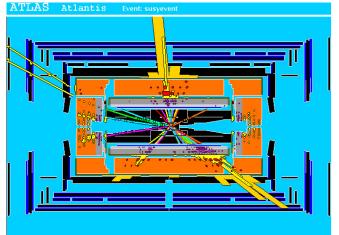
#### **CSIC Bilateral Agreement COOPB20472**

"Launching a platform of GRID Computing in Morocco to meet the new challenges of Physics Research"













#### Dr. José F. SALT CAIROLS

Profesor de Investigación CSIC Instituto de Física Corpuscular (Jose.Salt@ific.uv.es)



#### INTRODUCTION TO THE TRAINING COURSE

- The Distributed Computing Training course is within the COOPB20247 cooperation agreement between CSIC (IFIC-Spain) and Mohammed V University in Rabat (Morocco).
- The goal of the course was to teach the concepts of grid computing and its application in Physics. The course can be divided into two areas:
- I) One related to technical knowledge about grid computing in general and,
- II) The other addressed to High Energy Physics Grid computing, including the BigData of the LHC.
- The goals related to technical knowledge included understanding, explaining, and applying grid computing technology, in particular: concepts of grids, requirements of grids especially related to different disciplines, application and usage of grid technology on areas in different disciplines.
- In addition dedicated lectures of the ATLAS computing model, including data and Job management systems will be given to the High Energy Physics Phd student participants.

https://indico.cern.ch/event/606256/overview

### Today ( = Tuesday) Program

09:00	Introduction to Computing in Physics and e-Science	Jose Salt
	Valencia, Spain	09:00 - 10:00
10:00		
	Fundamentals of GRID Computing	Jose Salt
11:00	Valencia, Spain	10:15 - 11:15
12:00		
13:00		



17:00

## TRAINING COURSE – Bilateral Agreement COOPB20472

# Class # 1 INTRODUCTION TO SCIENTIFICAL COMPUTING AND E-SCIENCE

José Salt

#### Contents Class #1

- 1.- A brief history (ending in GRID Computing)
- 2.- GRID Computing : definition, objectives and more relevant aspects
- 3.- Functionality and features of GRID Computing
- 4.- Layers of GRID: Infrastructures, Network, Middleware and Applications
- 5.- e-Science: definition and activities. Classification
- 6.- The Computing ecosystem at present -Cloud Computing: basic concepts
- 7.- From GRID Computing to Big Data

#### 1.- A BRIEF HISTORY (ENDING IN GRID COMPUTING

#### Aggregation of resources:

- SHIFT system (RISC Unix "farms", L.Robertson, CERN)
- Clusters of PCs (Beowulf system, "factories ...)

#### Distributed resources:

- Condor System (M.Livny)
  - Management of the inactive time in Linux systems connected by local network.
  - Entropy Network, SETI@home program
- "Peer to Peer" systems.

#### Appearance of the Web:

- 1989: first proposal : CERN, Tim Berners-Lee and Robert Cailliau
- Firsts web servers at the European Physics Laboratories,
- 1991: a prototype of the WWW system delivered by the HEP community



Les Robertson (left) who received award on behalf of CERN



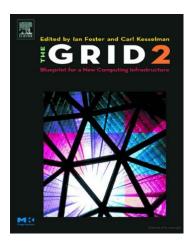
#### 1995: Supercomputing '95

- I-WAY Experience: 17 centers in USA connected at 155Mbps
- Firsts GRID initiatives:
  - NASA Information Power Grid
  - Initiative of the NSF with centers of NCSA y SDC
  - Advanced Strategic Computing Initiative (DoE)

#### The era of the clusters/farms/factories of PCs

- Nodes with CPUs (dual)
- Local disks + access to servers (NFS-NAS, AFS)
- Limitation:
  - Interconection of networlk: Gigabit almost popular, with low latency requires Myrinet or similar, solution more expensive
  - Perfect for HTC (High Throughput Computing)
  - Applications in HPC (High Performance Computing) need to be adapted:
    - Memory is not shared
    - Tools: PVM, MPI
  - Instalation and control: they work fine for hundred of computer "homogenous", but the does it scale?







