

# **Comput-ER: l'infrastruttura e i servizi di calcolo e archiviazione distribuiti per le comunità scientifiche e non in Emilia Romagna**

Marco Bencivenni (IGI & INFN-CNAF)

On behalf of the DUCK collaboration – [www.comput-er.it](http://www.comput-er.it)

09/11/2011 – GARR Conference 2011 - Bologna

# Overview

- DUCK collaboration
- Grid
- Comput-ER infrastructure and the Italian Grid Infrastructure
- Ported Applications
  - Bioinformatics
  - Chemistry
- Conclusion

# DUCK

## (Distributed Unified Computing for Knowledge)

- Collaboration between **multidisciplinary** Academic and Research Institutions located in the Emilia Romagna region aiming to:
  - exchange knowhow to solve scientific computing problems
  - contribute to the development of software services and of distributed computing/data infrastructure in collaboration with the Italian Grid Infrastructure (IGI)
  - extend the services and the infrastructure to other communities in the region like medicine, public administrations and private organizations.

# DUCK Partners

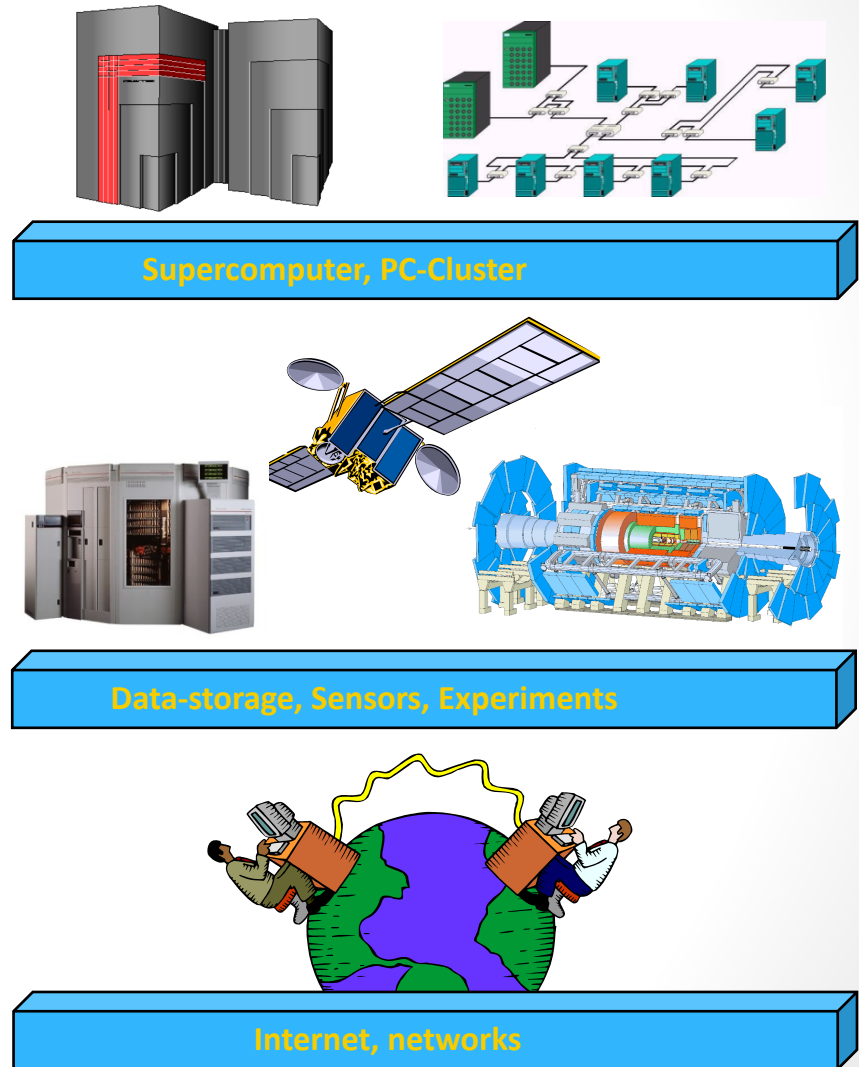
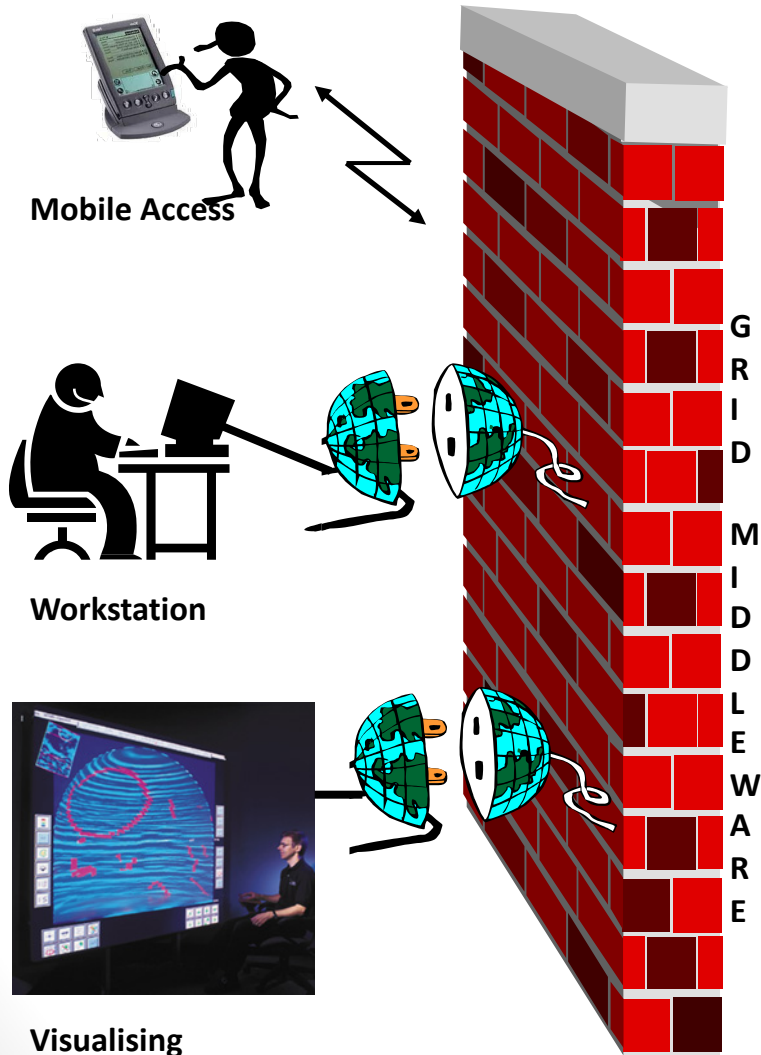
1. National Institute of Nuclear Physics, units INFN-BO and INFN-CNAF
2. National Institute of Geophysics and Vulcanology (INGV), unit in Bologna
3. The Euro-Med Center for Climate Change (CMCC), unit in Bologna
4. Interdepartmental Center for Research on Cancer "GIORGIO PRODI" – University of Bologna
5. Bologna Computational Biology Network / Department of Evolutionary Experimental Biology, University of Bologna
6. CeIRG, Interdepartmental Center for Genomics Research, University of Modena and Reggio Emilia,
7. National Research Council,CNR, and National Institute of Astrophysics (INAF) in Bologna Area
8. Physics Department, University of Ferrara
9. Physics Department of Alma Mater Studiorum-University of Bologna
10. Physics Department, University of Parma
11. Department of Computer Science, University of Bologna



