INAF
ISTITUTO NAZIONALE DI ASTROFISICA
NATIONAL INSTITUTE FOR ASTROPHYSICS

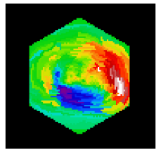
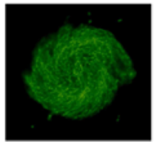
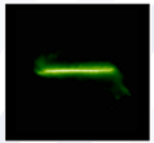
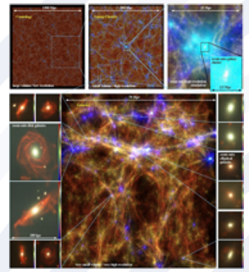
# Exascale Computing & Technology

Giuliano Taffoni on behalf of **EXACT (& daughters)**

# Scientific and Technical challenges

## High Performance Scientific computing for Numerical Astrophysics

- Next generation simulations
- Next generation Instruments

- Capture the complexity of the formation of cosmic structures and Astrophysical phenomena;
- Interpretative framework for the “tsunami” of observational data;
- **Re-design** to profit of new computing platforms
- Improve the “dynamical range” (from cosmological scales down into galaxies)

**The EXASCALE CHALLENGE**

**$10^{18}$ floating point operations per sec with increased power-efficiency**

# Scientific and Technical challenges

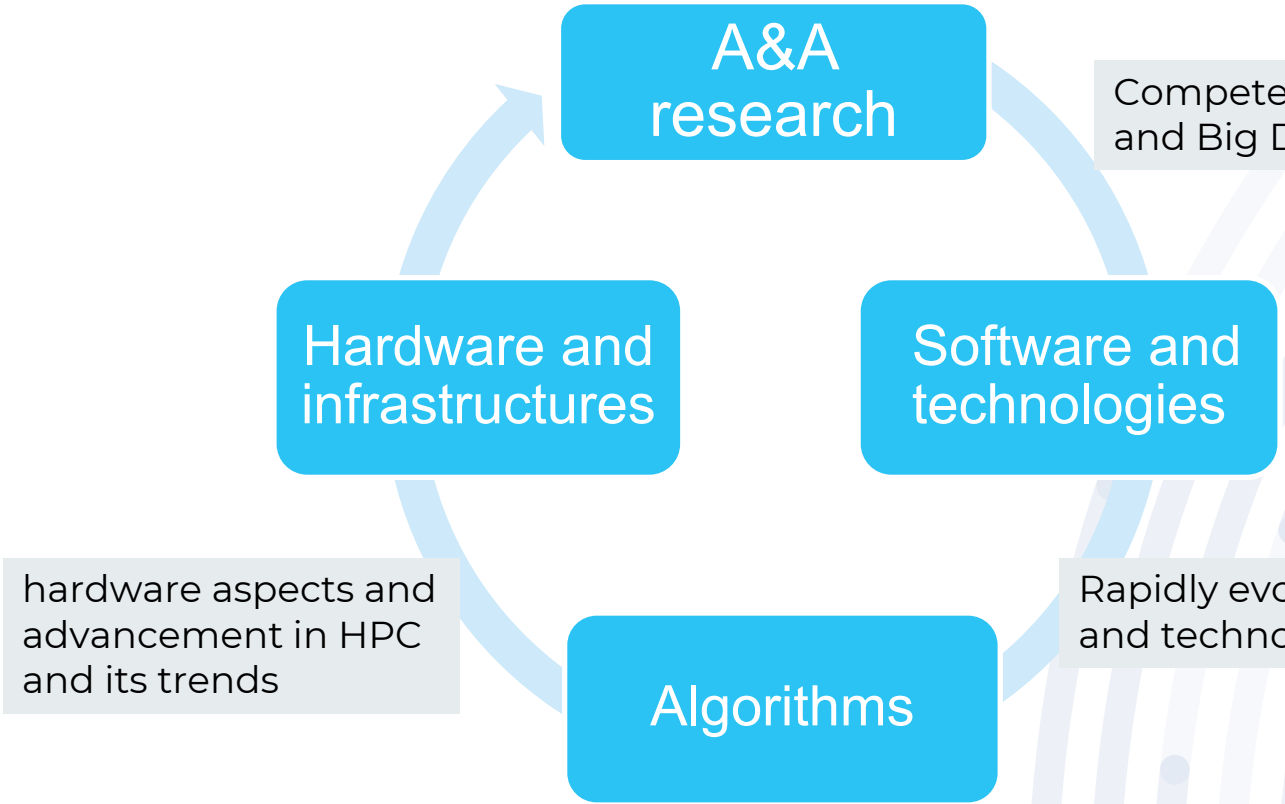
## Convergence of HPC and Data Analysis

- Next generation simulations
- Next generation Instruments

**10^20 Bytes of data**

**Cutting edge computing systems will be the sole approach to process datasets**

- New approach to data handling and analysis;
- New Algorithms
- Computing close to data & Science platforms;


