HPC at INFN: theory

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INFN and The Future of Scientific Computing - Episode I: The HPC Opportunity

4 May 2018, Accademia delle Scienze, Torino

Outline

- HPC@INFN-Th: scientific projects
- HPC(Th)@INFN: computational resources (2018-2020,…)
- Conclusions

HPC@INFN (The early days)

- **~1980 Lattice Gauge Theories**, relevant contributions from the INFN community

  - K. Wilson 1974: Introduces LQCD.
  - M. Creutz 1979: C. Rebbi 1980 First Monte-Carlo simulations.
  - H. Hamber and G. Parisi 1981, D. Weingarten 1982: Quenched approximation.
  - N. C., G. Martinelli, R. Petronzio 1983: Simulation of weak interactions.

  screenshot from Nicola Cabibbo "The APE experience" , GGI - Firenze, 8 Feb 2007

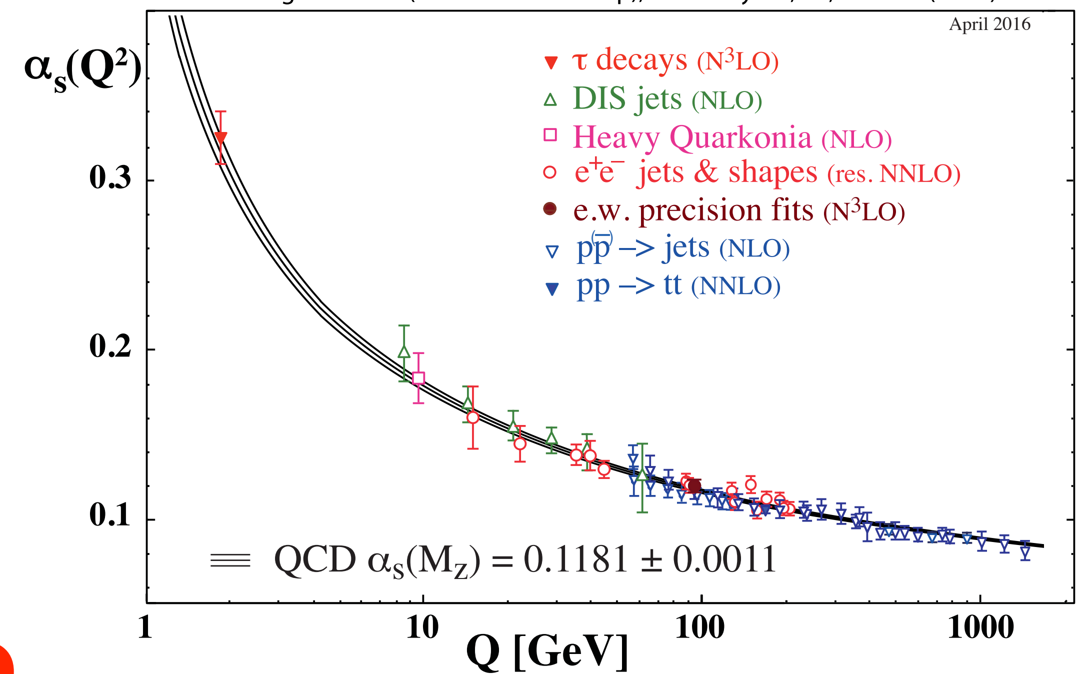
- **~1983-2003 The APE project**, development of parallel computers dedicated to LGT's (~2 Meuro/year actual value)

~1986	**APE**	**—>**	**1 Gflops**	**(~Cray XMP)**
~1994	**APE100**	**—>**	**100 GFlops**	**(~Cray T3D)**
~1998	**APEmille**	**—>**	**1 TFlops**	**(~Cray T3E)**
~2003	**apeNEXT**	**—>**	**10 Tflops**	**(~ASCI white)**

