CRESCO HPC

Energy Technologies Department – ICT Division
http://www.eneagrid.enea.it

Italian National Agency for New Technologies, Energy and Sustainable Economic Development

CRESCO: ENEA, the Italian National Agency for New Technologies, Energy and Sustainable Economic Development operates in a range of R&D sectors, including energy technologies, new materials, life and environmental sciences. In support of the institutional research activities, the ENEA IT division provides computing and storage resources. The computing core of ENEAGRID is represented by the HPC CRESCO clusters.

CRESCO HPC clusters

Cluster name (Linux x86_64)	Network	Cores/Tflops
CRESCO6 INTEL/SKL	OPA	20832/~1400
CRESCO4 INTEL/SNB	IB QDR	1024/~20
CRESCO4F INTEL/SNB	IB QDR	1024/~20
CRESCO4C INTEL/SNB	IB QDR	512/~10
CRESCO5F AMD/EPYC+NVIDIA/A100	IB EDR	1280/~100
XCRESCO IBM/PPC+NVIDIA/P100	IB EDR	2560/~250
Total		**~27232/~1800**

CRESCO Storage

Storage Systems CRESCO	Bandwidth GB/s	network	Capacity raw/net PB
2 x DDN SFA7790	20	IB EDR	4 /3.5
2 x DDN SFA7700	15	IB QDR	1 / 0.75
7 x RAID Servers	1.25	10 GEth	3.2 / 2.9
4 x RAID Servers	12.5	100 GEth	0.96 / 0.72
Total			~9 / ~8
Tape Library IBM 3500	LTO4/6	FC/8Gb	2.5 PB

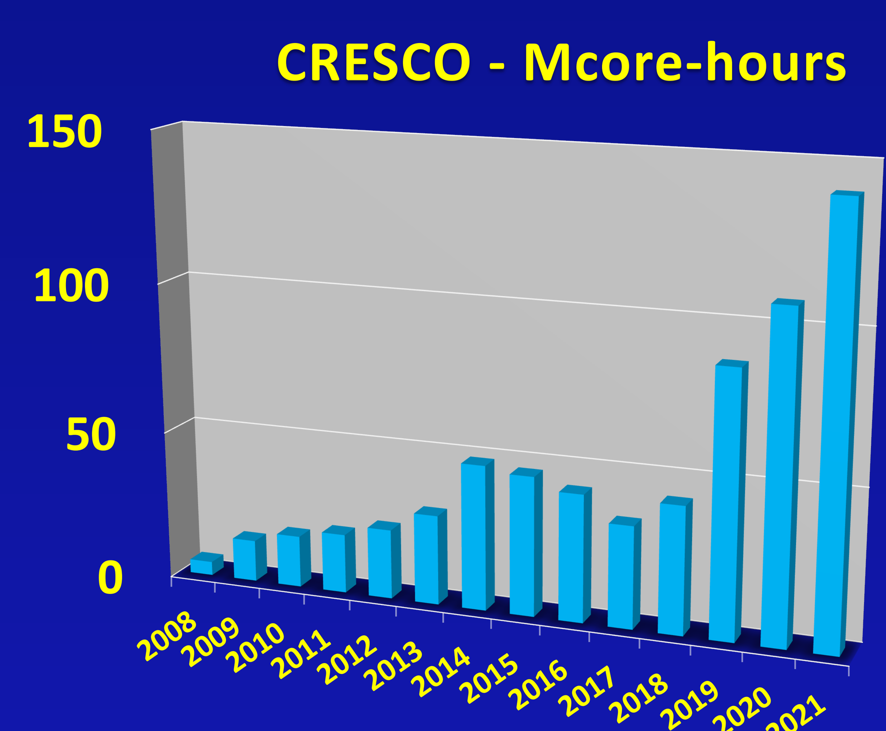
High performance storage systems based on DDN Infiniband QDR/FDR/EDR and GPFS Spectrum Scale parallel filesystem.