A&A research
Competences in HPC and Big Data
Software and technologies
Rapidly evolving paradigms and technologies
Algorithms
hardware aspects and advancement in HPC and its trends
Hardware and infrastructures

# Hardware Technologies

- Prototype **Exascale platforms**: **lead integration** of European prototypes.
- New hardware (FPGA, Vector accelerators).
- Platforms based on **"reconfigurable" computing**
- **Micro-clusters** for EDGE computing: heterogeneous MPSoC boards
- Computing infrastructure for the Italian SDC of the EUCLID project
- **High performance storage** (Luster, BeeGFS, SWIFT ObjectStorage)
- "Classical" computing and storage platforms

**Projects:**

**ExaNeSt**

**EuroEXA**

**ESCAPE**

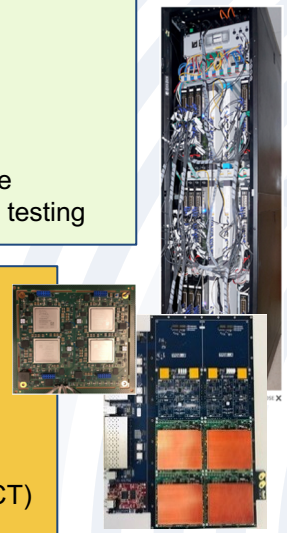
**LOFAR_IT**

**EUPEX**

**Results:**

Reference group for HW Exascale devel
MPSoC cluster
LOFAR_IT Computing infrastructure
EUCLID SDCIT Computing Infrastructure
Testbeds for software development and testing

**Impacts**
**COORDINATE EXSCALE HPC in EUROPE**
Cosmological Simulation
LOFAR_IT
EUCLID
INAF Infrastructures (CHIPP, Pleiadi, ICT)



# Software Technologies for HPC

- Parallel programming for distributed and shared memory platforms;
- **Programming frameworks** e.g. OpenMP, OpenCL, OpenACC, CUDA, OmpSs;
- New generation **accelerators**: FPGAs, GPUs, mixed;
- **Optimization, profiling** and energy profile of codes and algorithms
- **Machine learning** techniques on climate code for the study of exoplanets;
- HPC **containerized** algorithms and software.
- Quantum Computing…just started

**Projects**

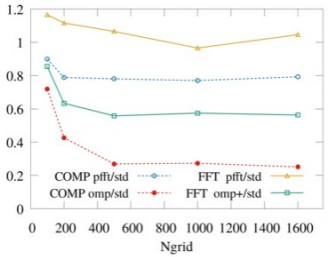
**EuroEXA** | **ExaNeSt** | **EUPEX**

**Results**
Enhanced codes, better algorithms & alg. implementations, acquaintance of new and leading-edge technologies

**Code of reference**: GADGET, OpenGADGET, ExaNBody, ESTM

**Impact**
General know-how in computation to upscale INAF role in international projects and collaborations

Cosmological simulations (INCC)
LOFAR data reduction
Exoplanet habitability (ClimHab)
....



# Software and Algorithms

**Re-engineering** and development of software for new hardware architecture (Arm, FPGA and **MPSoC**)

- **Hybrid** MPI / OpenMP / OpenACC parallelization to exploit accelerators, interconnect and memory hierarchy.
- Task-based parallelization and numa awareness: highly **hierarchical architectures** of the "Exascale" class.

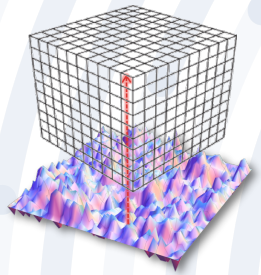
**Projects:**

| | |
|---|---|
| **EUROEXA** | **EUPEX** |
| **ESCAPE** | **ExaNeSt** |

**Results:**
*Continuous enhancement* of code capabilities:
- to exploit forthcoming and on-the-edge computing platforms
- to process larger volumes of data