# Grid: what is it ?

- Computational Grid is a collection of distributed, possibly heterogeneous resources which can be used as an ensemble to execute large-scale applications
- The three fundamental properties of Grid computing:
  - 1) coordinating resources that are not subject to centralized control
  - 2) using standard, open, general-purpose protocols and interfaces
  - 3) delivering nontrivial qualities of service
- From “The Anatomy of the Grid: Enabling Scalable Virtual Organizations” *enable “groups of users (**virtual organizations**)” to share geographically distributed resources as they pursue common goals – assuming the absence of...*
  - central location, control, omniscience, existing trust relationships.

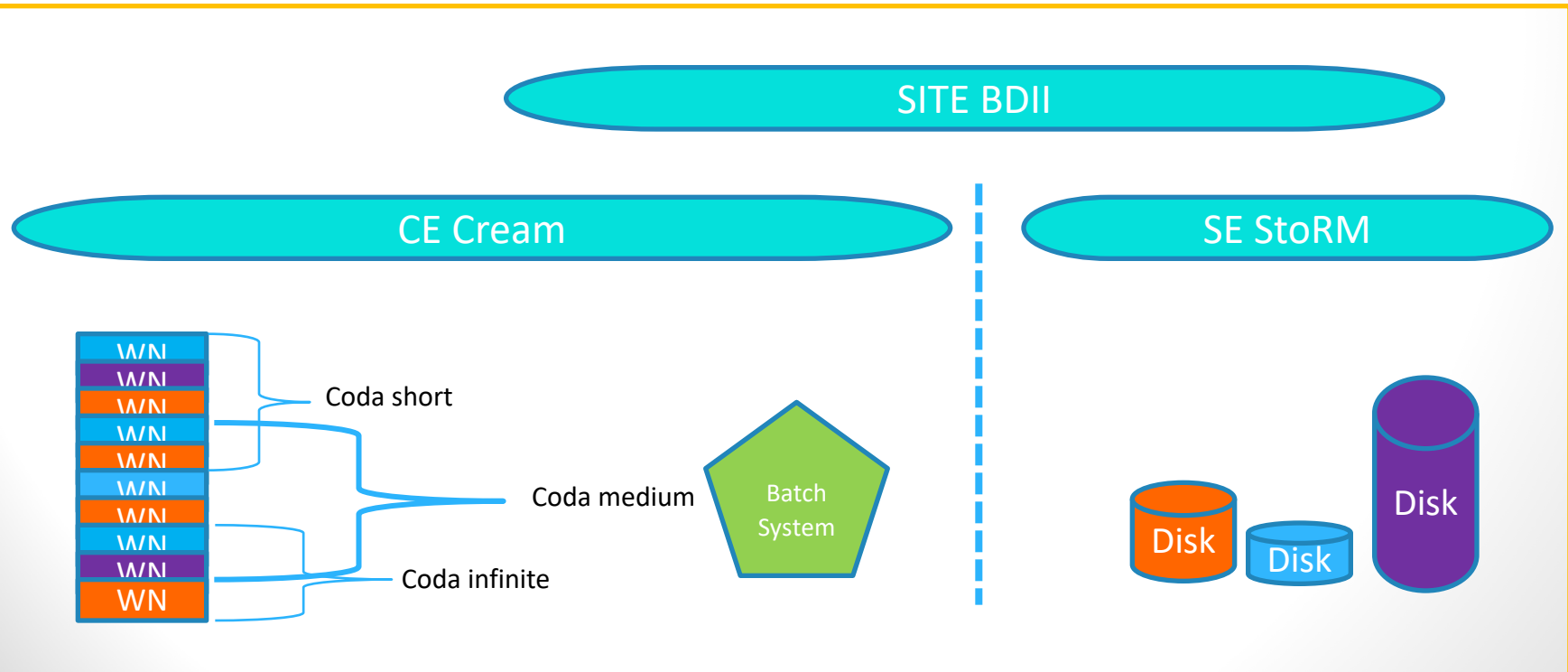
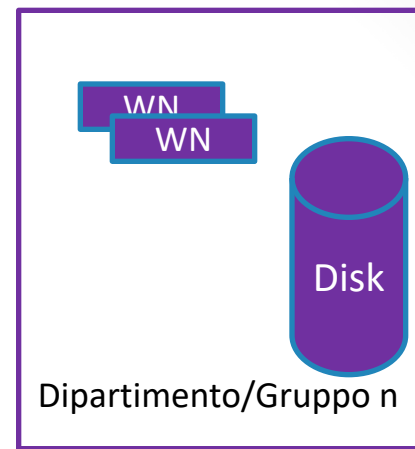
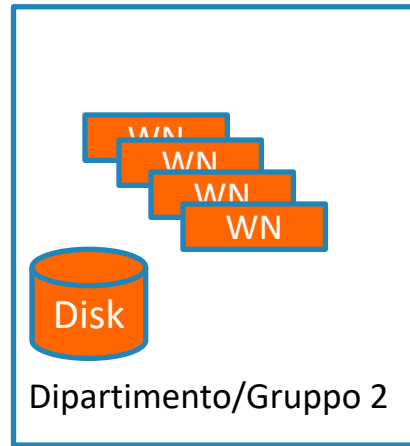
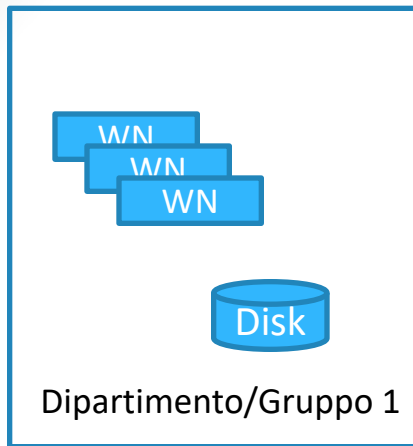
# The Grid Paradigm

