# Computational Theoretical Physics at INFN

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Roadmap of the High Performance Computing in Italy and the settlement of a Scientific Advisory Board in CINECA

23 March 2017, CINECA

# Outline

- INFN scientific projects
- HPC(Th)@INFN (2018-2020)
- Conclusions

# *Scientific Projects @ INFN (Th. Physics)*

**16 scientific projects  using HPC resources**
**~100 researchers  (16  young researchers on HPC_HTC )**

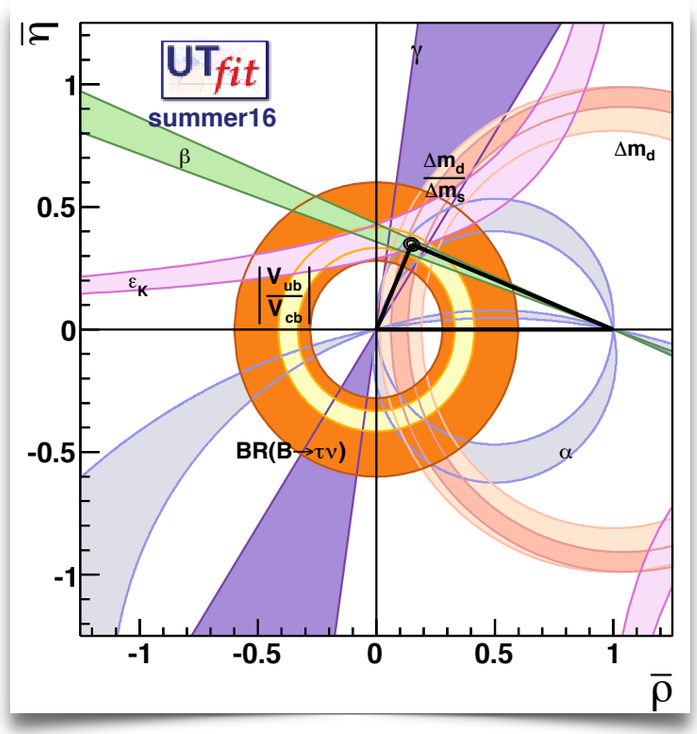
**Many areas of Theoretical Physics @INFN involved in HPC:**

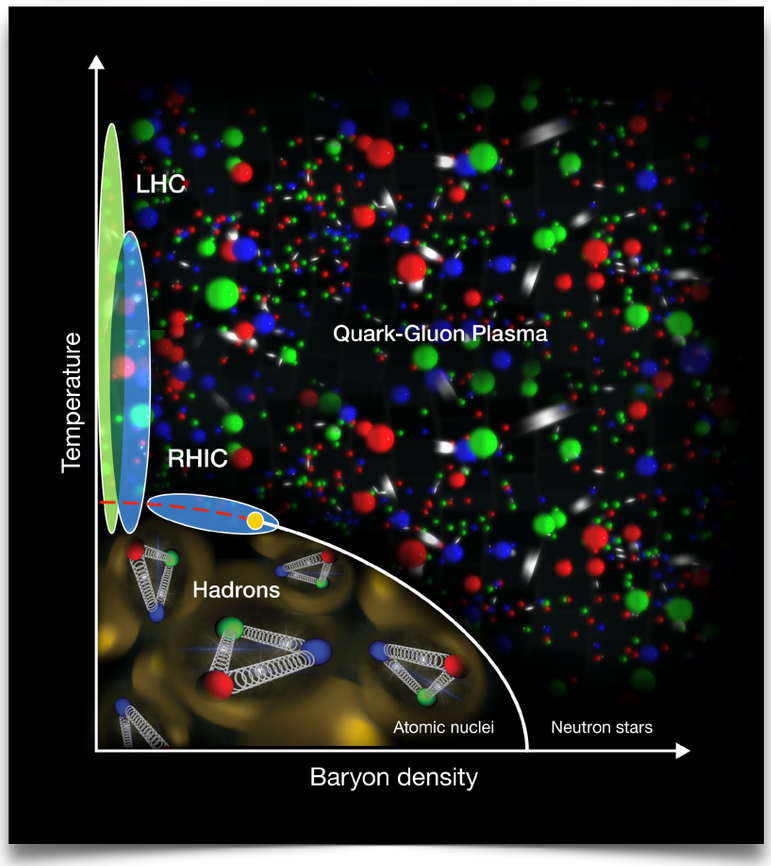
- **High Energy Physics - Lattice**
- **High Energy Physics - Phenomenology**
- **General Relativity**
- **Cosmology, Astroparticle Physics**
- **Nuclear Physics**
- **Fluid Dynamics**
- **Disordered Systems**

# High Energy Physics - Lattice

**Scientific Projects: LQCD123, NPQCD, QCDLAT, QFT_HEP, SFT**

- Flavour physics and Standard Model precision tests
- New Physics beyond the Standard Model
- Strong interactions under extreme environmental conditions (QCD at high temperature and density)
- Computational strategies and theoretical developments