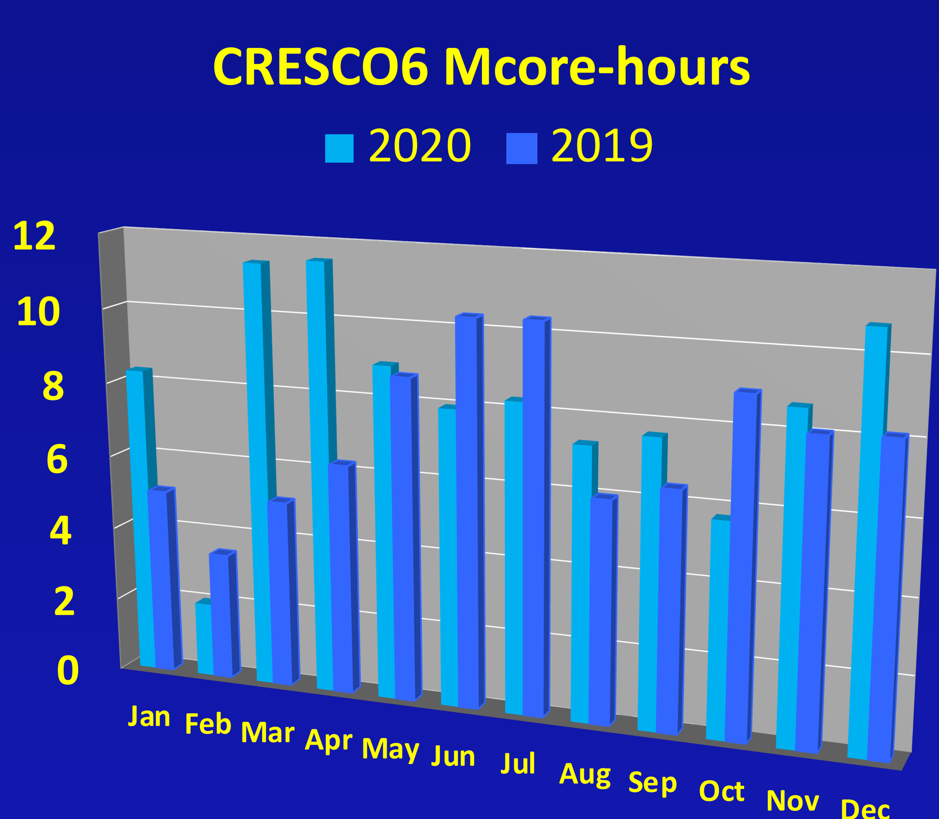
CRESCO HPC clusters are in operation in the 3 ENEA Research Centres: Portici, Frascati and Casaccia

CRESCO Usage in the time of COVID-19

CRESCO Usage in the time of COVID-19: High-Performance Computing and Data Analysis (HPC/HPDA) infrastructures contributed to face up the outbreak of SARS-COV2 in several research areas. Typical numerical applications include the design of new drugs and new physical barriers to reduce contagion, and the development of strategies based on epidemiological models to contain, mitigate and suppress the infection spread. Over the past two years, ENEA took part in this challenge with CRESCO, an HPC facility with 1.4 Pflops peak computing power. We made CRESCO available to projects requiring massive computing resources aimed at mitigating the impact of the COVID-19 pandemic. Since Spring 2020, CRESCO has run a large body of numerical simulations. It represented a powerful tool for the scientific community to model the molecular dynamics (MD) of drug-receptors. CRESCO made it possible to perform high-accuracy calculations of binding free energies and to carry out high-fidelity computational fluid-dynamics simulations of transport mechanisms and related fluid-dynamics of saliva droplets causing the virus contagion.

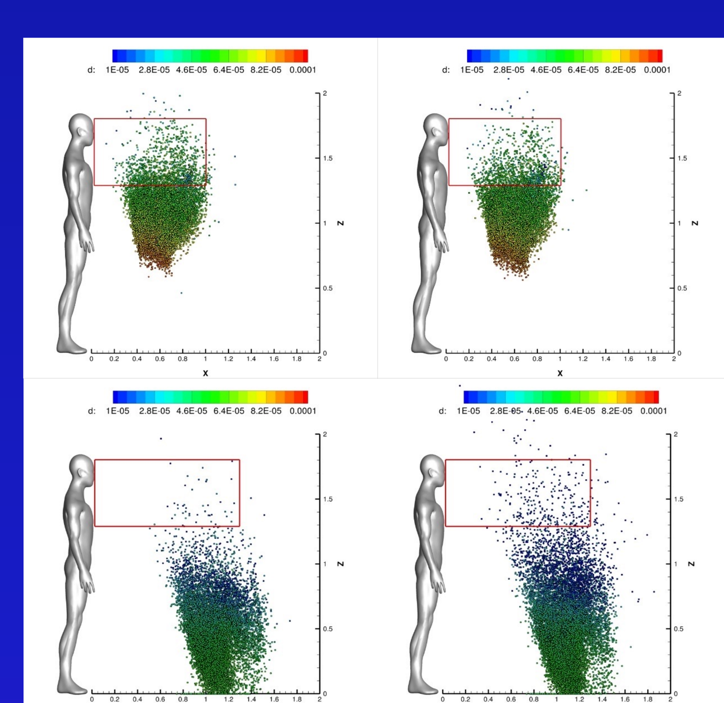
The plot on the right shows the computing work made by CRESCO (measured in terms of millions of core-hours) year after year over about a decade. Measurements include the activity of CRESCO1-2, the first ENEA HPC systems, installed in 2008 and featuring a peak power of 25 Tflops, that of CRESCO4, in operation since 2015 and featuring a peak power of 100Tflops, and the one of CRESCO6, with its peak power of 1.4 Pflops, running simulations since 2018.