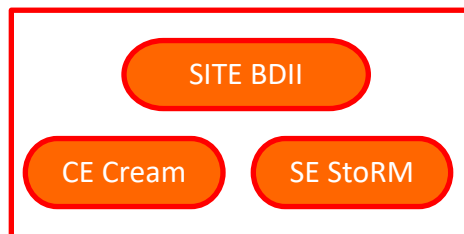
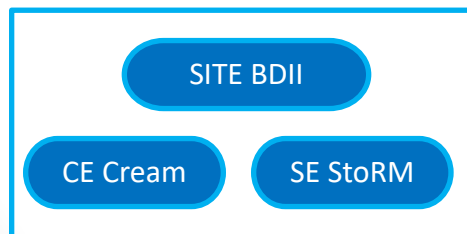
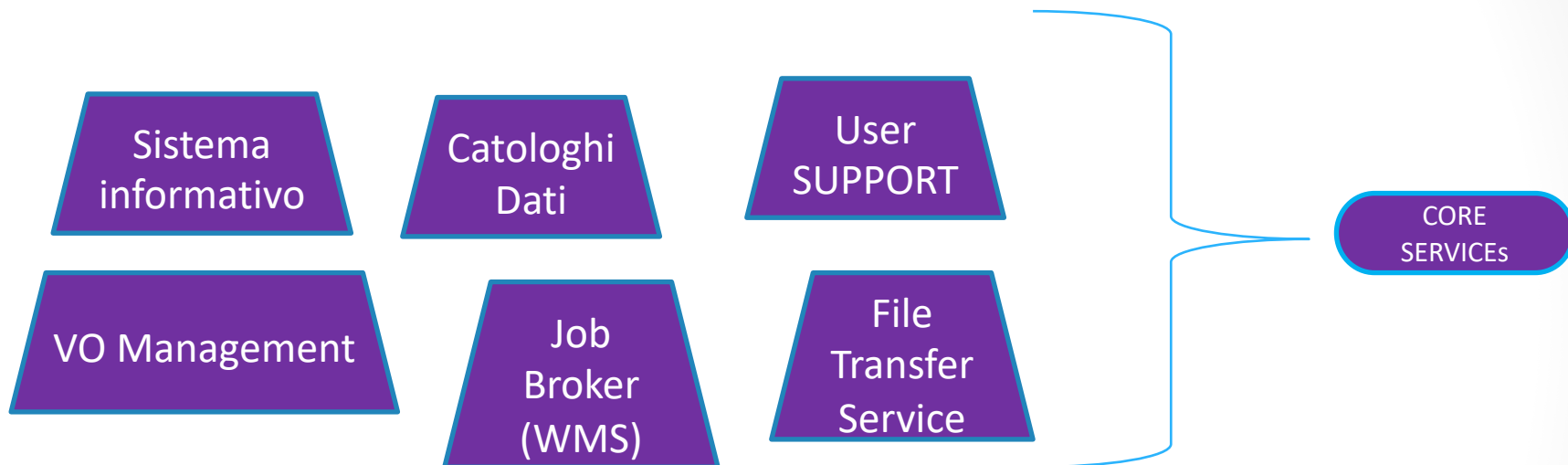


# Middleware Distribution



- **gLite** distribution is an integrated set of components designed to enable resource sharing. In other words, this is middleware for building a grid.
- The gLite middleware was produced by the [EGEE](#) project and it is currently being developed by the [EMI](#) project.
- The distribution model is to construct different services from these components and then ensure easy installation and configuration on the chosen platforms (currently [Scientific Linux](#) versions 4 and 5, and also [Debian 4](#) for the WNs).
- gLite middleware is currently deployed on hundreds of sites of different Distributed Computing Infrastructures (DCIs) and enables global science in a number of disciplines, notably serving the [LCG](#) project.  
<http://glite.cern.ch/>
- Middleware support is coordinated by IGI at Italian Level and by EGI-InSPire at European Level





~300 Resource Centers (~60 in Italia)

# The Job Submission Actors

**Grid Resources:** CE (Computing element), WN (Worker Node), SE (Storage Element)

**User:** ...well you know who you are...

**UI:** a machine containing a collection of clients to access the Grid services

**WMS:** responsible for dispatching user jobs selecting the best possible resource according to the job requirements

**LB:** contains detailed information about jobs lifecycle – tightly coupled to the WMS

**IS:** information system – contains an updated snapshot of what is contained in the Grid

**LFC:** a file catalog, links logical file names to physical locations

# Grid advantages: site

- Make better use of existing resource
- Monitoring tools
- Accounting tools
- Support for site managers
  - Installation, upgrading, problems, ticketing system
- Coordination of security aspects

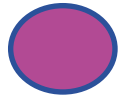
# Grid advantages: user

- Can solve larger, more complex problems in a shorter time
- Easier to collaborate with other organizations
- Support for users
  - Application porting