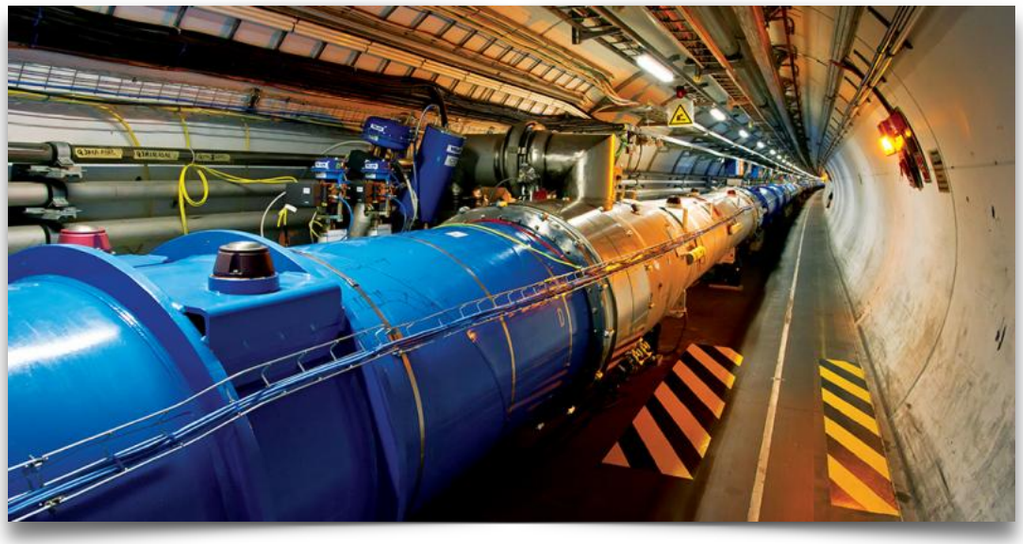


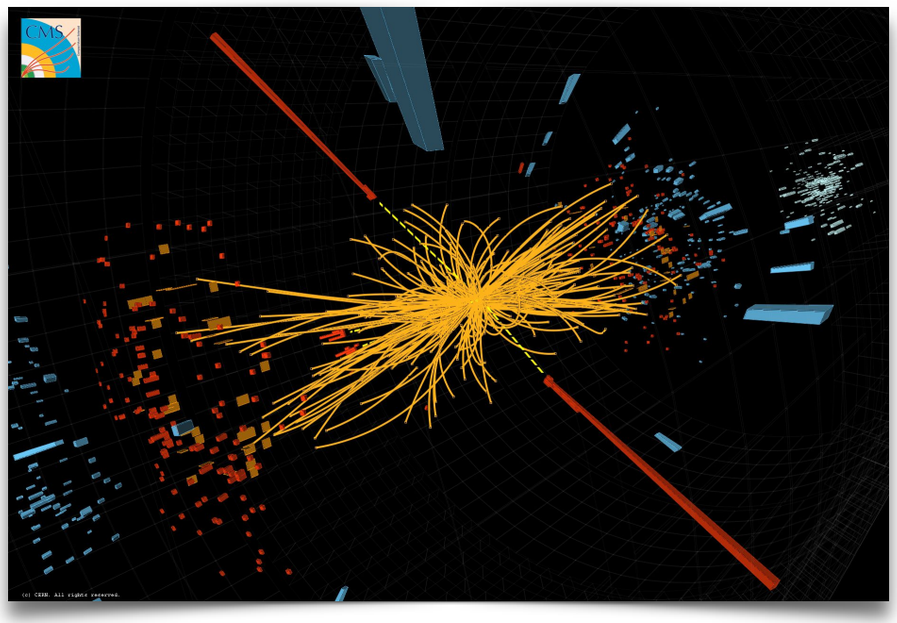
# High Energy Physics - Phenomenology

## Scientific Projects: QCD@Colliders

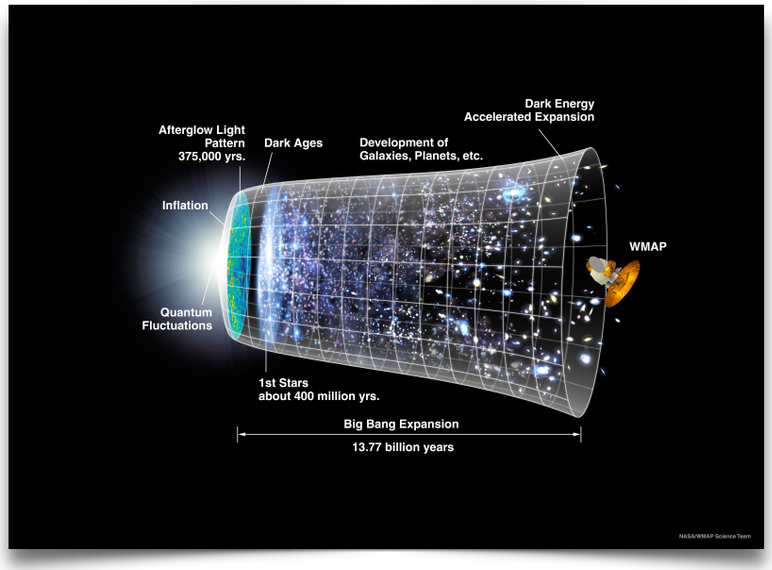
- Monte Carlo event generators to allow a systematic comparison between data and theory at LHC



