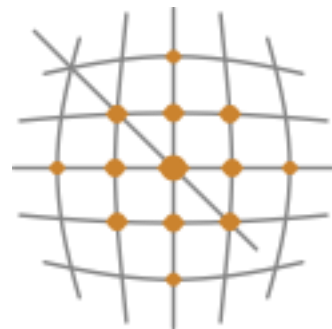
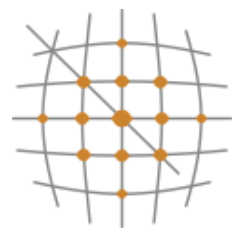


e-Infrastructures for scientific computing @ AUTH



Scientific Computing Center
Aristotle University of Thessaloniki

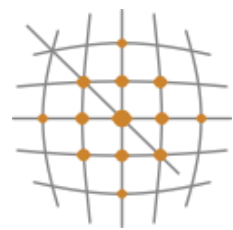


Overview

- Grid, Cloud, HPC and Big Data services
- Applications and Users
- Success stories



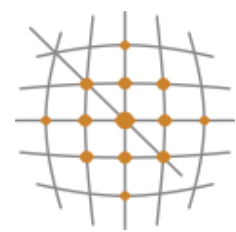
G rid



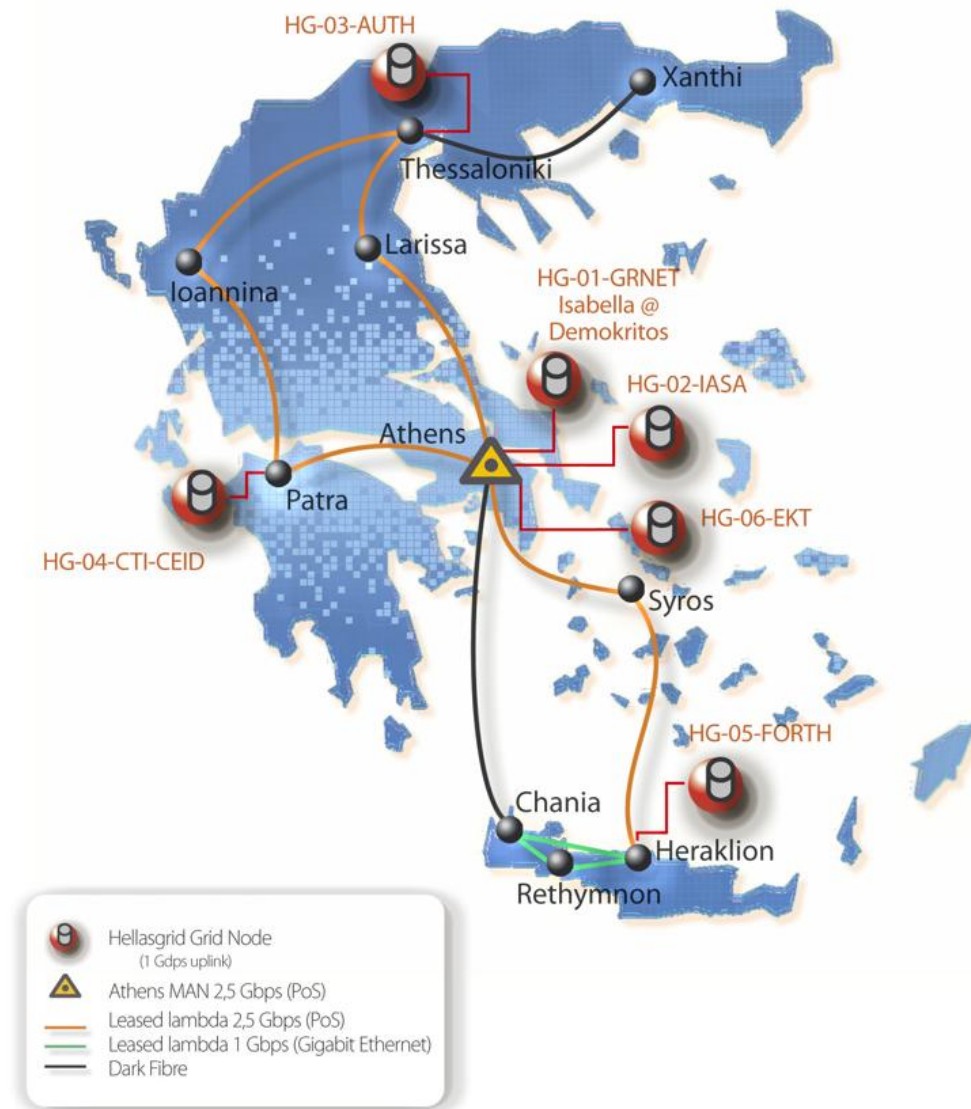
EGI overview



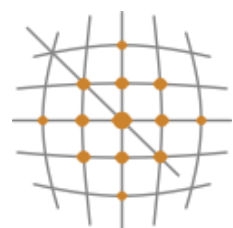
	Q1/2012	Q2/2012	Q3/2012	Q4/2012
Resource Providers	322	292	281	303
Cpu Cores	313795	306684	352612	333412
Resource centers supporting MPI	106	87	80	77
Jobs/day (million)	1.57	1.78	1.67	1.43
Wall clock (million hours/day)	5.3	5.8	4.8	4.9