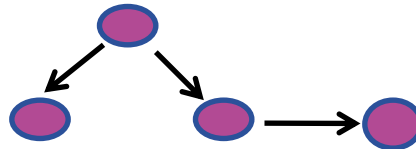


# WMS Supported Job Types

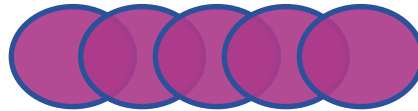
- Batch-like



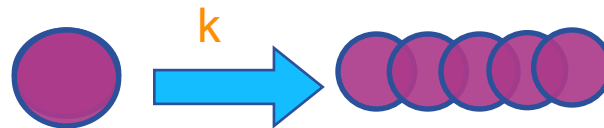
- DAG workflow



- Collection



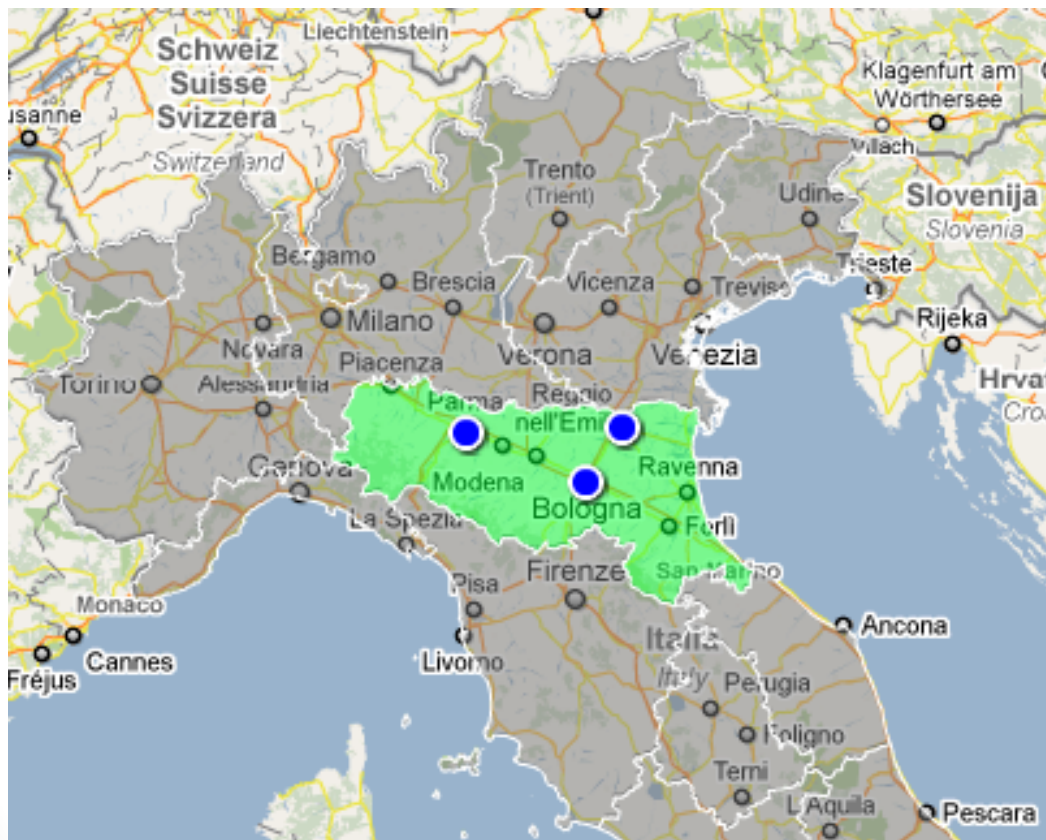
- Parametric



- MPI



# Comput-ER Sites and Resources (Computing in Emilia Romagna)



**Total Available Resources:**

**~1300 cores**

**~150 TB of storage space**

**8 SITES provided by  
DUCK partners**

• **INFN-CNAF**

• **INFN-BOLOGNA**

• INFN

• Dip. Fisica

• **INFN-FERRARA**

• INFN

• Dip. Fisica

• **AREA-BO**

• *IRA/INAF-BO*

• *OATS/INAF-BO*

• *ISMAR/CNR-BO*

• *ISOF/CNR-BO*

• **INFN-PARMA**

• Dip. Fisica

• **INGV**

• **CMCC**

# Comput-ER infrastructure

- Comput-ER is based mainly on commodity farms but new GPU-based servers for parallel applications are under testing.
- Comput-ER uses the gLite middleware.
- These resources are either based on real hardware systems, or are dynamically provisioned via virtual machines using the Worker Nodes on Demand Service (WNoDeS) grid/cloud virtualization system (Cloud Computing is foreseen in the near future).
- A **Virtual Organizations** (comput-er.it) has been setup and deployed on the resource sites provided by the DUCK partners
- Comput-ER is foreseen to be used by private organizations

Marco Bencivenni - GARR Conference 2011  
Bologna  
09/11/11

- $$\begin{bmatrix} 16 \end{bmatrix}$$



# Applications on Comput-ER

- Common characteristics :
  - Communities located in Emilia Romagna (even if belonging to national institution)
  - Owing limited hw resources compared to their computational needs
  - No or very limited previous Grid experience
- Research fields:
  - Bioinformatic/Biomedicine: protein annotation, genome sequencing
  - Geophysics: mid ocean ridge processes, ensemble methods for ocean forecasting
  - Computational Chemistry: Molecular Dynamics
  - RadioAstronomy/Astrophysics
  - High Energy Physics
  - Solid state Physics

# Example of Applications in the field of Bioinformatic/Biomedicine and Biocomputational Chemistry ported on Comput-ER



# Protein Annotation

(Biocomputing Group, University of Bologna)

Protein annotation is essential for understanding diseases at the molecular level