- Higher order QCD corrections and future colliders

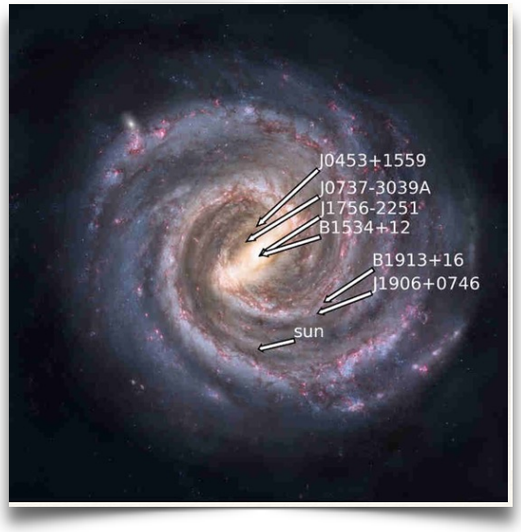


# General Relativity, Cosmology, Astroparticle Physics

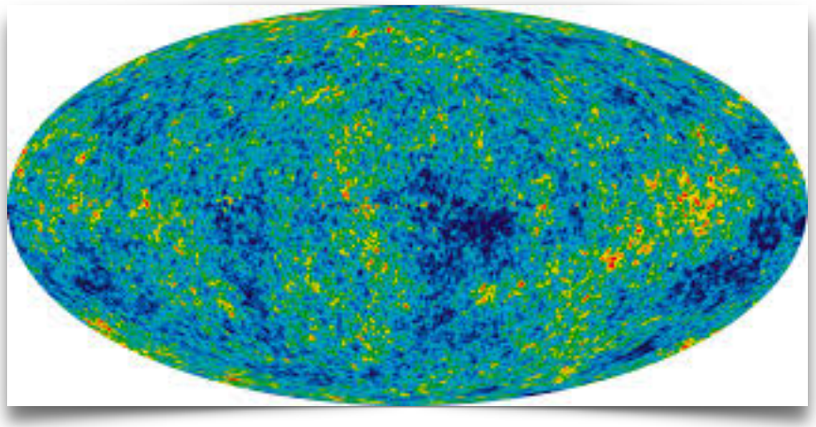



**Scientific Projects: INDARK, NEUMATT, TEONGRAV**

- **Numerical simulation of Binary Neutron Stars, Equation of State effects on the gravitational wave signal.**




- **Cosmic Microwave Background: tests of Inflation, fundamental and astroparticle Physics**



- **Large Scale Structure of the Universe: Dark Matter, Dark Energy, formation, growth and clustering of cosmic structures**

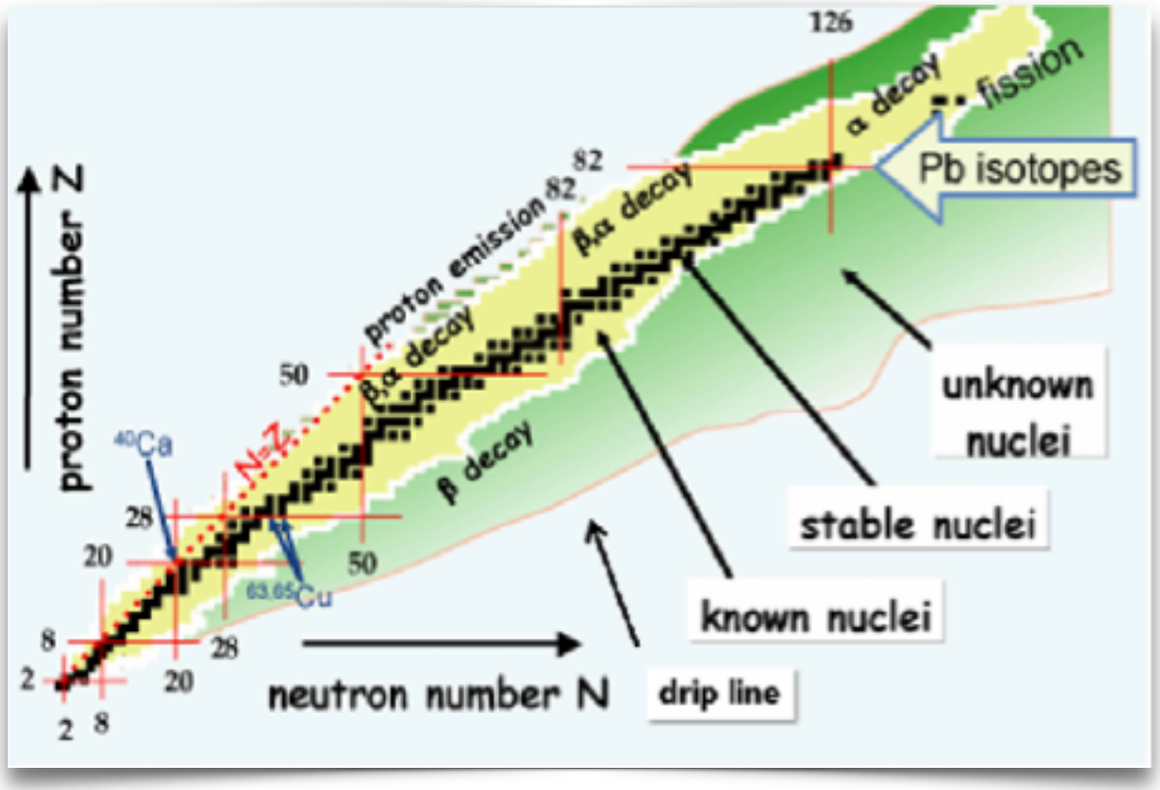
# Nuclear Physics

**Scientific Projects: FBS, MANYBODY, STRENGTH**

- Electron and neutrino interactions with nuclei, Equation of state of dense nuclear matter and neutrino propagation in nuclear matter, Monte Carlo techniques to compute ground- and excited-state properties of many-body systems.