HellasGrid infrastructure

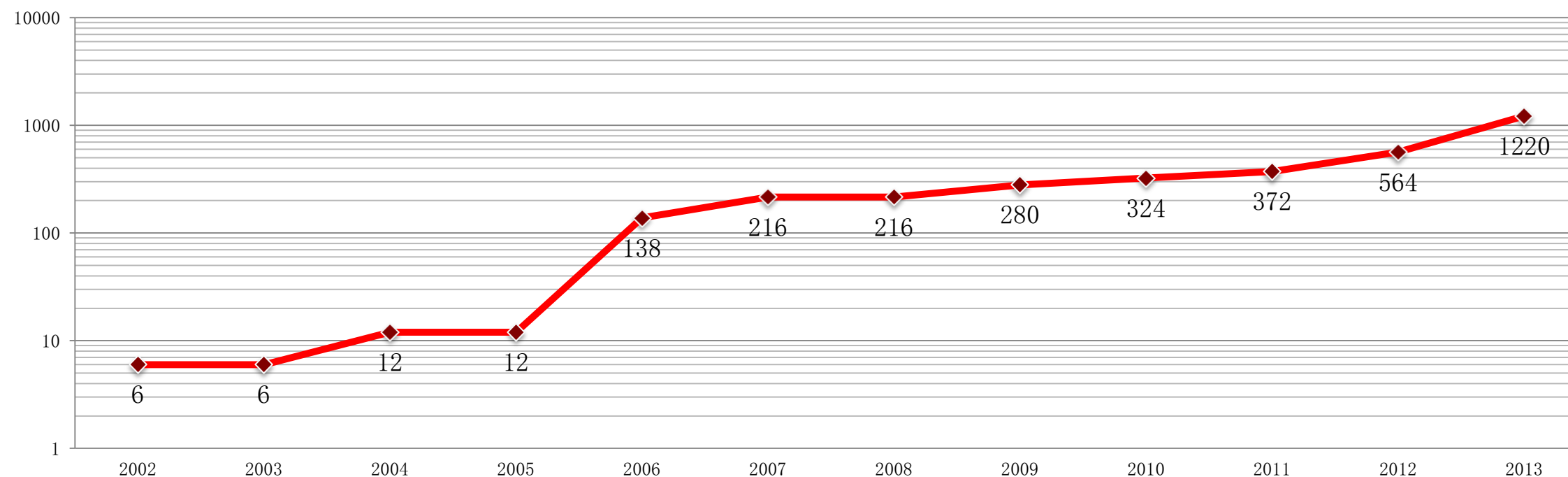


HellasGrid overview		
	Job slots	Storage [TB]
HG-01-GRNET	64	20
HG-02-IASA	120	4
HG-03-AUTH	620	8
HG-04-CTI-CEID	120	4
HG-05-FORTH	120	4
GR-01-AUTH	600	234
GR-04-FORTH-ICS	10	–
GR-06-IASA	20	2
GR-07-UOI-HEPLAB	28	20
GR-09-UOA	10	2
GR-10-UOI	400	2
Total	2112	300