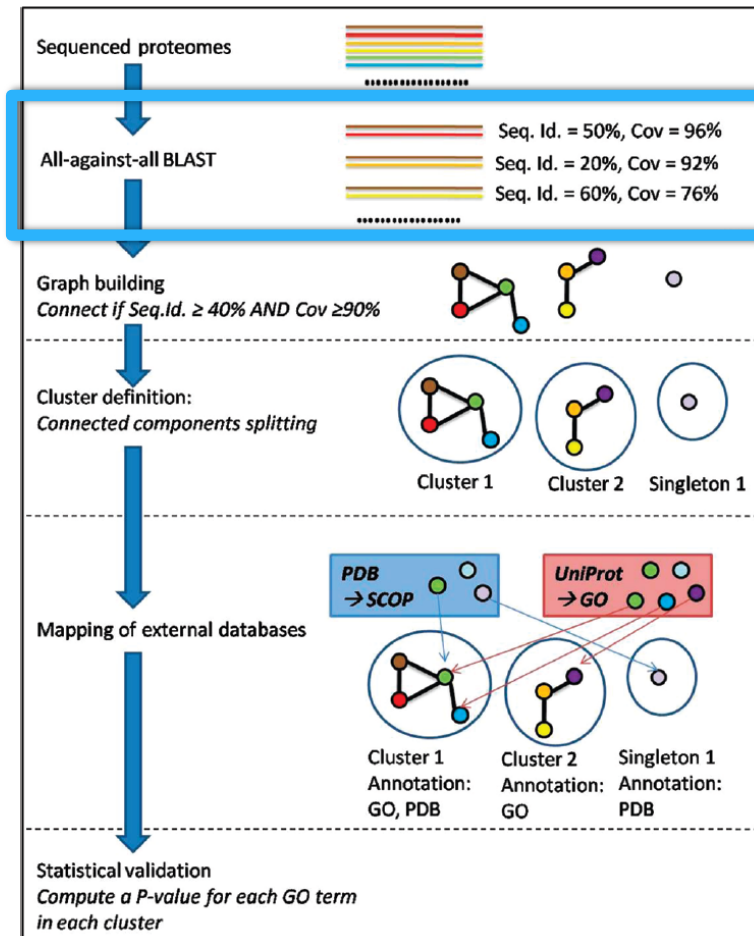
Bologna Annotation Resource (BAR) method was used

BAR uses the BLAST software for aligning the sequence: the number of computations is the Cartesian product of the number of the input sequences.

$\sim 17 \times 10^{13}$

Problem: the amount of time to do these alignments is estimated in seven years on the local resources of the group