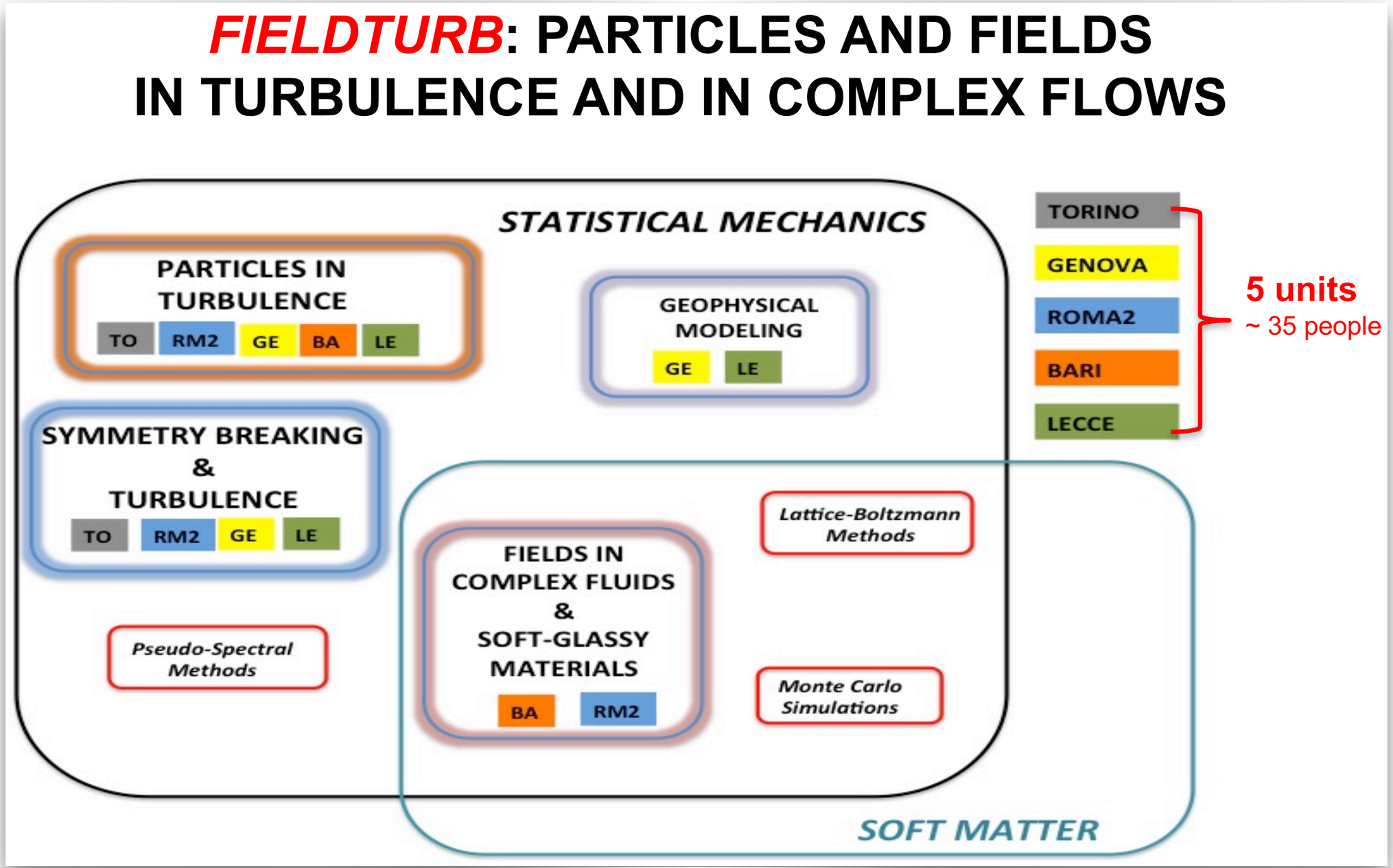
- Development and application of models for nuclear structure studies: Shell Model, Density Functional Theory, Microscopic and algebraic cluster models.

- Development of accurate methods to study the bound and continuum states of few-body systems using realistic interactions.