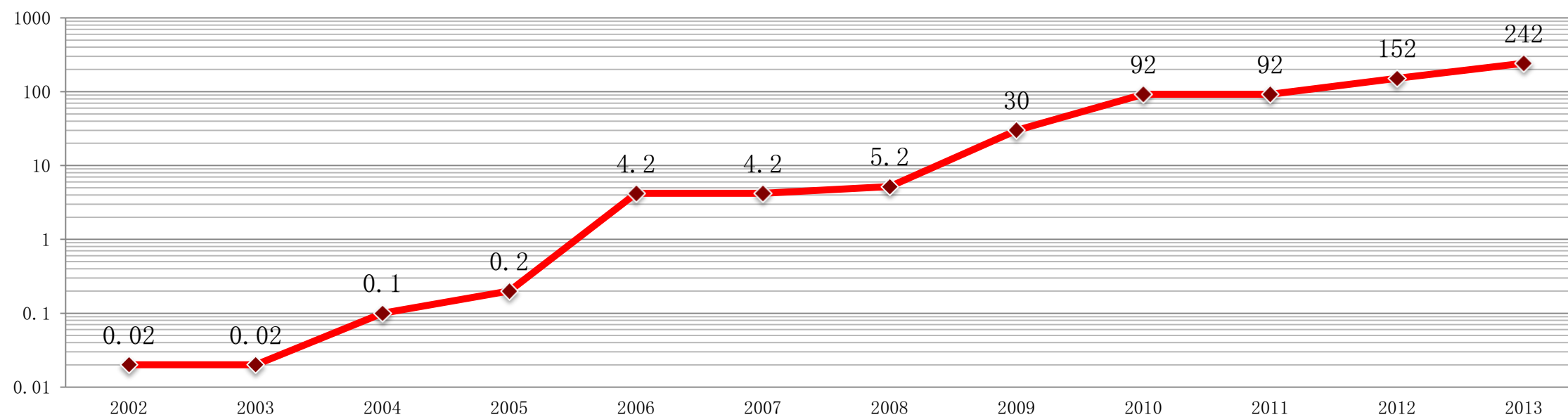


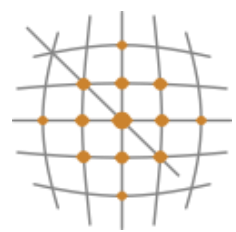
Grid Clusters @ AUTH

Number of CPU Cores from 2002 until today

