREGI 超高速コンピュータ網形成プロジェクト National Research Grid Initiative
Grid Applications
Grid Middleware
Networking
国立情報学研究所グリッド研究開発推進拠点 NII -The National Institute of Informatics
GridLab

Applications

- Type
  - Computation
  - Large volumes of data
  - Distributed collaboration
- Common aspects
  - Size or complexity of the problem
  - Inter-organizational collaboration
  - Sharing of computational resources, data, and instruments.

Index

- Introduction
- How does this work?
- More than just a “virtual supercomputer”
- Applications on the Grid
- Globus Toolkit 4
- I want to know more!

What is the Globus Toolkit?

- A collection of solutions to problems that come up frequently when building collaborative distributed applications
  - Job management, data management, information services, metascheduing, etc.
- Does not provide turnkey solutions. It provides building blocks for software developers and system integrators.
- http://www.globus.org/toolkit/

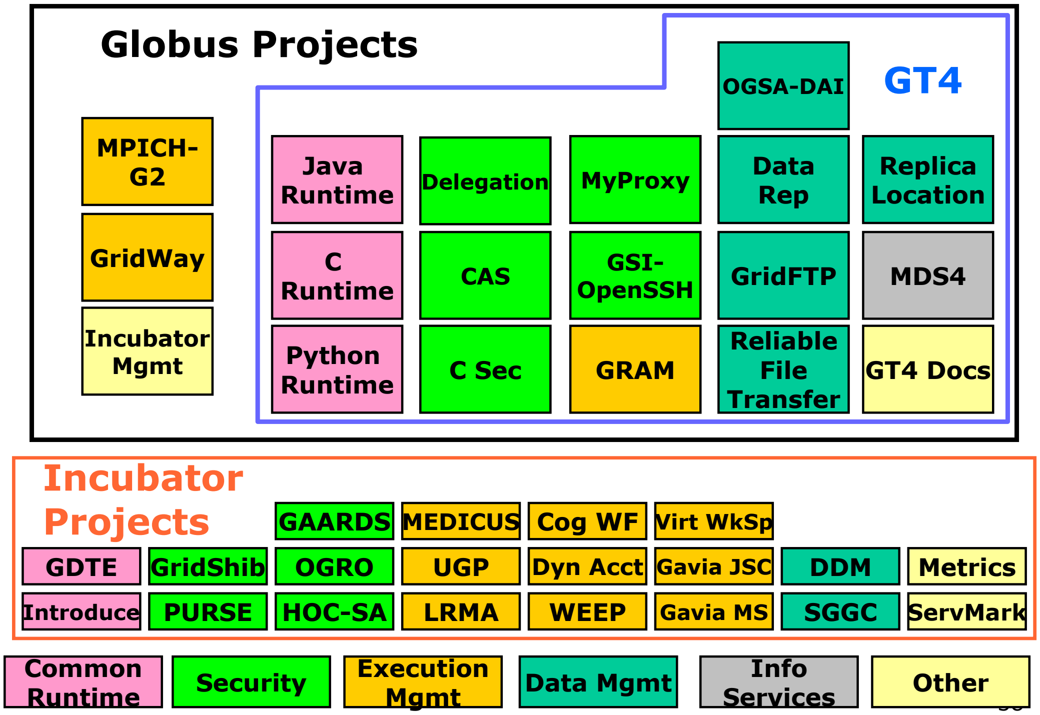
Globus Philosophy

- Globus was first established as an open source project in 1996
- The Globus Toolkit is open source to:
  - Allow for inspection
    - for consideration in standardization processes
  - Encourage adoption
    - in pursuit of ubiquity and interoperability
  - Encourage contributions
    - harness the expertise of the community
- The Globus Toolkit is distributed under the (BSD-style) Apache License version 2

dev.globus

- Governance model based on Apache Jakarta
  - Consensus based decision making
- Globus software is organized as several dozen "Globus Projects"
  - Each project has its own "Committers" responsible for their products
  - Cross-project coordination through shared interactions and committers meetings
  - New projects can be proposed by anyone through an incubation process.
- A "Globus Management Committee"
  - Overall guidance and conflict resolution

Globus Software: dev.globus.org



Globus Projects

GT4

MPICH-G2

GridWay

Incubator Mgmt

OGSA-DAI

Java Runtime

Delegation

MyProxy

Data Rep

Replica Location

C Runtime

CAS

GSI-OpenSSH

GridFTP

MDS4

Python Runtime

C Sec

GRAM

Reliable File Transfer

GT4 Docs

Incubator Projects

GAARDS

MEDICUS

Cog WF

Virt WkSp

GDTE

GridShib

OGRO

UGP

Dyn Acct

Gavia JSC

DDM

Metrics

Introduce

PURSE

HOC-SA

LRMA

WEEP

Gavia MS

SGGC

ServMark

Common Runtime

Security

Execution Mgmt

Data Mgmt

Info Services

Other

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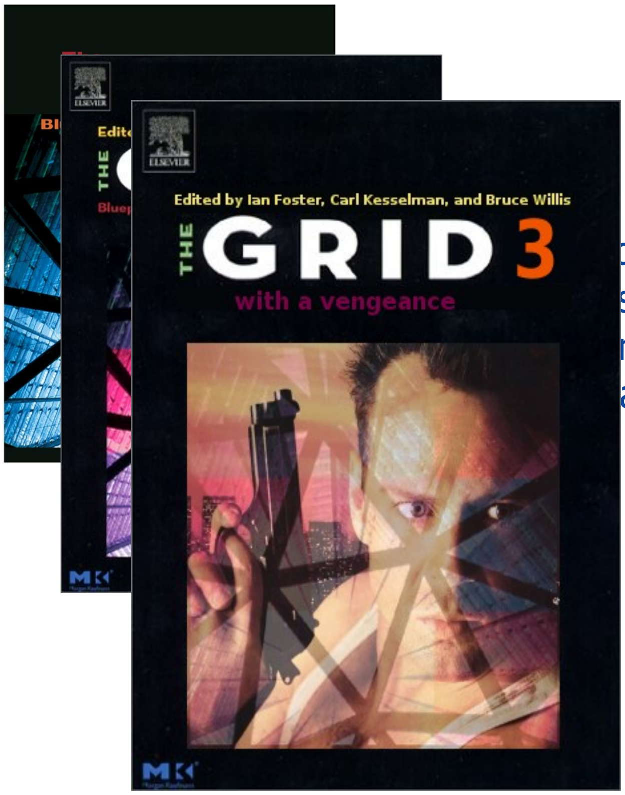
I want to know more!

- GridCafé provides a good introduction to Grid Computing
  - http://gridcafe.web.cern.ch/
- Books…



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ster and Carl
man. Morgan
ann, 2003.

I want to know more!

- Books
  - "Grid Computing: The Savvy Manager's Guide". Pawel Plaszczak, Richard Wellner, Jr. Morgan Kaufmann, 2005.
  - "Globus Toolkit 4: Programming Java Services". Borja Sotomayor, Lisa Childers. Morgan Kaufmann, 2005.
- Websites
  - The Grid Index: http://www.gridindex.org/
  - Grid Gurus blog: http://gridgurus.typepad.com/
  - Ian Foster's blog: http://ianfoster.typepad.com/

Questions?

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