# Fluid Dynamics

## Scientific Projects: FIELDTURB



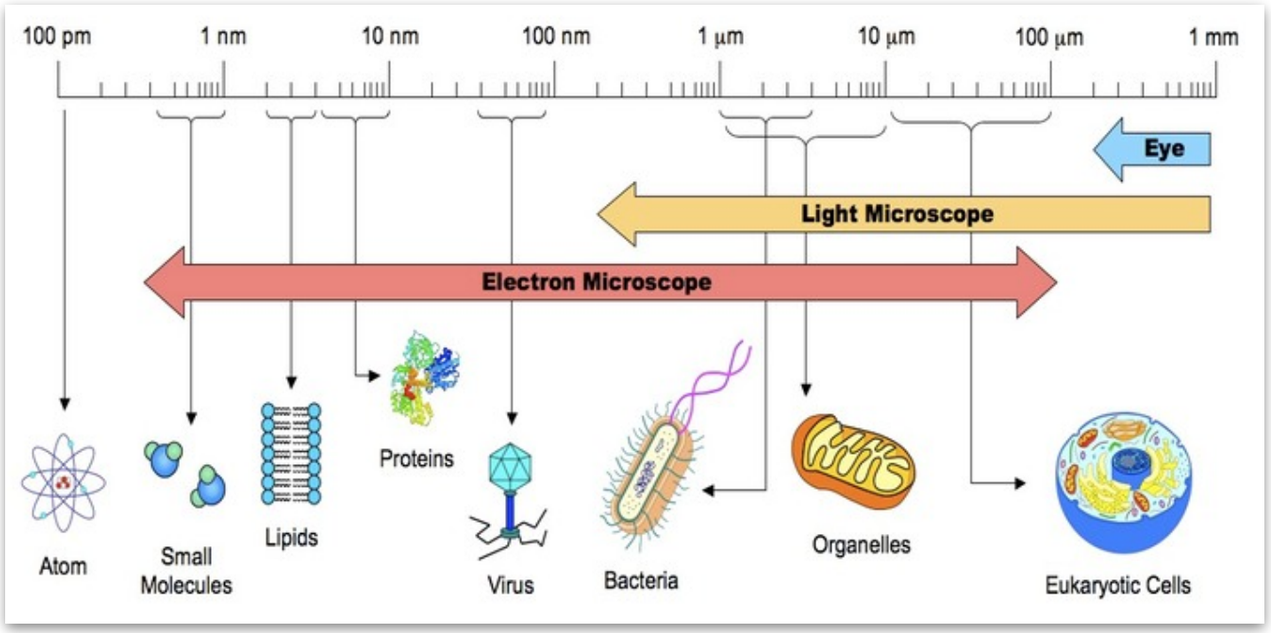

G. Boffetta @ SM&FT 2017, Bari 15 December 2017

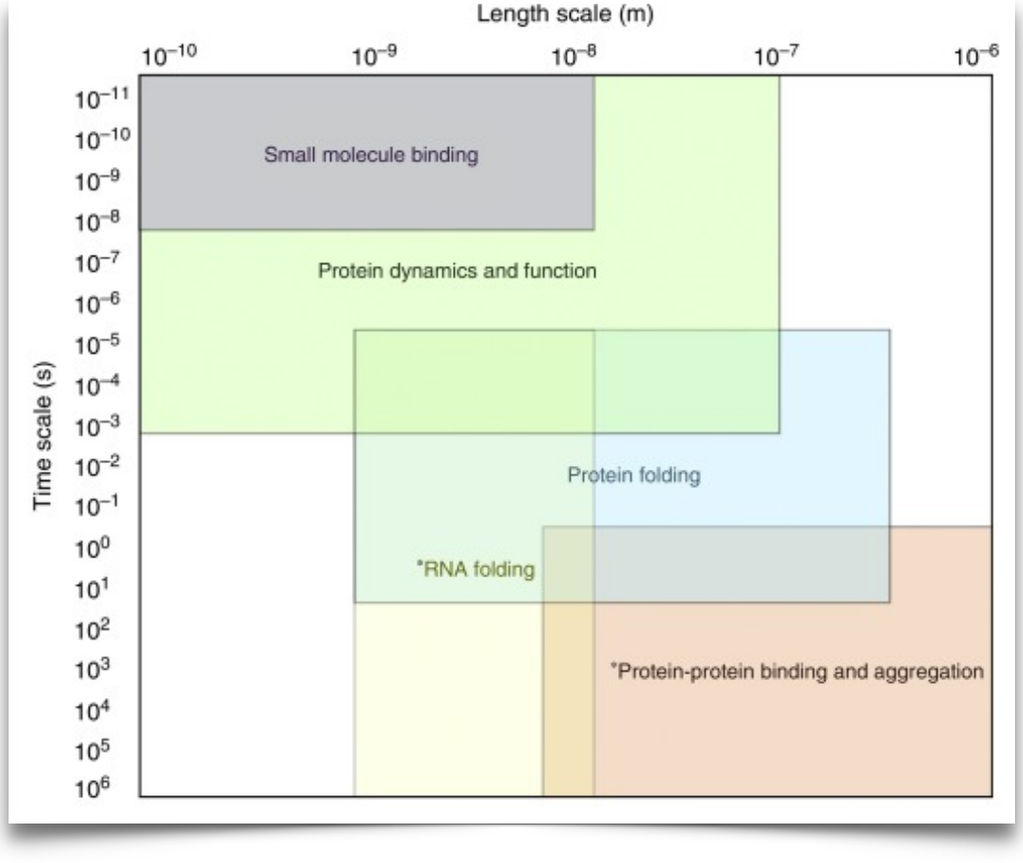
# Quantitative Biology

## Scientific Projects: BIOPHYS

**Quantitative Biology: quantitative approaches and numerical methods to gain a deeper understanding in life sciences.**

- **Characterization of biomolecules and their interaction**
- **3D organization and regulation of genome**
- **Regulatory networks of molecules, cells and neurons**