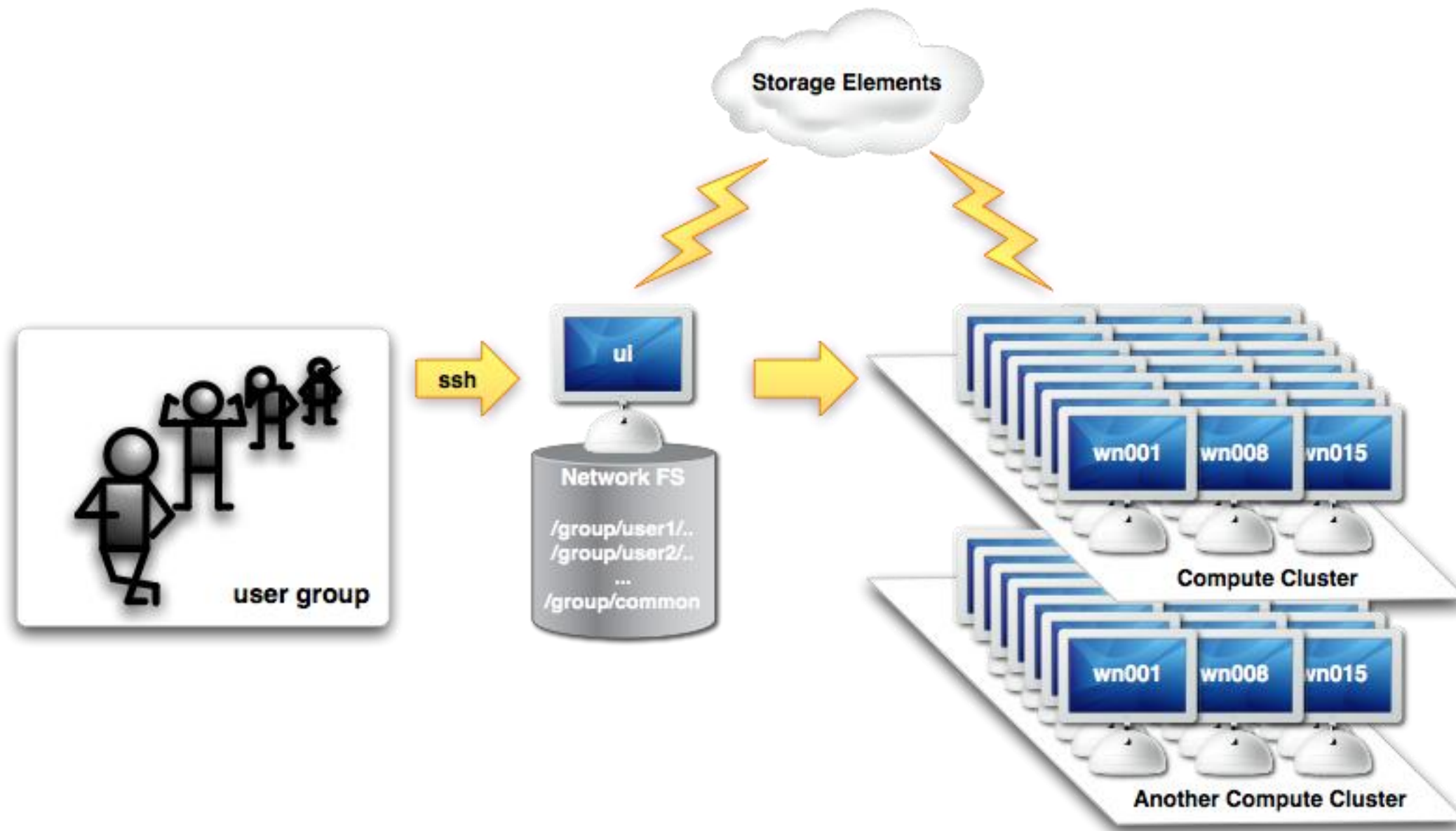


Storage [TB] from 2002 until today

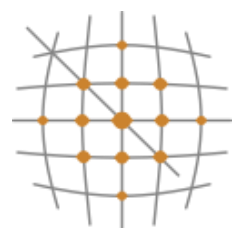




The Grid in a snapshot



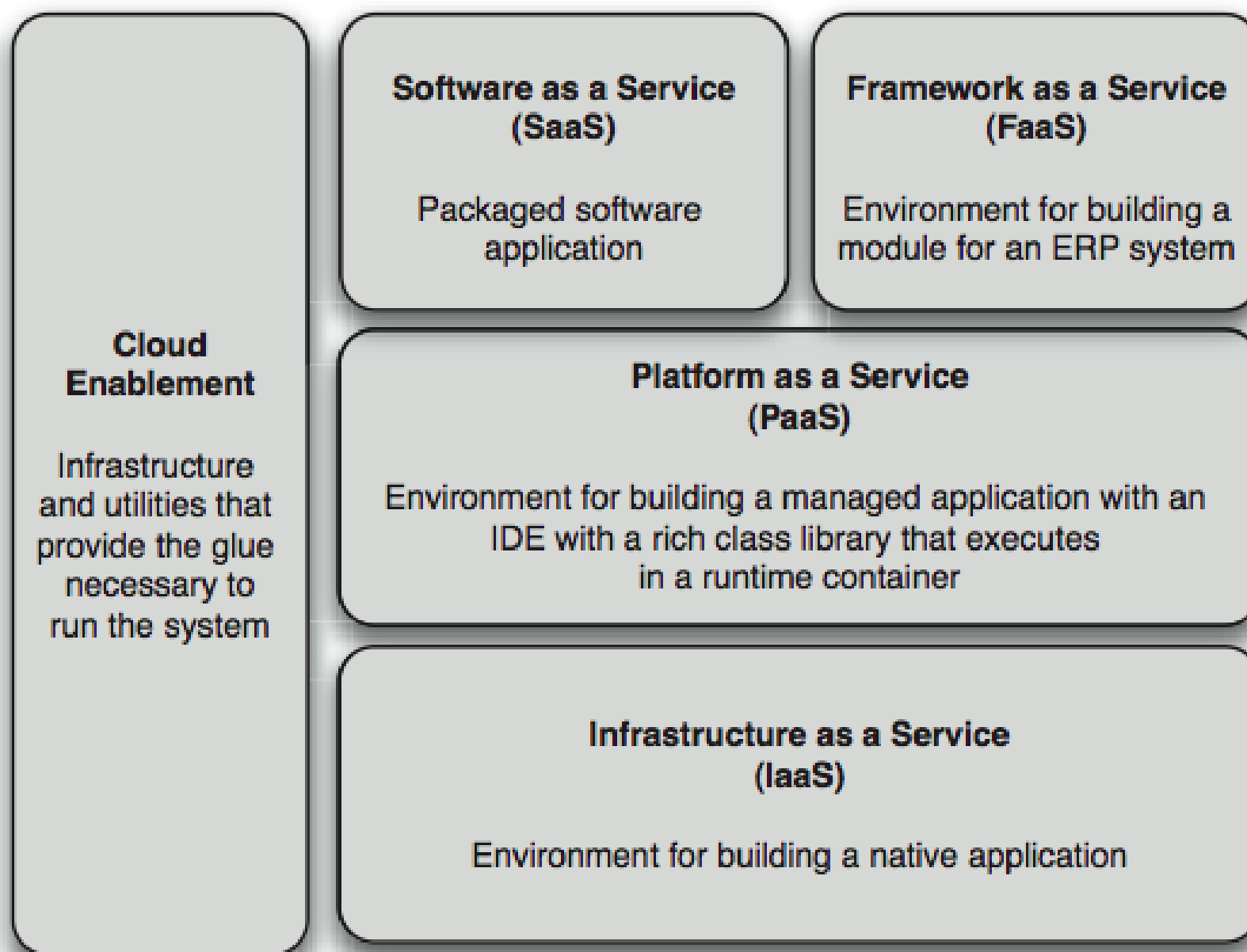