## BAR Method

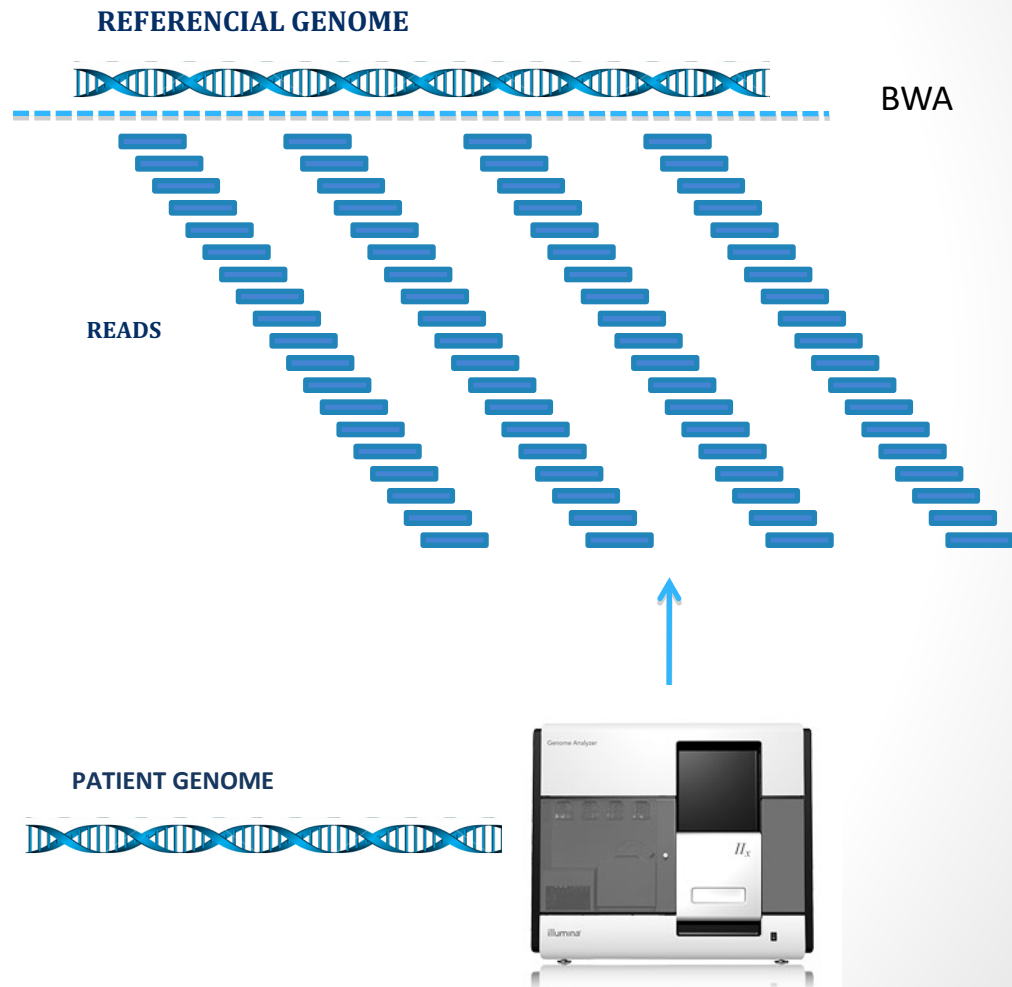


The alignment step was the gridified one

# Massively Parallel Genome Sequencing

(Biocomputing Group, University of Bologna & “Giorgio Prodi” Cancer Research Center)

- Used in the study of cancer diseases
- Next generation sequencing technology allows a massive amount of DNA or RNA fragments to be sequenced in a single experiment.
- For the *massively parallel sequencing* it is used **BWA** tool (Burrows-Wheeler Aligner) for indexing and alignment
  - Memory request ~ 3,5 GB
  - Total time ~ 50h using the group local resources
- Problem: it is more the time to elaborate the data than the time to produce them. With the consequence to accumulate data in storage element.





# Results for BLAST and BWA

Application	Local	DUCK Grid	GPU preliminary
BLAST	7 yrs	1/120 (3 weeks)	½ CPU result (1 cpu core vs 1cpu core + 1 TESLA GPU) (high memory demanding)
BWA	50 h	1/4	

**Same solution:** parametric jobs were used to parallelize the computation.  
In this way it is the WMS doing most of the work.

**Authors: Biocomputing Group, University of Bologna**

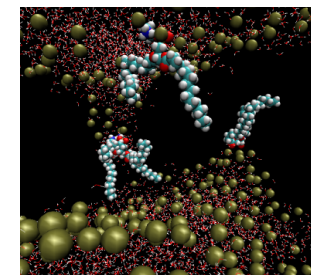
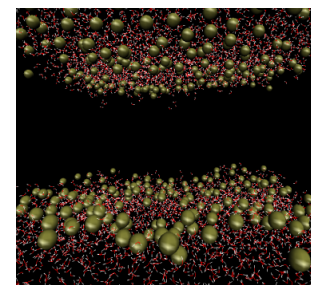
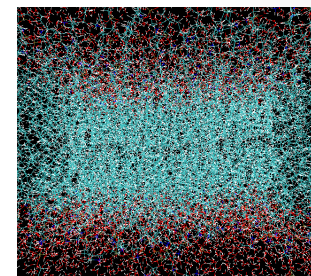
CASADIO Rita , INDIO Valentina, FARISELLI Piero, ZAULI Andrea, MARTELLI Pier Luigi,  
PIOVESAN Damiano, ROSSI Ivan

# Molecular Dynamics

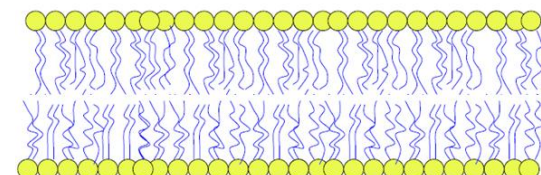
(ISOE-CNR - National Research Council-Institute for the OrganicSynthesis and Photoreactivity, Bologna Unit)



- Electroporation through dynamics of a lipid bilayer induced by electric fields.  
It is a widely used technique for permeabilization of cell membranes.
- Applications :
  - DNA Transfection or Transformation
  - Direct Transfer of Plasmids Between Cells
  - Induced Cell Fusion
  - Trans-dermal Drug Delivery
  - Cancer Tumor Electrochemotherapy
  - Gene Therapy