- ... And besides, in a distributed way by means of connection to clusters:
  - Thanks to the network interconnection,
  - The idea is to achieve the feeling of working with a Virtual Supercomputer formed by a lot of computer clusters (Metacomputing)



## 2- GRID COMPUTING: DEFINITION, OBJECTIVES and MORE RELEVANT ASPECTS

- Definition: GRID Computing is an evolution of Distributed Computing; its basis rely in the technologies which allow the organizations to share computing resources to face different kinds of needs. In general, these resources are geographically distributed and connected by internet. This network gives the impression of being working with a unique and virual computing system.
- Distributed Computing, Paralelism and GRID: review of concepts and establishment of concepts and meanings.
- Try to solve the present problems within the Information Society:
  - Fast access to the DataBases/Storage
  - To provide its processing and analysis using Distributed
     Computing power and analysis and visualization facilities
  - By using the network

#### What is NOT GRID?

- NOT an INTERNET upgrade (not at the same level)
- •It is NOT a project but a set of technologies that will allow the access of the users of the network to distributed computing resources
- NOT a cluster or computer farm
  - The development of the vast majority of scientific projects requires collaboration in distributed computing tasks on a global scale.
  - Scientific-Technological Areas: High Energy Physics,, Biomedicine / Medical Diagnostics, Bioinformatics, Earth Observation, Computational Chemistry, Analysis of Observational Astrophysics

#### Computational GRID - Eléctricity GRID

#### **Electricity GRID**

Power Plants

Hierarchical distribution of the electric flow



#### **Electrical Substation**

Electrical lines

 Final User: access to the electricity supply for home/industrial appliances









#### Computacional GRID

Big center with storage & computing power

(Supercomputers/ Big Computing centers)

Hierarchical Distribution
 (Computing Centermedium size)

Network -Internet

Fiber Optic branch



Final users: access to the computing services/ applications

- Recently (20 years ago),
  - when important computing resources were needed, a computer was purchased that suited that demand for resources and only to meet that demand;
  - We had more or less large 'computing generators' but they were not interconnected between them
- THEN The capacity of calculation that we possess at the individual level, in the Companies, university or research centers, etc. is not being used all the time;
  - it could be globally managed to be used when needed
  - When we use computing power we will not care where it comes from or the infrastructure behind (as in the case of electricity service)

#### **GRID Clasification**

#### National GRIDs :

- Strategic computing reserve for times of crisis
- Catalyst of scientific or engineering collaborations at the national level

United Kingdom: very important e-Science program

#### • Private GRIDs:

- Useful for hospitall
- Small scale infrastructure http://www.entropia.com

#### • GRID associated to projects

- Meet the needs of research teams
- Teams that collaborate with each other on short / medium term and highly oriented projects
- Example: LCG Project (LHC Computing GRID)

#### • GRID Goodwill

- Donation of computing capacity for certain investigations
- Examples: '@home' projects, SETI @ HOME
- Using BOINC Distributed Enclosure

#### • GRIDs Peer to Peer

- Designed for data distribution between computers
- There is no central control
- You get in 'kind' something that they are all making available if all Napster and Gnutella

#### • GRID Consumer

 Companies or institutions that rent distributed resources and charge for their use

# 3- FUNCTIONALITY AND FEATURES OF GRID COMPUTING 3.1 How does GRID work? 3.2.-The pillars of GRID

#### 3.1.- How does GRID work?

- GRID is based esentially in a special software, called middleware, which ensures the transparent comunication between different computers geographically distributed;
- There is a search engine which not only finds the data that the user needs, but also the tools to analyze them and the computing power needed to use them;
- At the end of the process, GRID processing Al final del proceso el GRID will distribute the computing tasks to every site connected by the network where available capacity could be found and GRID will submit the results to the users.