Clo u d

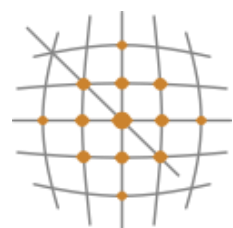


Cloud services “heat map”

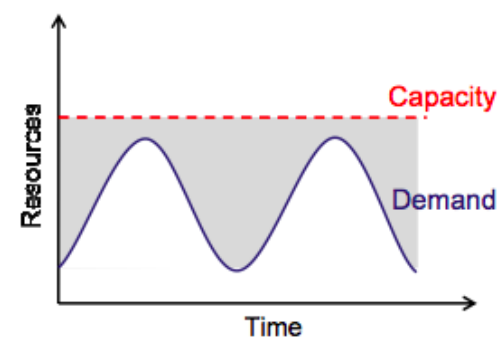
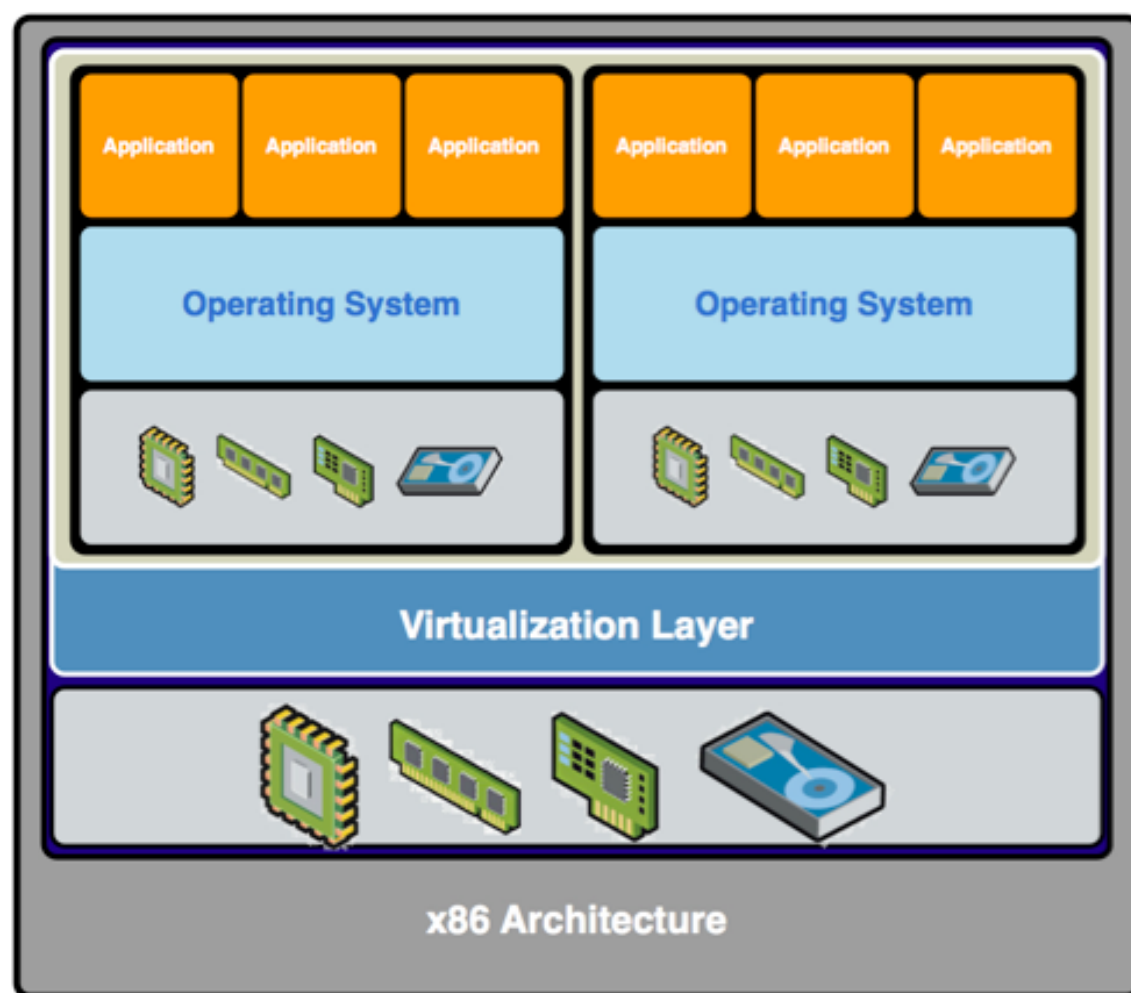