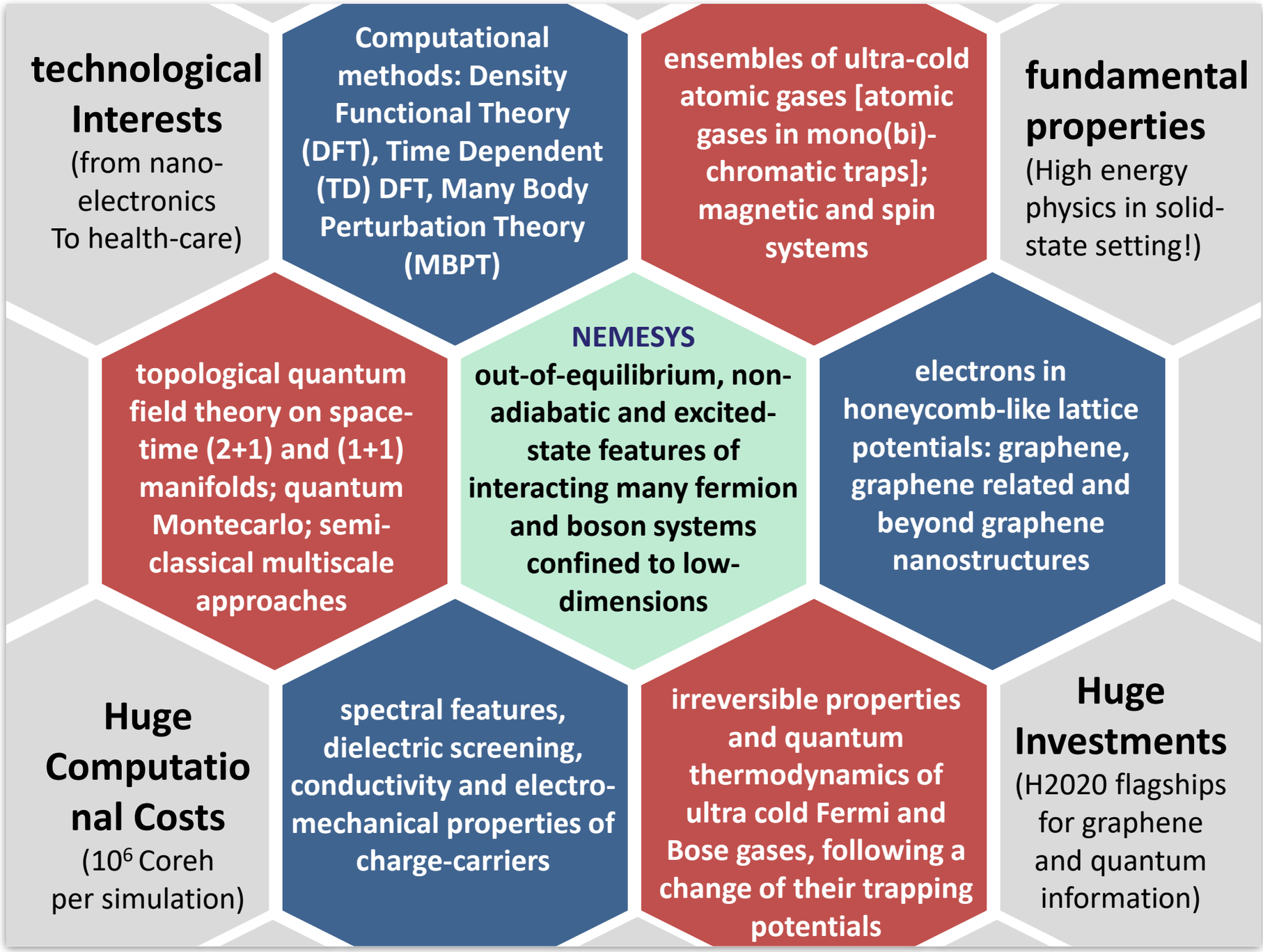


# Condensed Matter

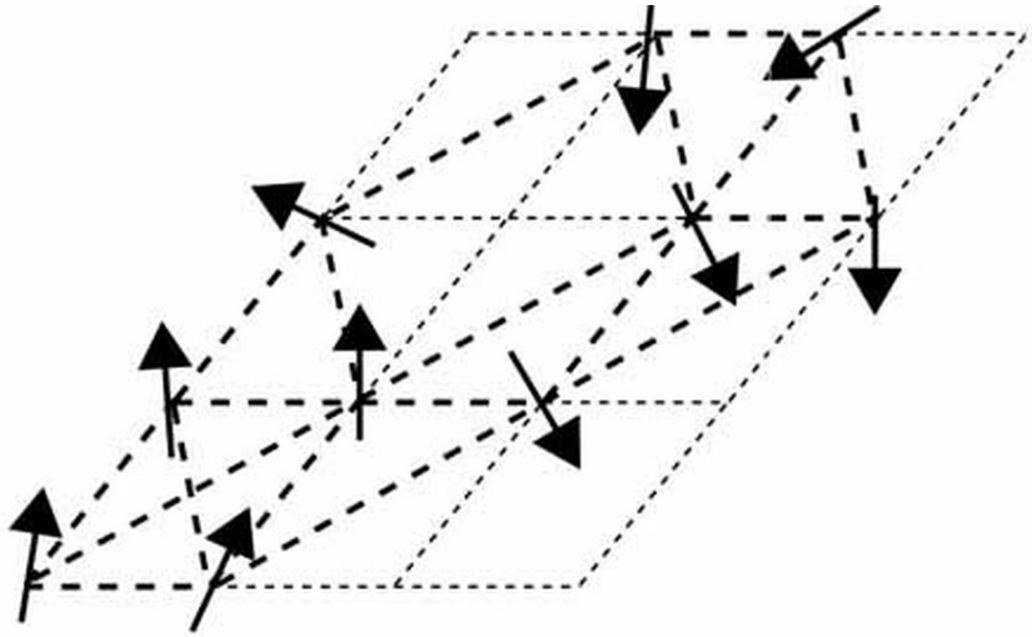
**Scientific Projects: NEMESYS**

- **Condensed matter phenomena in low dimensional systems**



# Disordered Systems

## Scientific Projects: DISCOSYNP



- Large scale simulations of spin glasses

- Hard spheres jamming and low-temperature glasses

- High resolution cortical simulations in the Human Brain Project

# ISCRA , EU-PRACE (since ~ 2012)

- ~18 projects EU-PRACE
- ~30 projects ISCRA (B-C)
- ~1000 Mcorehours (in BG/Q Fermi units)