#### 3.2.- The pillars of the GRID

This working is based in 5 pillars:

#### 1)Posibility of sharing resources:

- direct access to software, computing resources and remote data/ access and control of other devices (sensors, telescopes, etc).
- differente domains and , a lot of times, heterogeneous, different access and security policies,
- adventage of sharing resources/ mechanisms of trust between users

#### 2) Security – Safe access

- a) Authentication: procedure to establish the identity of an user or a given resource (computer element, Storage element,...)
- b) Authorization: procedure to determine if a given operation is consistent with the relationships defined previously with the aim of Sharing resources

#### 3) Efficiente usage of resources:

 In a system with jobs in queue coming from the users, which need mechanisms to share the jobs in an automatic and efficiente way in an environment with a big quantity of resources reducing notably the waiting time => MIDDLEWARE

#### 4) Stable Communication Networks

The existence of high speed connections is the main corner stone which permits the GRID at world scale

#### 5) Open Standards:

The so-called Open Source contribute in a evident and esencial way to GRID development since it can be obtiened benefit from all the participant agents.

Importance of GGF( Global GRID Forum) and OGSA (Open GRID Services Architecture)

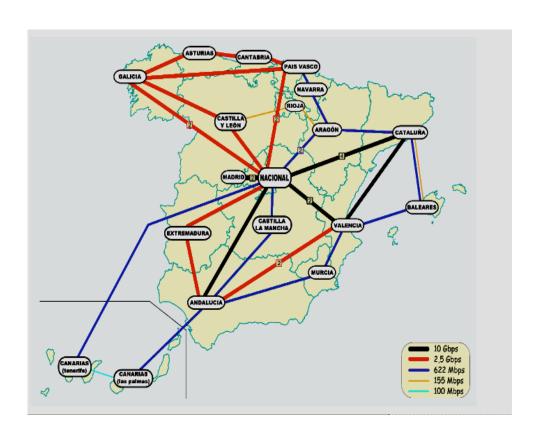
Globus Toolkit: it is a tool in open source developed by Globus Alliance

#### 4.- THE LAYERS OF THE GRID :

- 4.1.- The Network
- 4.2.- The resources
- 4.3.- The Middleware
- 4.4.- The applications

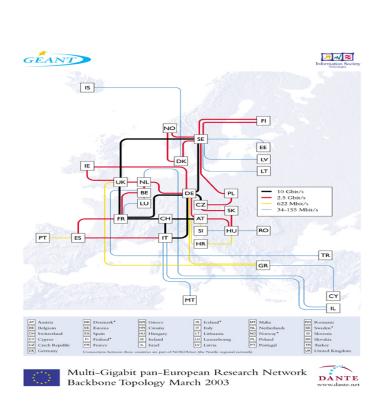
#### 4.1- The Network

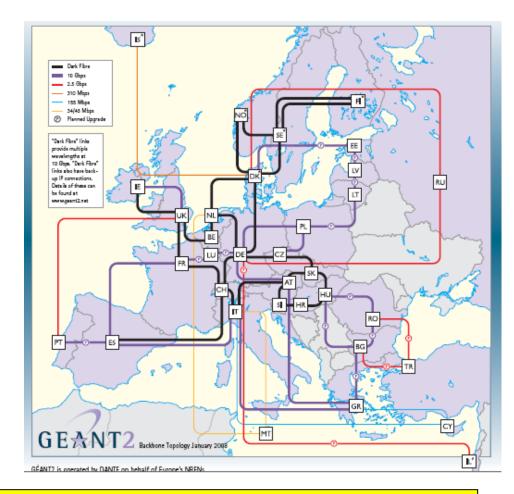
- El GRID could not have been developed without an adequate network
- Network agencies have ensured the resources forming the GRID
- Comunications:
  - Internet Protocols: IP, DNS, routing, etc.
- Big effort at the european level (DANTE y NRENs) and at spanish level (RedIris)
- Project RedIRIS-Nova: deployment of optic fiber



Mapa de la Infraestructura de la Red en España (RedIris)

## Academic and Research Pan-European Network





2003 GEANT

. 2008 ....