Cloud Computing: “Everything as a Service”

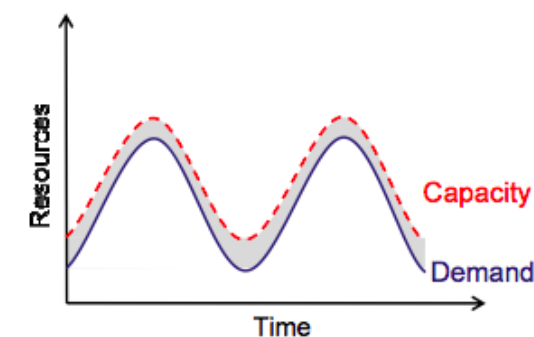




Cloud relies on virtualization

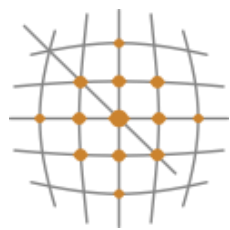


Static data center




Data center in the cloud

Unused resources



okeanos

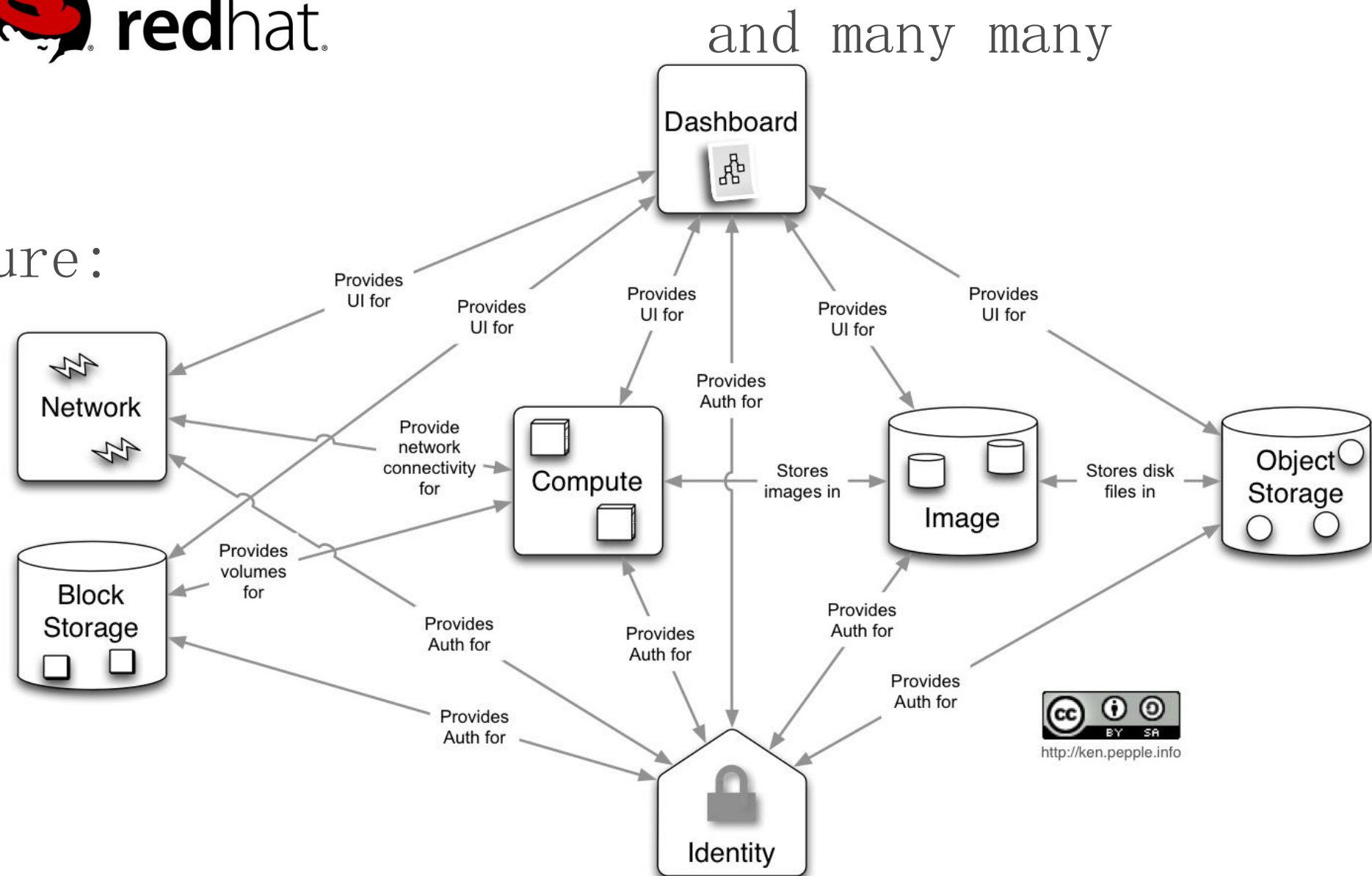
- okeanos is Greek for ocean
 - *Oceans capture, store and deliver energy, oxygen and life around the planet*
- Powered by GRNET
- IaaS type of cloud based 
- Build with **Simplicity & Flexibility** as basic principals

