

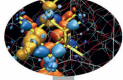
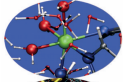
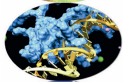
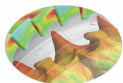
# HPC methods for Engineering

**HPC facilities: overview and the engineering production environment**

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- **Cineca** is a non profit Consortium, made up of 70 Italian universities, 4 Italian Research Institutions and the Italian Ministry of Education.
- Today it is the largest Italian computing centre, one of the PRACE Tier-0 hosting site, one of the most important worldwide.
- With more 700 employees, it operates in the technological transfer sector through high performance scientific computing, the management and development of networks and web based services, and the development of complex information systems for treating large amounts of data.
- Cineca has three locations: Bologna, Milan and Rome

**Mission:** Cineca offers support to the research activities of the scientific community through supercomputing and its applications



- **SCAI**(SuperComputing Applications and Innovation) is the High Performance Computing department of CINECA, the largest computing centre in Italy and one of the largest in Europe.
- The mission of SCAI is to accelerate the scientific discovery by providing high performance computing resources, data management and storage systems, tools and HPC services, and expertise at large
- aiming to develop and promote technical and scientific services related to high-performance computing for the Italian and European research community.
- CINECA enables world-class scientific research by operating and supporting leading-edge supercomputing technologies and by managing a state-of-the-art and effective environment for the different scientific communities.
- The SCAI staff offers support and consultancy in HPC tools and techniques and in several scientific domains, such as physics, particle physics, material sciences, chemistry, fluid dynamics



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Cineca is currently one of the Large Scale Facilities in Europe and it is a PRACE Tier-0 hosting site.

<http://www.hpc.cineca.it/content/hardware>

- 1 FERMIL (Tier-0): It is a IBM BG/Q supercomputer, classified among the most powerful supercomputers in the Top500 List: rank 7th in June 2012. On June 2012 it was ranked 11st in the Green500's energy-efficient supercomputers list.  
It will be replaced by a new Tier-0 system at the end of the 2015
- 2 GALILEO (Tier-1): it is a IBM NeXtScale cluster accelerated with Intel Phi's and (GPUs): in full production February the 2nd, 2015. It will be upgraded shortly with a bunch ( $\simeq 100$ ) Nvidia K80 Gpu. It will reach around 100th position in the next top500 list.
- 3 PICO: BigData infrastructure has been recently acquired (Nov 2014) devoted to "Big Analytics".



High-end system, devoted for extremely scalable applications

- IBM power2@1.6 Ghz
- 10240 computing nodes, 16 core each (163,840 total)
- 16 GB or RAM per computing node, 163 TB of Total RAM
- Proprietary Network (5D torus)
- Peak performance 2PFlops

x-86 based system for production of medium scalability applications

- Intel Xeon E5-2630 v3 @2.4 GHz (a.k.a Haswell)
- 516 computing nodes, 16 core each (8,256 total)
- 128 GB of RAM per computing node, 66 TB of Total RAM
- Infiniband QDR ( $\simeq 40\text{Gb/s}$ )
- 768 Intel Phi 7120p (2 per node)
- Nvidia K80 ( $O(100)$ )
- 8 nodes devoted to login/visualization
- Peak performance 1.2 PFlops
- $\simeq 480$  GFlops single node LINPACK (only CPU) sustained performance



## Processing system for large volumes of data

- Intel Xeon E5 2670 v2 @2.5 GHz (a.k.a Ivy Bridge)
- 66 computing nodes, 20 core each (1320 total)
- 128 GB or RAM per computing node, 8.3 TB of Total RAM
- Infiniband FDR ( $\simeq 56\text{Gb/s}$ )
- 4 nodes devoted to login/visualization
- Peak performance  $\simeq 40\text{Tflops}$
- $\simeq 400\text{GFlops}$  single node LINPACK (only CPU) sustained performance

- Each system has:
  - a */home* area
  - a */scratch* area
  - a */work* area (project-based)
- a common */gss* area ( $\simeq 3PB$ )
  - shared by all login nodes
  - shared by all PICO computing nodes
  - Tape subsystem (LTFS, up to  $\simeq 12PB$ )

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User Portal: <http://www.hpc.cineca.it/content/users>

It is organized in sections:

- Getting started: you have to register yourself to the UserDB portal to get a valid login, once you have an active project (see next talk) you can access to CINECA facilities
- Get in touch: register to the mailing list to be upgraded about the status of the machine
- Help desk: [superc@cineca.it](mailto:superc@cineca.it) for any problem/help/support
- Documentation: User Guide, FAQ et al....