**Impact**
INCC
CliMHab

Next-generation cosmological / astrophysical simulations



# Distributed computing, Cloud, Containers

- **Containerization** of software environments for data analysis and scientific computing in the cloud and HPC cluster.
- **Science Platform** as enabling technology for data access and processing;
- Services and protocols to associate **Data, software, and platforms**: reproducibility, accessibility, sw preservation;
- **HPC as a Service:** HPC as “nodes” in the very large network of computing **;**
- **Distributed infrastructure** prototypes;
- Virtual Observatory standards for: Auth&Authz, data storage**,** software/Algorithms, interoperability and FAIR (**Vobs.it and IVOA project**)

**Projects**

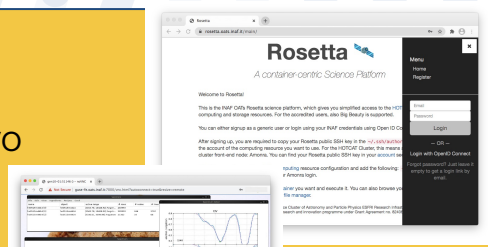
| | | |
|---|---|---|
| **ESCAPE** | **LOFAR_IT** | **SKARC** |
| **EuroVO** | **IVOA** | |

**Results**

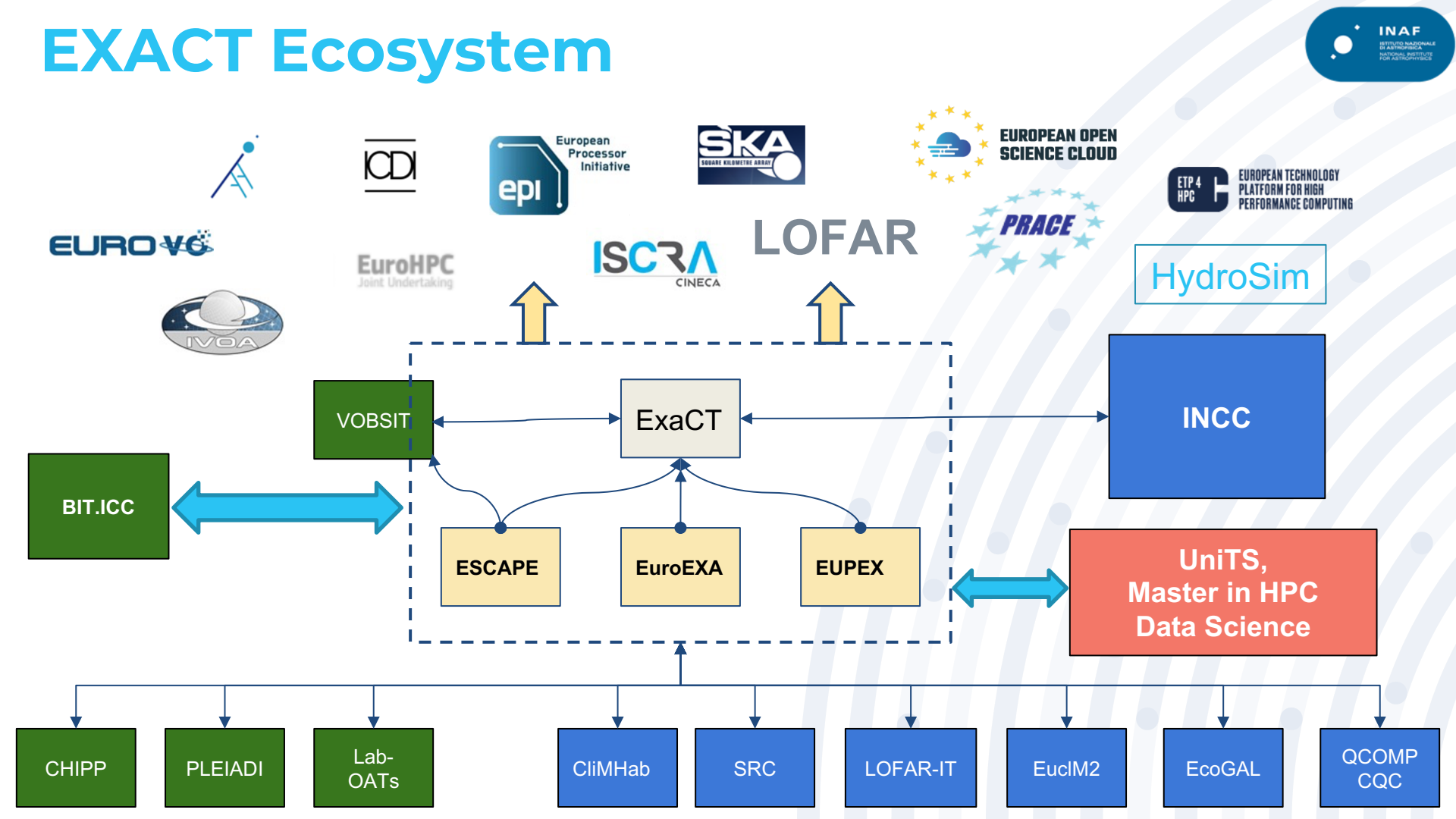
Rosetta Science platform for interactive data analysis
Canfar-INAF platform for data sharing
EOSC Data Lake
HPC as a Service testbed