Spawned VMs	Active VMs	Spawned Networks
234,183	6,421	64,754
- Statistics:

- IaaS solution

- Power by  redhat.
more

- Architecture:



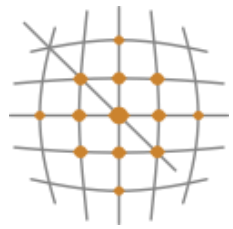


HP C



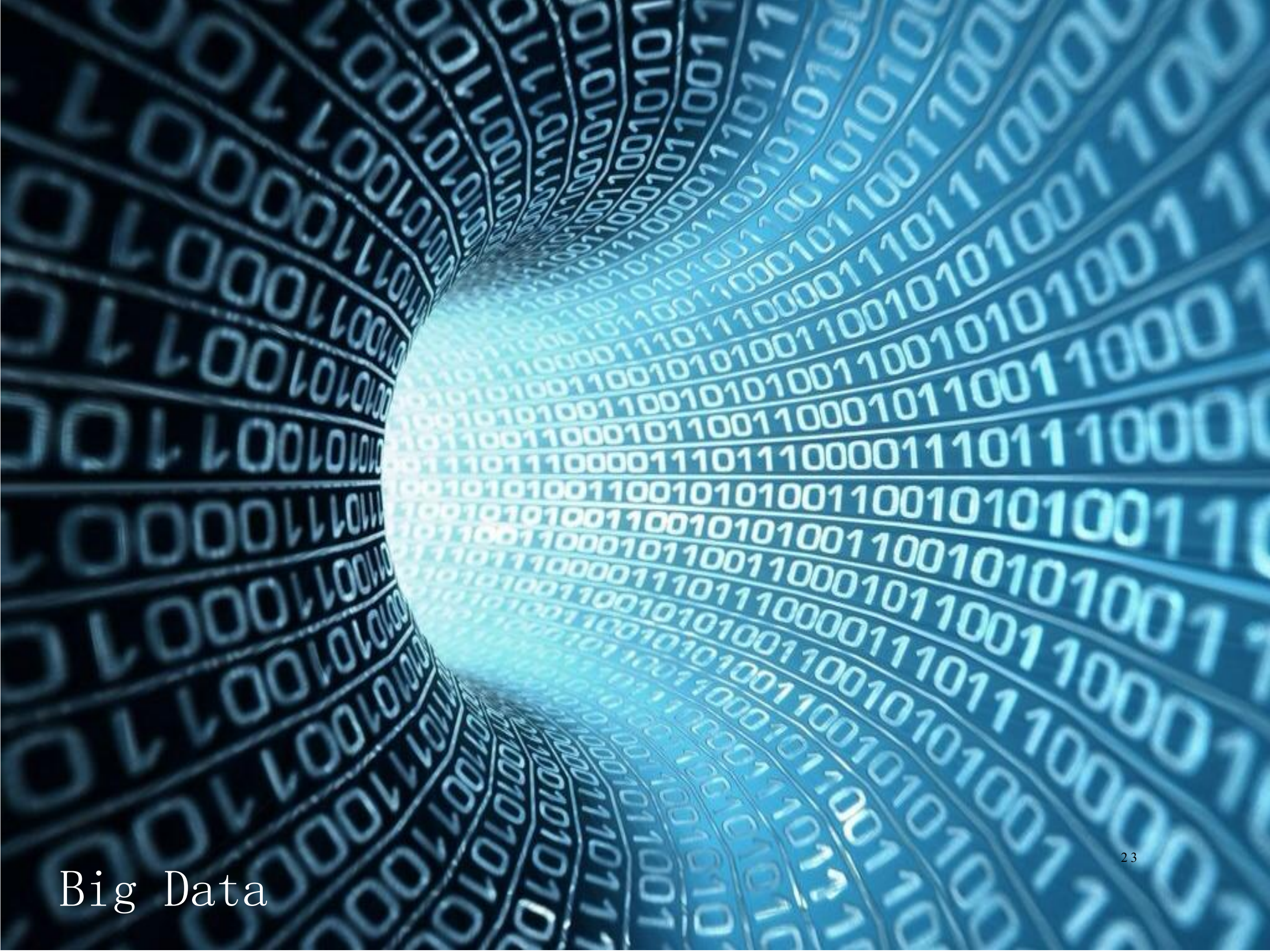
HPC activities

- AUTH has been involved in PRACE since 2009
- GRNET oversees the procurement and installation process of a national Tier-1 infrastructure (currently underway)
- to be installed centrally at Athens
- will be available for academic and research community

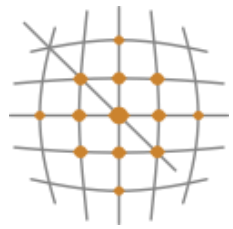


PRACE access calls

- PRACE runs a continuous call addressed towards European researchers. Types of access are:
 - DECI calls (runs continuously/cut-off every 3mo)
 - access to Tier-1 resources
 - Type-C Preparatory access call (runs continuously/cut-off every 3mo)
 - access to Tier-0 resources for a time period of 6mo

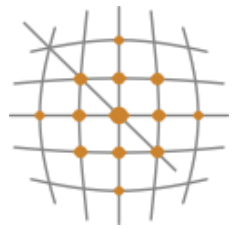


Big Data



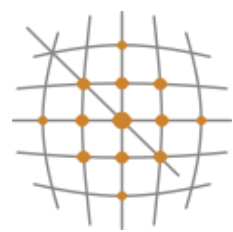
Big Data services

- Big Data infrastructure operational since April 2011
- So far used primarily for internal purposes
 - Log parsing and statistics extraction
- Based on Hadoop MapReduce/HDFS
 - Built on top of Cloudera software stack
- Additional tools include: Hive, Hue, Pig, Hcat, Oozie



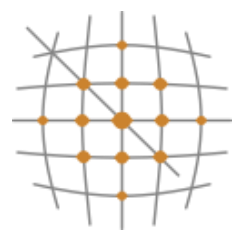
Supporting activities @ AUTH

- More than 150 researchers and domain experts (with approximately 20-40 being active)
- More than 30 scientific applications from several research fields supported (i.e. use case examples, sample files etc)
- Core support activities include:
 - Grid computing related support (1st and 2nd level)
 - Support for Big Data (Hadoop) applications
 - HPC support for successful PRACE applicants



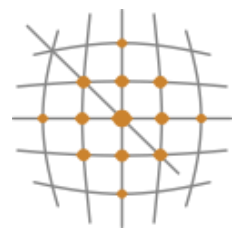
Applications from Chemistry/Materials

Application Name	Application Version	Compilers used	Parallel API used	Architecture	Status
CP2K	2.1	Intel (11.1)	mpich2	x86_64	Production (use case available)
NAMD	2.9	Precompiled	mpich2	x86_64	Production (use case available)
LAMMPS	Trunk	Intel (11.1)	mpich2	x86_64	Production (use case available)
VASP	5.2	Intel (11.1)	mpich2	x86_64	Production / Licensed
Gaussian	g03	Precompiled	linda	x86_64	Tested / Licensed
Abinit	6.10.2	Intel (11.1)	mpich2	x86_64	Tested
DL_POLY	4.01	Intel (11.1)	mpich2	x86_64	Production (use case available)
Siesta	2.0.1	Intel (11.1)	mpich2	x86_64	Tested
VMD	1.8.6	Precompiled	—	x86_64	Production



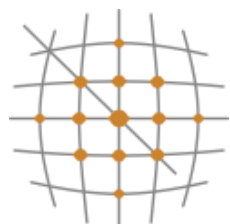
Applications from Engineering/CFD

Application Name	Application Version	Compilers used	Parallel API used	Architecture	Status
FLOW-3D	9.4.5, 10.1	Precompiled	<u>openmp</u>	x86_64	Production
NUMECA	8.8.2	Precompiled	Intel-MPI, <u>mvapich</u>	x86_64	Production
ANSYS/Fluent	12.1	Precompiled	Intel-MPI, HP-MPI, SMP	x86_64	Testing
ANSYS/CFX	12.1	Precompiled	Intel-MPI, HP-MPI, SMP	x86_64	Testing
<u>Code_Saturne</u>	2.0.1	GNU (4.1.2)	<u>mpich2</u>	x86_64	Production
OpenFOAM	2.1	GNU (4.4.0)	<u>openmpi</u> , <u>cuda</u>	x86_64	Testing
<u>Sphysics</u>	2.2.1	GNU (4.1.2)	<u>mpich2</u>	x86_64	Production
ANSYS	12.1	Precompiled	Intel-MPI, HP-MPI, SMP	x86_64	Production
Code_Aster	10.6	GNU (4.1.2)	<u>mpich2</u>	x86_64	Testing