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## The module eng

- Available on Galileo, HPC cluster for production

```

*
* Welcome to GALILEO @ CINECA - NeXTScale cluster - CentOS 7.0!
*
*
*
* 516 Compute nodes:
* - 2 octa-core Intel(R) Xeon(R) CPU E5-2630 v3 @ 2.40GHz per Compute node
* - 128 GB RAM per Compute node
* - 2 16GB Intel Xeon-Phi 7120P Accelerator per Compute node
*   (only on 384 nodes)
*
*
* 8256 Total cores
* Intel QDR (40Gb/s) Infiniband high-performance network
* PBSpro 13 batch scheduler
*
*
* http://www.hpc.cineca.it/content/galileo for a guide on GALILEO
* mailto: superc@cinca.it for support
*
*
*****
This system is in full-production.
Since February 23rd, the accounting of the consumed budget is active.

IMPORTANT: The Xeon Phi accelerators are available for production runs.
Please refer to our online guide for further info.
*****
[ispisso@node166 ~]$ module load profile/eng
[ispisso@node166 ~]$ module av
----- /cinca/prod/modulefiles/profiles -----
profile/advanced profile/base(default) profile/eng
----- /cinca/prod/modulefiles/eng/interpreter -----
----- /cinca/prod/modulefiles/eng/environment -----
autoload/0.1
----- /cinca/prod/modulefiles/eng/libraries -----
----- /cinca/prod/modulefiles/eng/compiler -----
intel/cs-xe-2015--binary
intelmpi/5.0.2--binary
intelmpi/5.0.3--binary
openmpi/1.8.4--intel--cs-xe-2015--binary
----- /cinca/prod/modulefiles/eng/tools -----
----- /cinca/prod/modulefiles/eng/applications -----
abaqus/6.14          consol/4.4          starccm+/9.02
ansys/150           openfoam/2.3.0     starccm+/9.04
ansys/160           pointwise/17.3R1  starccm+/9.06
[ispisso@node166 ~]$ █

```

- and much more: matlab, octave, tecplot, paraview hyperworks, Marc, Nx, ... (profile/advanced)

- List of (some) eng software available on Galileo: Linux 64 bit, Centos 7.0.

Software	Type	License	Version
Pointwise/GridGen	Meshing tools	ISV (Owner)	17.3R1
Ansys*	CFD/Mech	ISV (Hosting)	16.1
Starccm	CFD	ISV (Hosting)	
CFD++	CFD	ISV (Hosting)	
OpenFOAM	CFD	GPL (open-source)	2.3.0
Abaqus	multi-physic	ISV (Owner)	6.1
Comsol	4.4	ISV (Hosting)	4.4
matlab	prototype language	ISV (Hosting)	R2014a
octave	prototype language	GPL (open-source)	
Marc	structural mechanics	ISV (Hosting)	
Nx	structural mechanics	ISV (Hosting)	
paraview	cfD post-process	GPL (open-source)	
Tecplot	Post-processing CFD	ISV (Owner)	

\* not working internode with Infiniband only Ethernet waiting for next release

For the licensed software, this is the actual policy:

- CINECA hold only (some) pre- and post-processing software:  
Pointwise, Tecplot
- For some specific grant/agreement (example: LISA) the licenses can be purchased to be used by the beneficiaries of the grant
- Generally the policy is: *bring/use your own license*: Owner or Hosting
  - Owner
  - Hosting



## Experience:

- OpenFOAM **installed and tested** on our clusters: GALILEO, FERMI, PICO
- Used in **Several Academic project**: 37 ISCRA + 10 LISA + 1 PRACE (under evaluation)
- OpenFOAM in **FORTISSIMO** for the Enabling Manufacturing SMEs to benefit from HPC and Digital Simulation.
  - **Cloud-based Computational Fluid Dynamics Simulation** in collaboration with Konigsegg, ICON, CINECA and NTUA. DES solvers for Drag and Lift prediction of supercars.
  - **Shape Optimization under Uncertainty through HPC Clouds** in collaboration with Optimad Eng, University of Strathclyde and Automobili Lamborghini (OF + Dakota)
- Support for **industrial development**: 14 projects.
- CINECA has hosted two edition of the 'HPC enabling of OF for CFD applications', in November 2012 and March 2015



OpenFOAM can be installed for many users (network installation) or for a single user (local installation):

- **Network installation:** This installation is suitable when a group of people is supposed to use OpenFOAM, and when not everyone wants to learn how to install and compile it. All users will use exactly the same (base) installation.

Pro: A single installation for each version of OpenFOAM, maintained by the CINECA UserSupport.

Cons: limited to major release and most common used tools (swak4foam, pyfoam, dakota).

- **Local installation:** This is the most common way of installing OpenFOAM. The installation will be located in `HOME/OpenFOAM/OpenFOAM-3.x.y`.

Pro: Each user will 'own' his proper installation and may update it any time. For info on [installation](#)

Cons: Requires extra disk space for several users with their own installations (minor issue), and all users have to know how to install OpenFOAM and the Third-Party products (major issue)

## CINECA policies:

- Network installation only major 2.3.0, 2.4.0, ... 2.n.0 by default.
- Minor installation 2.3.1, 2.3.2, ... 2.3.4 upon request.
- profile base  $\Rightarrow$  last two majors + 1 minor.
- profile advanced  $\Rightarrow$  other versions
- Git and .x only local installation

## Network Installation status on HPC platforms:

- FERMI  $\Rightarrow$  version 2.1.1 (no upgrade possible due to issues with bgq-gnu/4.7.2 compiler)
- GALILEO version 2.3.0 + swak4foam/0.3.1 + pyfoam/0.6.4 + dakota 6.1
- PICO version 2.3.0

- RCM, Remote Client Manager
- Enginframe