**Impact**

LOFAR_IT
SKARC
IVOA, EuroVO



# EXACT Ecosystem



# EXACT daughters

## Exascale Projects

*ExaNeSt, EuroEXA, EUPEX*

International collaboration with large industrial partnership. Total of ~**70 M€**

Develop a novel computing platform for Exascale with European technologies.

Based on Co-design HW/SW.

Lead platform Integration and application co-design.

## ESCAPE

*European Science Cluster of Astronomy & Particle physics ESFRI research infrastructures*

SKA, CTA, KM3Net, EST, ELT, HL-LHC, FAIR, CERN, ESO, JIVE.

- connect ESFRI projects to EOSC ensuring integration of data and tools;
- foster common approaches to implement open-data stewardship;
- establish interoperability within EOSC as an integrated multi-messenger facility for fundamental science.

Lead VO and HPC Tasks
Science platforms for SKA and LOFAR

# People involved

| Tecnologie software per calcolo ad alte prestazioni | Calcolo distribuito, cloud containers | Codici e algoritmi | Tecnologie HW |
|---|---|---|---|
| **Chaitra Chaitra**, **David Goz**, Giuseppe Murante, **Antonio Ragagnin**, Giuliano Taffoni, Luca Tornatore | **Sara Bertocco**, **Chaitra Chaitra**, **Gianmarco Maggio**, Marco Molinaro, Fabio Pasian, **Stefano Alberto Russo,** Claudio Vuerli | Stefano Borgani, **David Goz,** Gianluigi Granato, Giuseppe Murante, **Antonio Ragagnin,** Giuliano Taffoni, Luca Tornatore | **Sara Bertocco,** Igor Coretti, Federico Gasparo, **David Goz, GianMarco Maggio,** Fabio Stocco, Giuliano Taffoni, Claudio Vuerli |

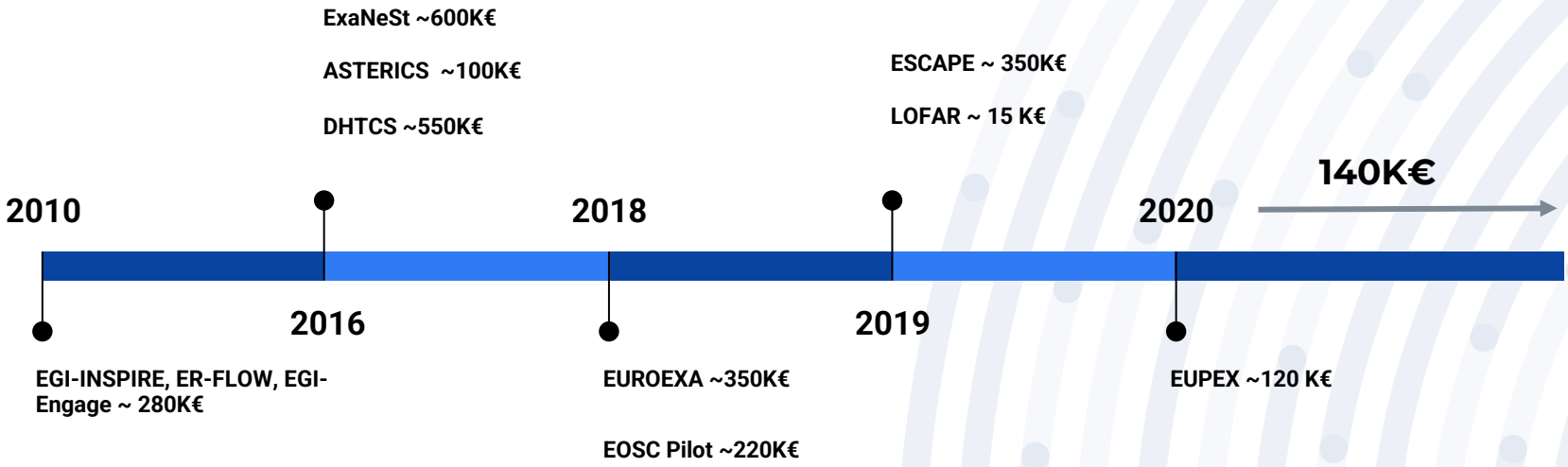
Total FTE ~80
Total for 21-23: ~3 FTE per year **more than 50% TD**

Different scientific and technological Background
**Cross-cutting activities**

# Funding and perspectives

Total budget since 2004 ~2M€

From: European projects, PRIN,  research projects (LOFAR, EUCLID, PLANCK, SKA, etc.)