# Suggestions (from the INFN community):

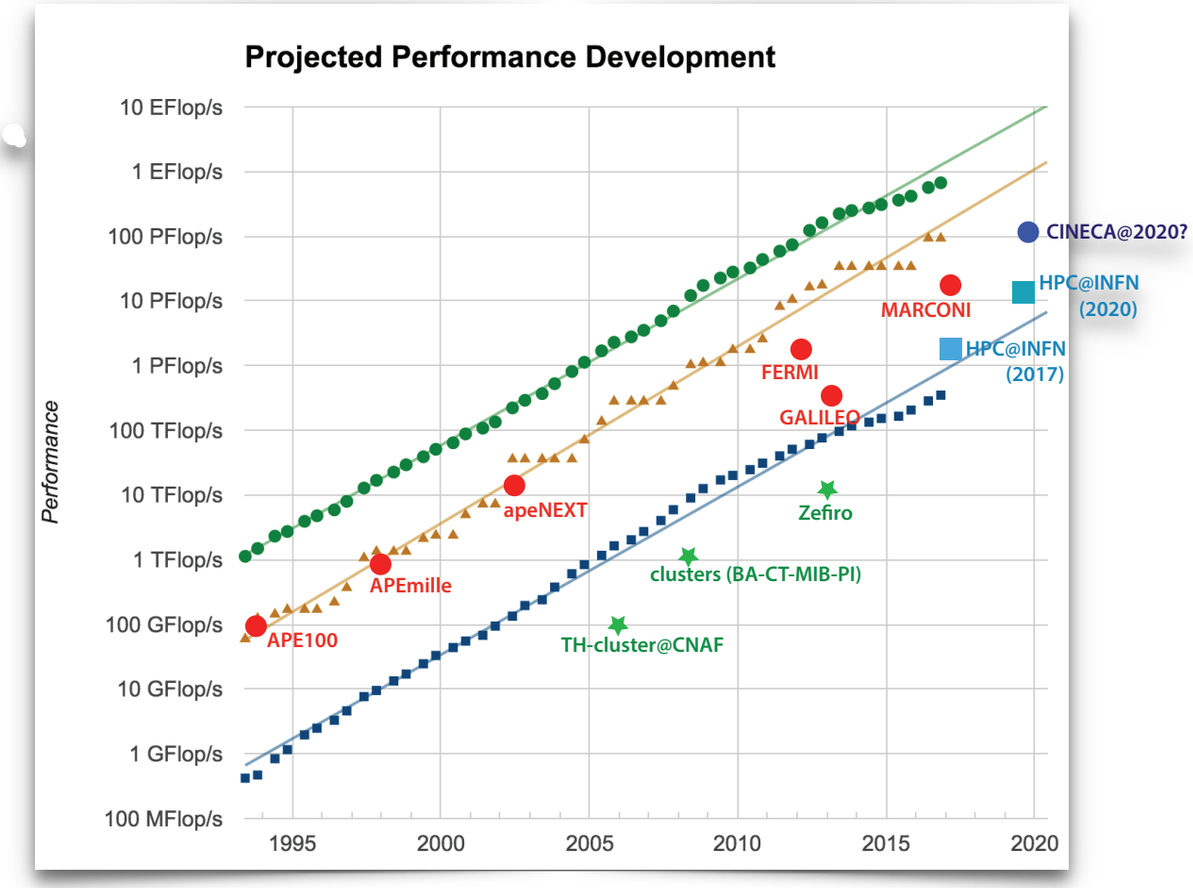
- **Scientific board: the national resources should be managed by the national community. The board should be made up of affiliates from Universities and Italian Institutions (as is the case everywhere).**

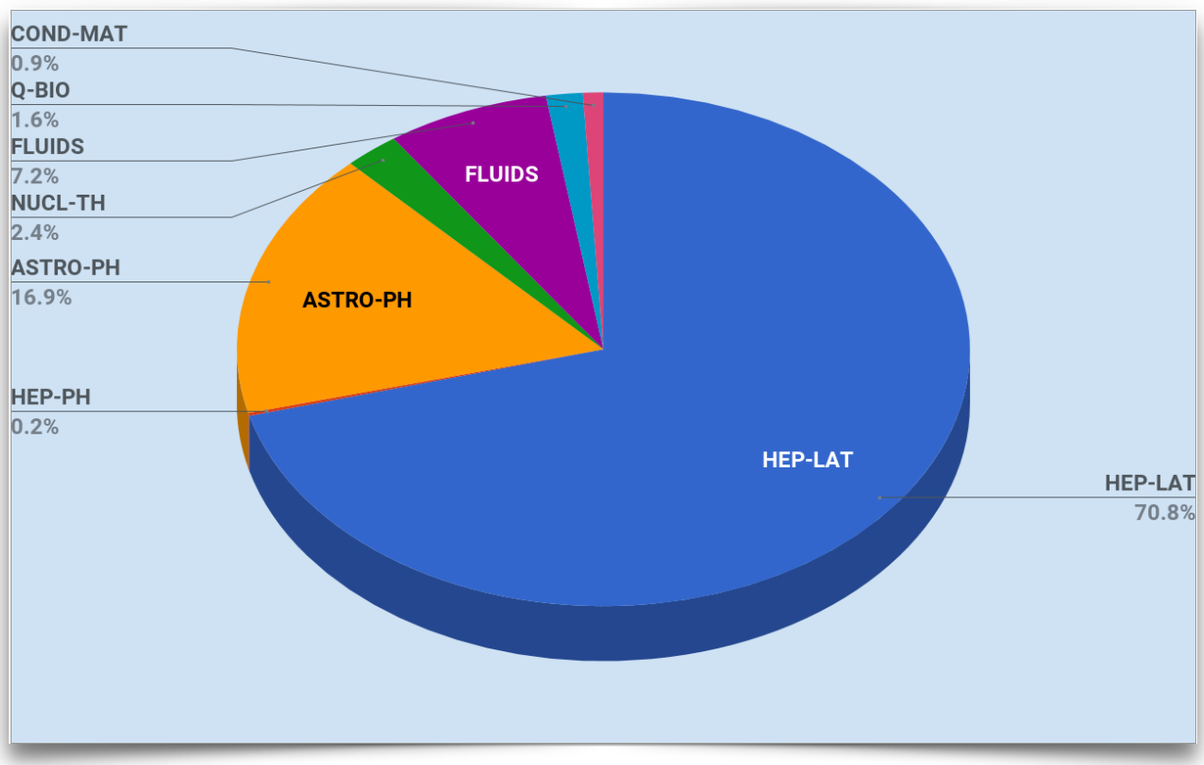
- **Since PRACE seems to be moving in the direction of approving less and less projects but with very high demands (~ 60 Mch), it would be the case to have ISCRA projects maximum requests higher than the current ones.**
  ***At the moment there is a gap between the maximum that can be requested with the national calls (4 Mch on KNL) and the minimum that can be asked with PRACE (e.g. minimum 30 Mch on Marconi KNL, bearing in mind that a minimum request on PRACE could be easily rejected because not ambitious enough).***