The usage of CRESCO HPC systems in 2020 was ca. 110 Mcore-hours. What happened during the pandemic year 2020 is shown in the plot on the left. CRESCO6 usage peak in 2020 was in the months of March and April, during the first Italian lockdown, whilst the usage peak in 2019 was in the months of June and July

The main numerical simulations, carried out during the years of pandemic, have used Molecular Dynamic (MD) codes. Several of these codes belong to the open-source material-science community. They have undergone a process of code-refactoring in order to run efficiently on exascale heterogeneous systems. The main codes used in numerical simulations on CRESCO over the pandemic years are: GROMACS, CP2K and LAMMPS.



SARS–CoV–2 can be transmitted through airborne diffusion of saliva micro-droplets, travelling in the air via thermo-fluid dynamic interactions with it. Numerical simulations using CFD/OPENFOAM codes provided a contribution to thermo-fluid dyamic modelling of saliva droplets diffusion produced by coughing. A wide range of HPC computations were performed on CRESCO to give a better insight on:

- ✓ saliva droplets diffusion physics;
- ✓ the effectiveness of the social distancing rules adopted in Italy during the pandemic

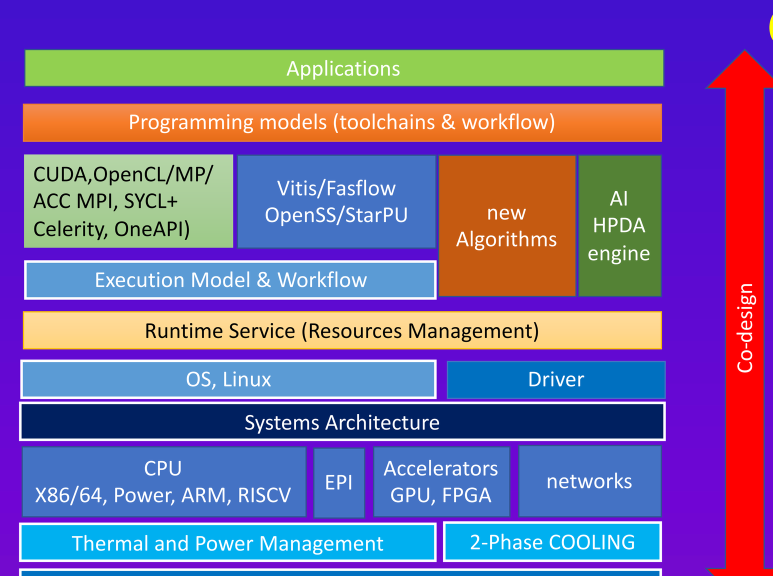
Supported Project: Towards EXtreme scale Technologies and Accelerators for EuroHPC hw/Sw Supercomputing Applications for exascale (http://textarossa.eu)

textarossa

EuroHPC Joint Undertaking

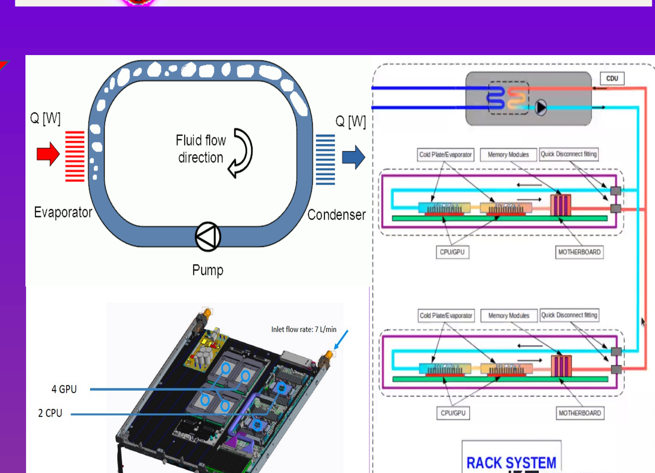
In the near future, Exascale systems will need to bridge three technology gaps to achieve high performance while remaining under tight power constraints:

- energy efficiency and thermal control;
- extreme computation efficiency via HW
- acceleration and new arithmetic;
- methods and tools for seamless integration of reconfigurable accelerators in heterogeneous HPC multi-node platforms



From a methodological standpoint, TEXTAROSSA adopts a co-design process as a key strategy for Fast Forward and Exascale computing, considering the entire system stack from underlying technologies to applications. The co-design process concerns five layers covering the whole HPC stack: 1. *User Application;* 2. *Runtime Services;* 3. *Programming Models;* 4. *System Architecture; Platforms;*

GPU/FPGA architectures



The HPC community provided several programming models that have demonstrated their potential to develop efficient applications. However, parallelization models are used separately, and most of them target CPUs or combinations of CPUs/GPUs, but not FPGAs. However, FPGAs open new possibilities that can be highly beneficial to almost any HPC application, providing toolchains to handle heterogeneous architectures.

2-Phase Cooling

In TEXTAROSSA, an optimized two-phase cooling solution for HPC is being developed and customized to fit the requirements of node and rack levels for Exascale applications