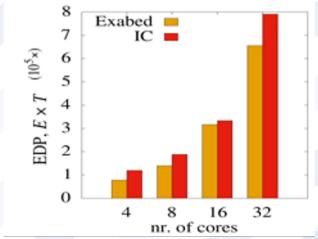


# Leadership

- **Co-design of the European Exascale platform prototypes** (application and integration).
- Development team of two of the **main cosmological simulation software** GADGET and OpenGADGET and develops many of the astrophysical modules.
- Standards and services for computing and storage in IVOA (**GWS Working Group**) and EuroVO framework.
- **Lead WPs and Tasks** of Exa-projects and ESCAPE.
- **LOFAR** - INAF Astron agreement for re-design of pipelines and codes, containerization and software distribution.
- LOFAR-IT leading **Data Working Group**
- Coordinate the HPC activities in ESCAPE.
- Lead the Astrophysics community participation to main European efforts on **Exascale**.
- Co-lead in Quantera **Quantum Computing** project.

# Results in the last 5 years

## Publications ( >50 direct and > 100 indirect)

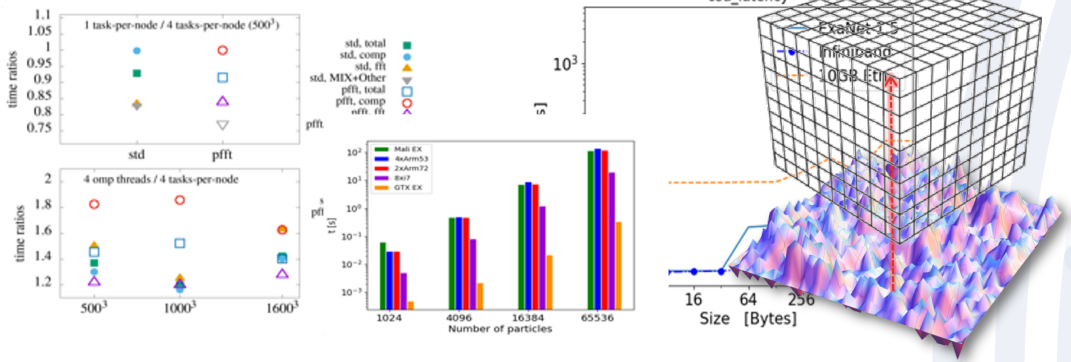


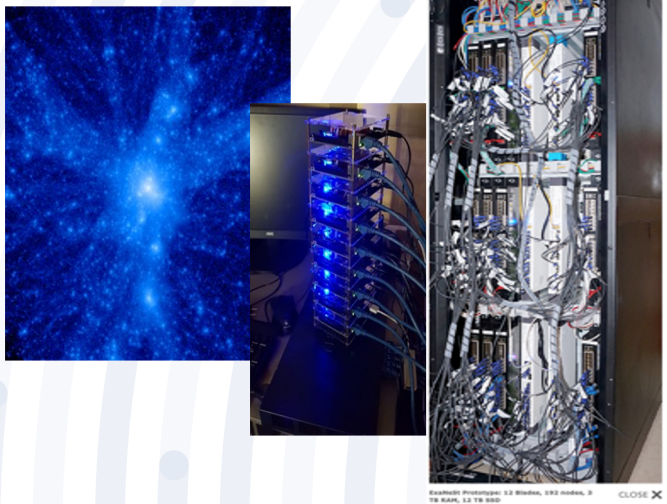

Software packages (codes and services) (~10)

International collaborations particularly on Exascale (BSC, Athos, FORTH, EPI, LRZ, etc.)

International recognition of our role in HPC and exascale

Main Scientific results (see **INCC presentation**)



# Criticalities

- Access to  testing platforms (T2.5) and innovative devices for R&D (HW/SW co-design);
- Support new research lines (e.g. Quantum Computing);
- Improve coordination among INAF groups;
- Need for INAF support;

# Know-how to retain....and further develop

- Code development and HW/SW co-design for Exascale  applications
- Distributed computing and infrastructures
- Increase # of professionals who have **astrophysical and software** design skills on HPC;
- Machine-learning methods;
- Quantum computing: Co-lead in Quantera proposal
- **Consolidate distributed competence on HPC**