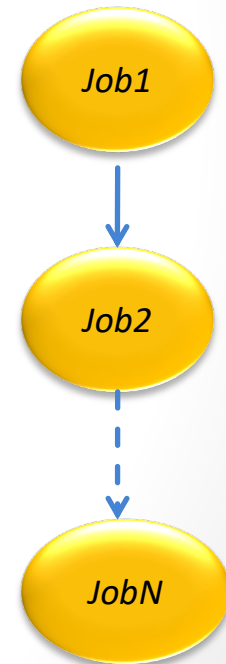
**z** ↑



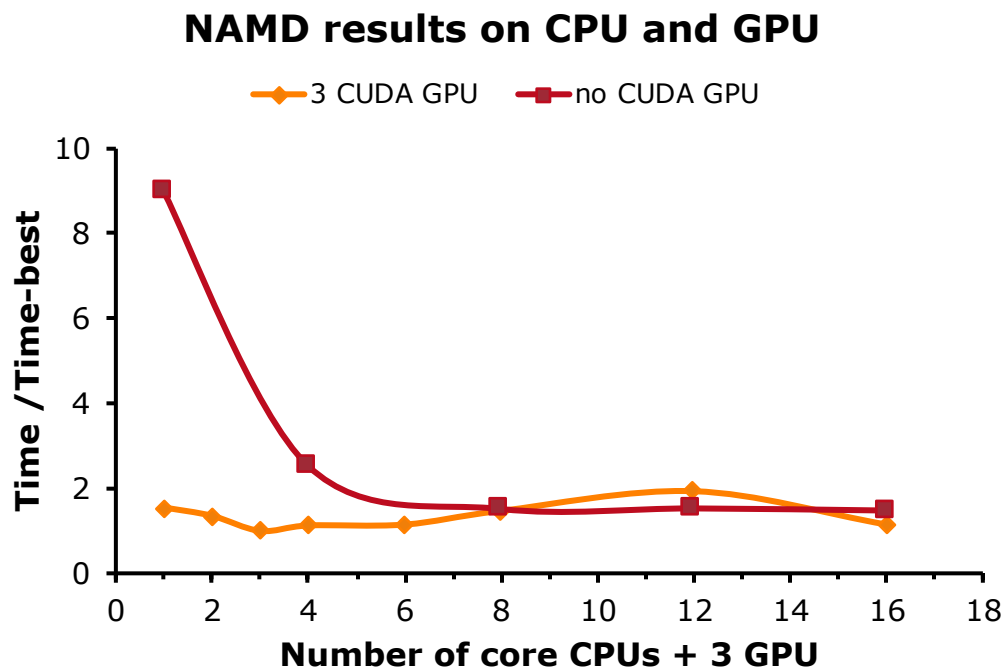
External field of 0.35, 0.5 and 1.0 V/nm was applied parallel to the membrane normal z

# Molecular Dynamics Computational Problem

- Huge molecular systems to be simulated: from 35 to 65 katoms
- NAMD package used (<http://www.ks.uiuc.edu/Research/namd/>)
- OPENMPI long parallel runs needed
  - Single run too long for a Grid job
    - 41 days (35katoms – 25 ns sym\_time) on 8 cores
    - 18 days (35katoms – 25 ns sym\_time) on 32cores
  - Computation split into N sequential MPI jobs
  - Two parameters influence the computational time:
    - N: number of jobs – set to 50
    - CPU\_NUM: number of required cores – set to 32
  - 1 day lost in Grid with respect to local run
    - Depends on the Grid load
  - Need bigger MPI enabled site



# Molecular Dynamics GPU tests



Preliminary results using a 16 cores + 3 TESLA GPU machine

Need further investigation

# Conclusion and future works

- DUCK and Comput-ER allowed to share computing resources between small, local communities
- The Comput-ER infrastructure together with the support of the NGI staff demonstrated to be a powerful and flexible tool for their research
  - Applications got benefits not only in sharing resources but also in knowledge-sharing from a multidisciplinary scientific computing environment
- For most of the applications the key solution is based on their execution as loose parallel applications. For some of them, MPI and GPU has been investigated, good results have been obtained but more testing is required
- DUCK is working to open Comput-ER services to private sectors
- IGI is developing a Grid web portal in order to easy the user in job submission, data management, certificate management and VO membership using Identity Federation (IDEM) attribute released by IDPs.

# Authors

- **Biocomputing Group, Bologna Computational Biology Network, University of Bologna**
  - CASADIO Rita , INDIO Valentina, FARISELLI Piero, ZAULI Andrea, MARTELLI Pier Luigi, PIOVESAN Damiano, ROSSI Ivan
- **“Giorgio Prodi ” Cancer Center Research , University of Bologna**
  - PANTALEO Maria Abbondanza, ASTOLFI Annalisa, BISCO Guido, INDIO Valentina, MARTELLI Pier Luigi, CASADIO Rita
- **CNR/ISOF (National Research Council-Institute for the OrganicSynthesis and Photoreactivity), Bologna Italy**
  - OTTANI Stefano, VENTURINI Alessandro
- **INFN–CNAF (National Institute of Nuclear Physics – National Computer Science Center)**
  - GHISELLI Antonia
- **INFN–CNAF & IGI (Italian Grid Initiative), Bologna Italy**
  - BENCIVENNI Marco, CESINI Daniele, VERONESI Paolo

# Questions?

[www.comput-er.it](http://www.comput-er.it)