# HPC@INFN (2018-2020) - cont'd

# HPC requirements for Th.Physics@INFN

| | 2018 | 2019 | 2020 |
|---|---|---|---|
| LGT: hadron physics | 54 | 108 | 180 |
| LGT: QGP and BSM | 207 | 432 | 648 |
| LGT: flavor physics | 117 | 234 | 387 |
| Colliders Phenomenology | 1 | 2 | 3 |
| General Relativity | 142 | 182 | 227 |
| Cosmology and Astroparticle Physics | 3 | 4 | 6 |
| Nuclear Theory | 18 | 27 | 36 |
| Fluid Dynamics | 50 | 80 | 110 |
| Quantitative Biology | 9 | 18 | 27 |
| Disordered systems | 4 | 6 | 8 |
| Condensed matter | 2 | 4 | 6 |
| **Grand Total (Mcore-h)** | **607** | **1097** | **1638** |
| **Grand Total (Eq. Pflops)** | **4.6** | **8.4** | **12.5** |



# HPC@INFN (2018-2020)

## Computational theoretical physics at INFN: status and perspectives (2018-2020)

R. Alfieri, B. Alles, S. Arezzini, S. Bernuzzi, L. Biferale, G. Boffetta*, C. Bonati, G. Brancato, C.M. Carloni Calame, M. Caselle, P. Cea, A. Ciampa, M. Colpi, L. Cosmai*, L. Coraggio, G. de Divitiis, M. D'Elia*, R. De Pietri*, E. De Santis, C. Destri, G. Di Carlo, P. Dimopoulos, F. Di Renzo, A. Drago*, P. Faccioli, R. Frezzotti*, A. Gamba, A. Gargano, B. Giacomazzo, L. Giusti*, G. Gonnella, N. Itaco*, A. Kievsky, G. La Penna, A. Lanotte*, W. Leidemann, M. Liguori*, M.P. Lombardo*, A. Lovato, V. Lubicz, L.E. Marcucci, E. Marinari, G. Martinelli*, A. Mazzino, E. Meggiolaro, V. Minicozzi, S. Morante*, P. Natoli*, F. Negro, M. Nicodemi*, P. Olla, G. Orlandini, M. Panero*, P.S. Paolucci*, A. Papa*, G. Parisi*, F. Pederiva*, A. Pelissetto, M. Pepe, F. Piccinini*, F. Rapuano, G.C. Rossi, G. Salina, F. Sanfilippo, S.F. Schifano*, R. Schneider, S. Simula*, A. Sindona*, F. Stellato, N. Tantalo, C. Tarantino, G. Tiana, R. Tripiccione*, P. Vicini*, M. Viel, M. Viviani*, T. Vladikas, M. Zamparo

* *Conveners*

(Dated: April 26, 2017)

We present the status of computational theoretical physics at INFN, the results obtained by its research groups active in this field and their research programs for the next three years. Computational theoretical physics, besides its own importance, is a powerful tool in understanding present and future experiments. A continued support of INFN to computational theoretical physics is crucial to remain competitive in this sector. We assess the high performance computing resources needed to undertake the research programs outlined for the next three years.

https://drive.google.com/file/d/0BzOFbH1uCRZ1Y09CUHJUdlBJUUU/view?usp=sharing

https://agenda.infn.it/internalPage.py?pageId=0&confId=12156

# List of recommendation to INFN (*)

(*) from "Computational theoretical physics at INFN: status and perspectives (2018-2020)"

- Ensure that the needed computing resources are made available to the community. This is best done by renewing the current agreements with the National Supercomputer Centre (CINECA) that allow to use their HPC resources.

- Establish stronger scientific and institutional links with CINECA, with the goal of playing an active role in the definition of the computational requirements of the future HPC systems that CINECA plans to install.

- Make sure that the HPC computational skills needed to efficiently use current and future supercomputers are mastered by the community. This is best done encouraging young researchers to enter the computational arena; to this effect, we propose to support a specific programme of post-doc grants at the crosspoint between computational physics, algorithm development, code development and optimization.

- Support at every appropriate political level the continued operation of national (e.g., ISCRA) and international (e.g., PRACE) competitive access programs to HPC resources.