2017 ....

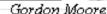
**GEANT2** 

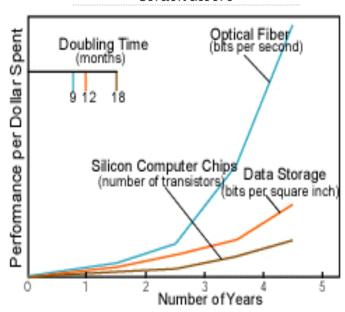
## 4.2- The Computing Resources: the GRID Infrastructures

#### **Technological Evolution.**

- Hardware:
  - Processors: compliance with the Moore's law: doubles every 18 months
    - doubles every 18 months!
  - Computing nodes:
    - PCs and laptops, Stations, servers Clusters, Blades, GPU's
  - Storage: doubles every 12 months !!
- Improvement of the network:
  - network performance sdoubles every 9 months!!
  - >>>10 GB ethernet
- Cost taking into account several factors:
  - space, electric suply, maintenance

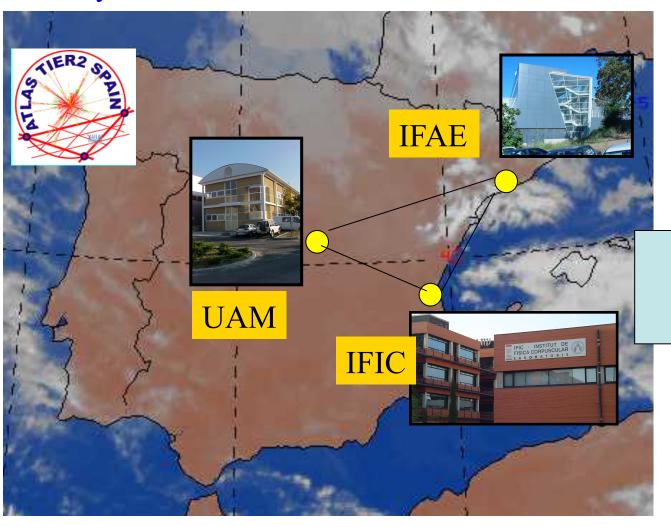






#### **Example: the Spanish ATLAS Tier-2**

#### Proyecto Coordinado del Plan Nacional de FAE de 3 centros:



IFAE (25%) UAM (15%) IFIC (50%)

4% del total Tier-2

**Equipment:** 

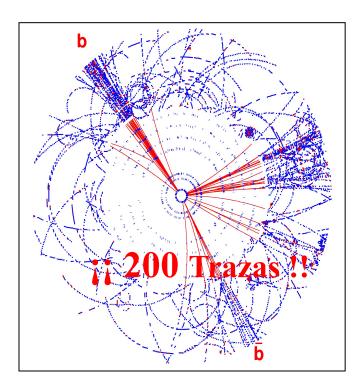
CPU = 18.000 KSI2k Disk = 2 PB

**Human Resources:** 

**12 FTE** 

**July 2017** 

## Complejidad de un suceso de LHC



Hits: señales de lo detectores; A partir de estos se reconstruyen Las trayectorias

#### More details: talks of Santiago and Farida



Europa: 267 institutos, 4603

usuarios

Resto mundo: 208 institutos, 1632

usuarios

#### GRID Computing and e-Science Group (2017)

Personal Permanente:

**MIEMBROS** 

A. Fernández Casani : Titulado Superior Informática- CSIC

S. González de la Hoz : Profesor Titular – UVEG
J. F. Salt Cairols, : Profesor Investigación - CSIC

J. Sánchez Martínez : Titulado Superior Informática- CSIC

PostDoc:

E. Fullana Torregrosa: Postdoc 'Severo Ochoa'

Personal Contratado ó Vinculado:

J. Lozano Bahilo Contratado Proyecto, CSIC

F. Fassi Doctora Vinculada.

Profesora Física Universidad de Rabat

C. García Montoro Técnico Apoyo Ministerio

J. Aparisi Pozo Contratado Proyecto(Doctorando)

Colaboradores externos/ Colaboradores Visitantes:

G. Amorós Vicente: Técnico Especialista en la AEMET (Agencia

Española de Meteorología)

Miguel Villaplana Postdoc en INFN-Milán

#### 4.3 - Middleware

More details: talk of Álvaro

Definition:

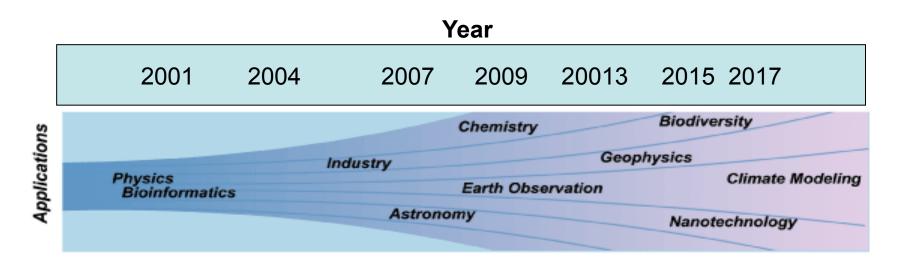
it Is a connectivity software that offers a set of services that enable the operation of distributed applications on heterogeneous platforms. It works as a distributed software abstraction layer, which sits between the application layers and the lower layers (operating system and network)

- Middleware abstracts us from the complexity and heterogeneity of the underlying communications networks, operating systems and programming languages, providing an API for easy programming and management of distributed applications
- but this definition is still too much general...
  - It is the differential feature of GRID Computing with respecto to another solutions of distributed computing
  - Purpose: 'virtualize' computing resources

- the Middleware functions are :
  - To find a adequate site to execute the tasks requested by the user
  - To optimize the usage the resources which can be distributed
  - Organize an efficient access to thte data
  - Authentication of differente elements
  - It deals with resource allocation policies
  - Execute tasks
  - Monitor the progress of running jobs
  - Manage system recovery against faults (Fault Tolerance)
  - Warns end of task and returns results
- The systems and resources involved can be heterogeneous (operating systems / hardware platforms / systems of different companies)
- It is the true 'brain' of GRID

#### 4.4 – The Applications

- 1) Some scientifical disciplines have been organized themselves during the past decades in big collaborations grouped in an big quantity of scientists in order to achieve the goals of high level (which would not be posible with smaller research.
- These groups have obtained scientifical results and discoveries of great impact; they have been linked to the solving of important technological challenges (i.e. HEP experiments, Genoma Project, Chemistry, etc)
- 3) In the filed of the ICT (Information and CommunicationTechnologies) they have evolved from 'mainframes' solutions, going through computer cluster, and now GRID and Cloud Computing.



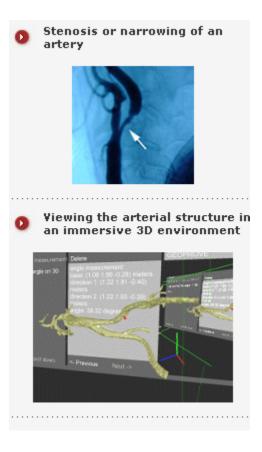
#### El GRID aplicado a enfermedades vasculares

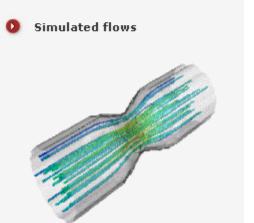
- Dos procedimientos: stent y bypass
- El cirujano se ayuda con imágenes 3D obtenidas con scanners CT y MRI
- Las simulaciones de una posible intervención ayuda a la toma de decisión por

parte del médico



El GRID permite lanzar los cálculos pertinentes. Se utilizan los recursos de los centros que participan en el proyecto (CROSSGRID)





Investigación coordinada por la Universidad de Amsterdam y con la colaboración Del CSIC y de todos los centros de CROSSGRID