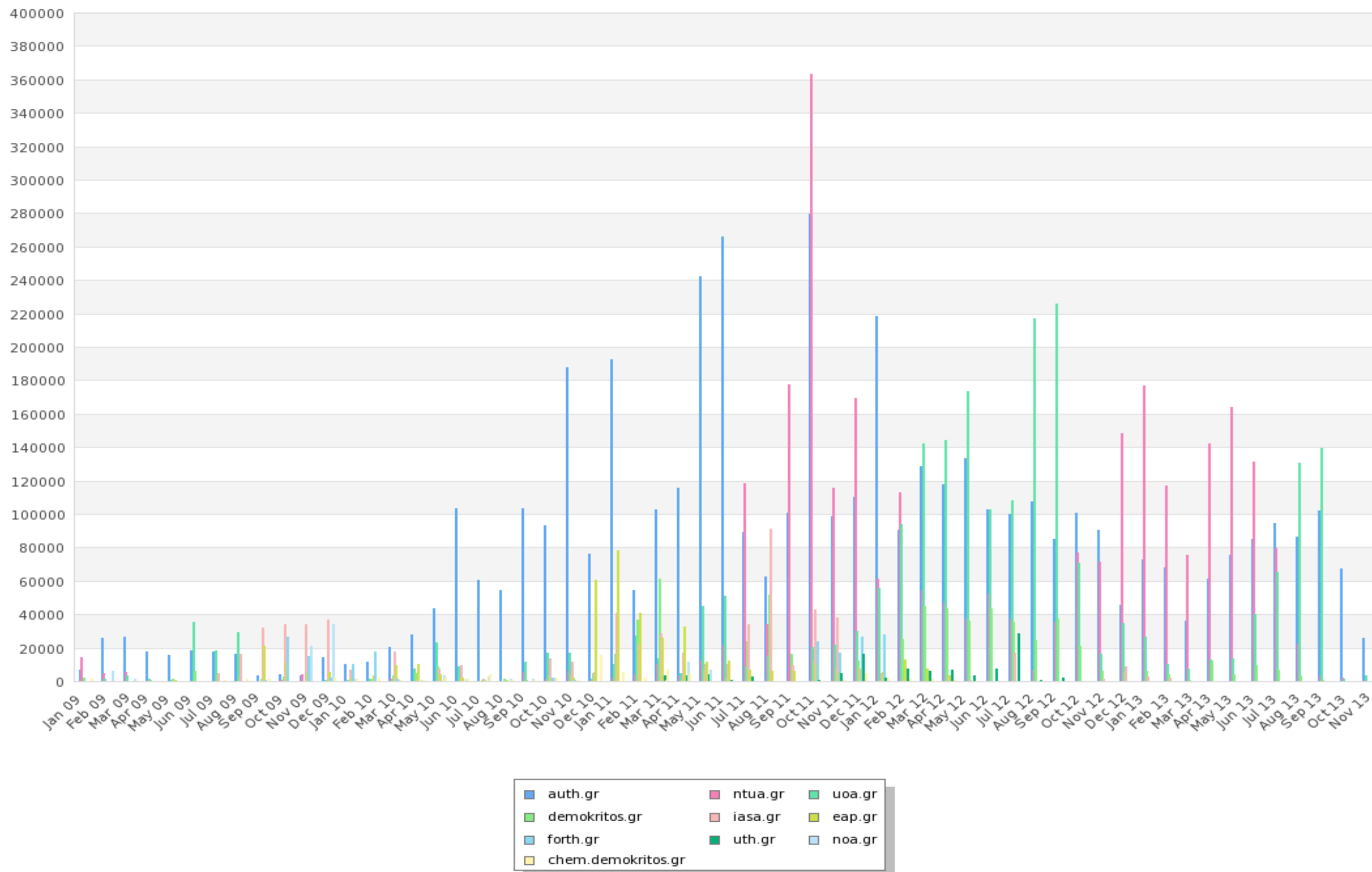
Tools/Libraries for development

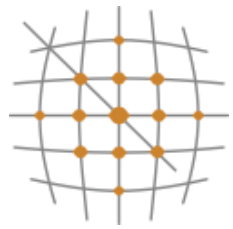
Libraries & Utilities	Version	Compilers	Architecture	Status
netcdf	4.1.1	GNU, Intel	i386, x86_64	Production
hdf5	1.8.4	GNU, Intel	i386, x86_64	Production
GSL	1.13	GNU	x86_64	Production
MKL	10.1.2.024, 10.2 (Update 2) καί 10.3.8	Intel	x86_64	Production
BLACS	1.1	GNU	x86_64	Production
ScaLAPACK	1.7.5	GNU	x86_64	Production
ARPACK	2.1	GNU	x86_64	Production
ATLAS	3.8	GNU	x86_64	Production
LAPACK	3.0	GNU	x86_64	Production
BLAS	3.0	GNU	x86_64	Production
Cuda toolkit	3.0, 4.2	–	gpgpu	Testing



Statistics

Top 10 HellasGrid Institutes (Sum CPU (hours))





Success stories

- Evaluating the impact of **climate change** on European air quality
- Spatial distribution of site-effects and **seismic wave** propagation properties in Thessaloniki (N. Greece) using a 3D finite difference method
- **Protein classification** algorithms over a distributed computing environment
- Investigating the nature of explosive **percolation transition**