#### **Architecture:**

#### ✓ Workload Management System

- Responsible for the distribution and management of tasks through GRID resources, such that the applications are convenient, efficient and effectively executed
- Essentially provides tools to coordinate jobs and ask about their status
- ✓ CE: Computing Element: it Is a set of services that provide access to the local batch system running on a farm. Typically the CEs provide access to a set of job queues within the batch system.
- ✓ Security Service: To use GRID, users must obtain and renew their 'certificates' from a CA -Certification Authority

#### ✓ Information Services:

✓ The information services publish and maintain data about GRID resources

- ✓ **Gestión de Datos: Data management** in the GRID, data files can be replicated in many sites. The users and the applications don't need to know where the files are placed, and they use Logical File Names (LFNs) in order to have a reference to them.
  - ✓ **SE:** is a logical entity which provides storage space for GRID-- Mass Storage System (MSS), disk cache or disk cache with tape.
- ✓ **Accounting:** The purpose of "Accounting" is to have an exact view of the use of the resources and services in the grid until that moment. The "Accounting" should not lose any data or registration. The main theme is to have a historical view so it is acceptable to delay information. However this should be as accurate as possible.
- ✓ Virtual Organisation Membership Services (VOMS): Is a system for managing authorization data within multi-institutional collaborations. VOMS provides a database of user roles and capabilities and a set of tools to access and manipulate the database and use the contents to generate user credentials when needed

#### 5- e-Science: Definition and activities. Classification

#### 5.1- Definition

\* The one given in the White Book in e-Science:

#### *€* (nhanced) Science:

is the set of scientific activities developed by means of the usage of distributed resources accessible through internet

 The term 'e-Science' denotes the systematic development of research method that exploit advanced computational thinking (Prof. Malcom Atkinson)

Such methods enable new research by giving researchers access to resources held widely-dispersed computers as though they were on their desktops. The resources can include data collections, very large-scale computing resources, scientific instruments and high performance visualization

#### ... or in a more detailed way....

- Distributed Computing
  - Masive simulations in international collaborations
  - Data processing and proposed estructures
- Storage of huge quantity of shared data
  - Data of Experiments and results from simulations
  - Digital repositories and Data Bases of common interest to several centres.
- Teleoperation of Scientific Instrumentation
  - Telescopies
  - Sensors and detectors
- Advanced collaborative Tools
  - AccessGrid Rooms
  - Teleinmersion and Virtual Reality

#### 5.2 e-Science projects

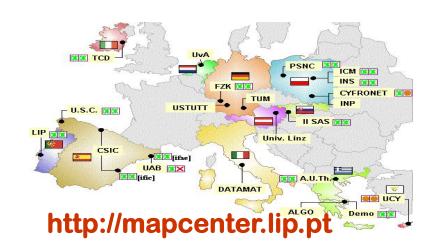


as R&D project (start)

as R&D GRID project

European Project 5PM. 21 partners. IFIC and IFCA (CSIC) Objective: Establishment of an interactive GRID with several applications in different Fields of Science (Particle Physics, Meteorology, Medicine, Atmospheric Pollution.

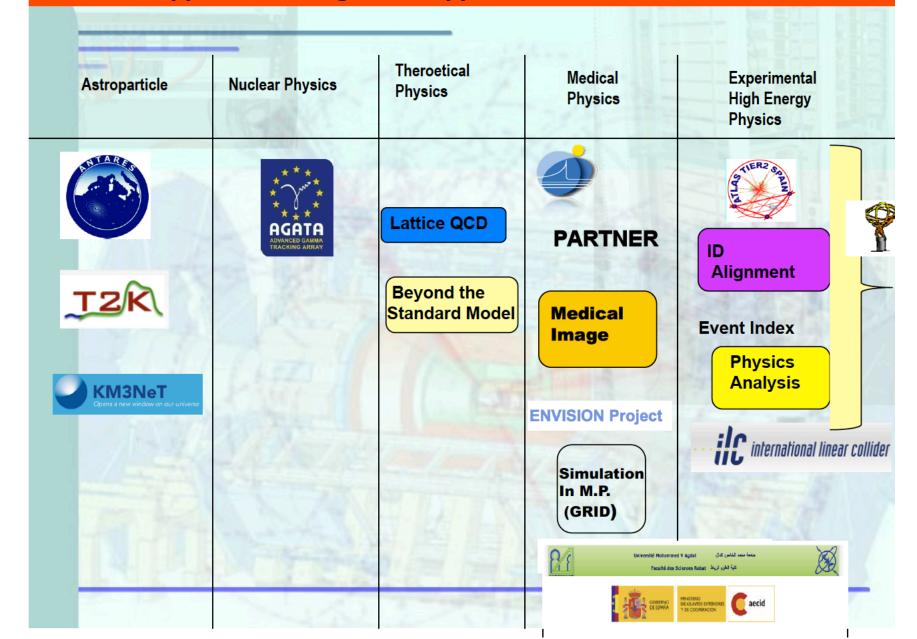
We have obtained many lessons from CrossGRID
The multidisciplinary aspect of the project has been very helpful







#### Scientific Applications migrated/supported in GRID at IFIC



#### **Historic Antecedent: IRISGRID**

#### Objetive

Launch a Thematic Network to promote the use of GRID technologies

Analyze the possibility of organizing an e-Science program in Spain

Review existing GRID initiatives

Support and promotion of participation in calls for proposals of the Sixth Framework Program of the European Union

- Involved Centers: 23 centers
- White Book of e-Ciencia







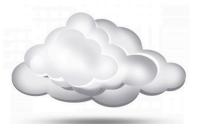


#### 6.- The computing Ecosystem at present

- The scenario has changed due to:
  - The very good performance of the network in terms of latency and bandwidth,
  - The improvement the quality/ cost ratio for the computer equipments (commodity solution)
  - Supercomputers has followed a growing trend during the last decades
  - Cloud Computing emerges as another solutions for given computing problems

Computer cluster





**Cloud Computing** 







Supercomputers

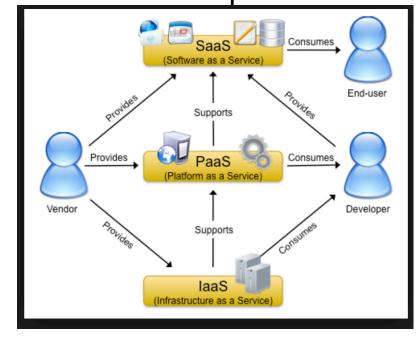
#### **CLOUD COMPUTING: Basic Concepts**

 According to NIST\*, Cloud Computing is a model for enablong ubiquitous, convenient, on-demand network access to a shared pool of configurable computing resources (e.g. networks, servers, storage, applications and services) that can be rapidly provisioned and released with minimal management effort or service provider

interaction

5 esential elements:

- On-demand self-service
- Broad network access
- Resource pooling
- Rapid elasticity
- Measured service
- 3 basic service models:



<sup>\*</sup>NIST = National Institute of Standard Technology

#### 7- From GRID Computing to Big Data

#### GRID

- : Las tecnologías GRID están suponiendo un gran avance en la forma de trabajar de los científicos y tecnólogos en los principios del siglo XXI
- También están proporcionando resultados operacionales muy relevantes
- El potencial del GRID es muy alto: quedan muchos aspectos a atacar y en perspectiva.

#### Cloud Computing- HPC

#### E-Ciencia:

- Los proyectos de e-Ciencia (DataGrid, CrossGrid, EGEE, Int.eu.grid, EELA, etc) han sido fundamentales para el desarrollo del GRID en el mundo
- La e-Ciencia se está desarrollando muy activamente en Europa. España posee la masa crítica para que se plantee un Programa de e-Ciencia. El primer paso se ha dado: se ha constituido la Red Nacional de e-Ciencia.
- Iniciativa GRID-CSIC:
- Big Data-Machine Learning-Data Mining

- The situation is now:
  - Open Science
  - New technologies are influencing in new initiatives and updates



- Thanks
- Questions