Lattice QCD and HPC

strongly coupled at low energies

C. Patrignani et al. (Particle Data Group), Chin. Phys. C, 40, 100001 (2016)

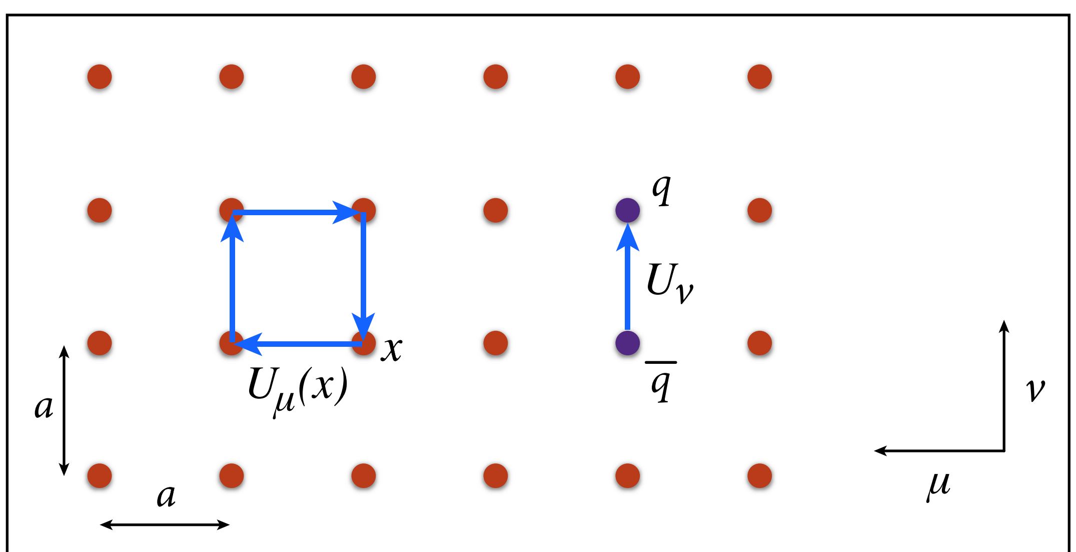


asymptotic freedom at high energies

LATTICE QCD

space-time discretisation —> lattice regularization of QCD —> non-perturbative calculations by numerical evaluation of the path integral that defines the theory

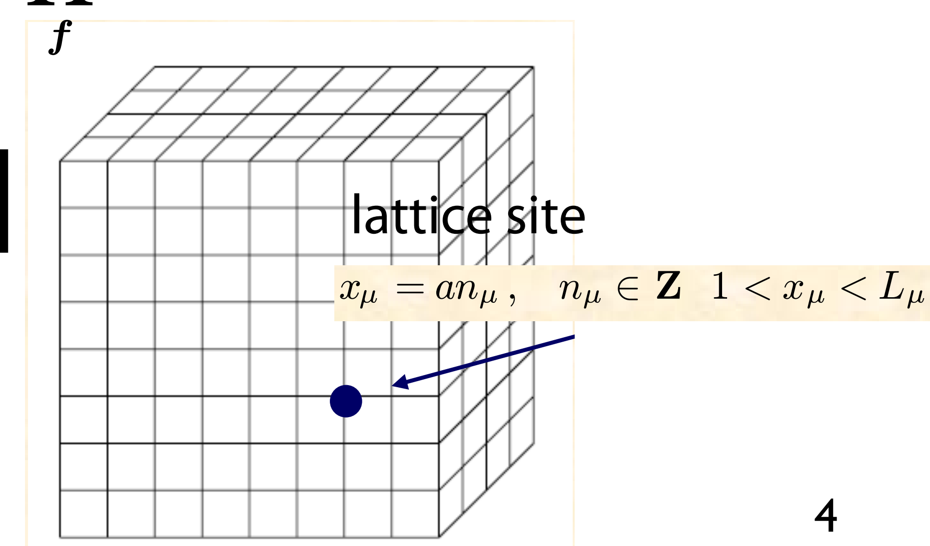
$$\langle \mathcal{O}(U,q,\bar{q})\rangle = (1/Z)\int [dU]\prod_f [dq_f][d\bar{q}_f]\mathcal{O}(U,q,\bar{q})e^{-S_g[U]-\sum_f \bar{q}_f(D[U]+m_f)q_f}$$



$$Z = \int [dU]e^{-S_g[U]}\prod_f \det(D[U]+m_f)$$

hyper cubic lattice

$$V_{\text{lat}} = N_s^3 \times N_t$$



Practical LQCD calculations:

- Monte Carlo methods to numerically evaluate the functional integrals
- limited by the availability of computational resources and the efficiency of algorithms
- LQCD results come with both statistical (Monte Carlo integration) and systematic (from discretization) errors
- computational cost of LQCD simulations: $\sim (V_{\text{lat}})^{1+\delta} \qquad \delta = 1/4$
- typically one aims to create an ensemble of ~ 10^3 statistically independent gauge configurations at each choice of parameters (*lattice volume, lattice spacing, quark masses*)
- Infinite lattice volume limit, continuum limit (lattice spacing —>0)

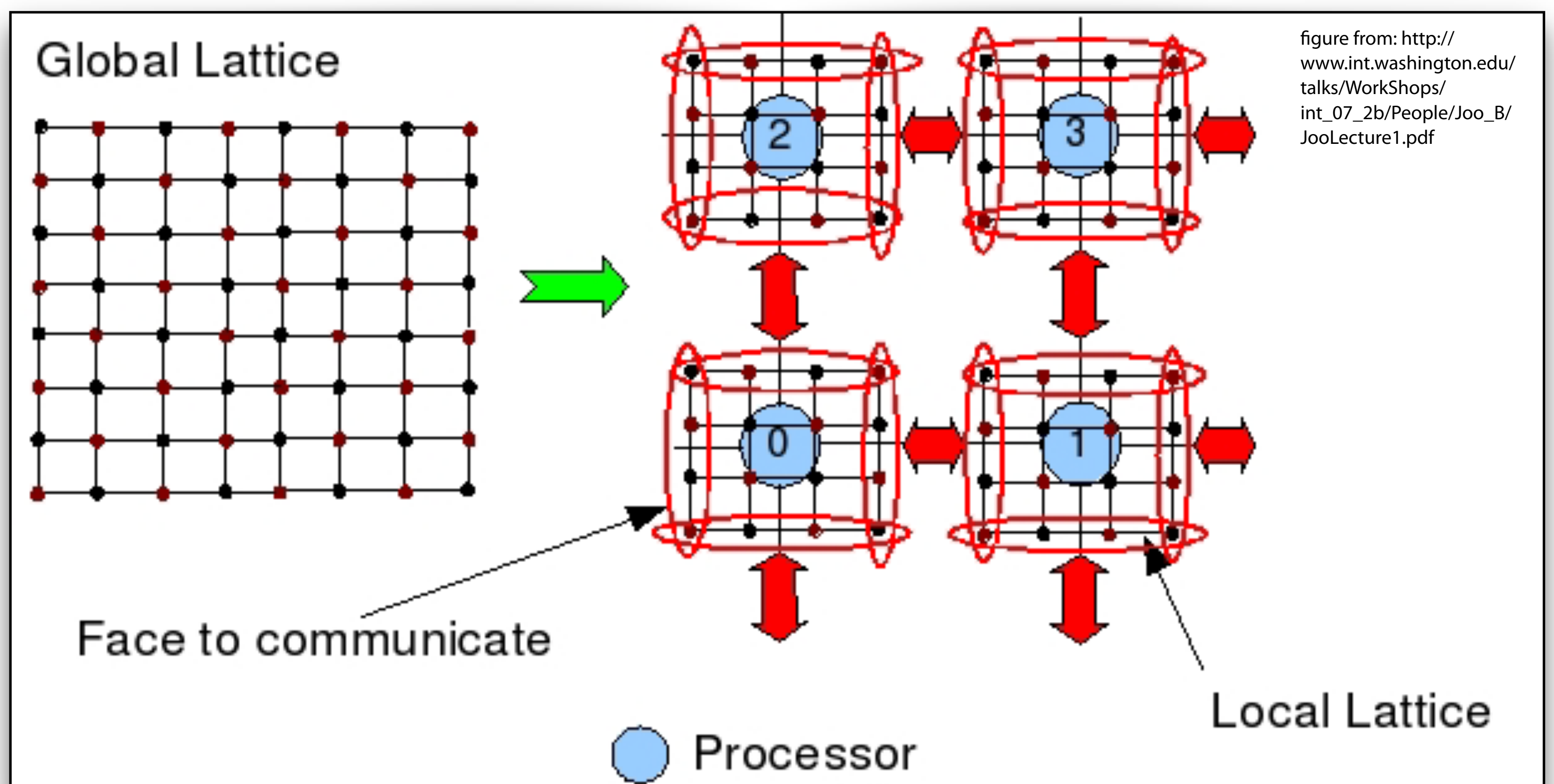
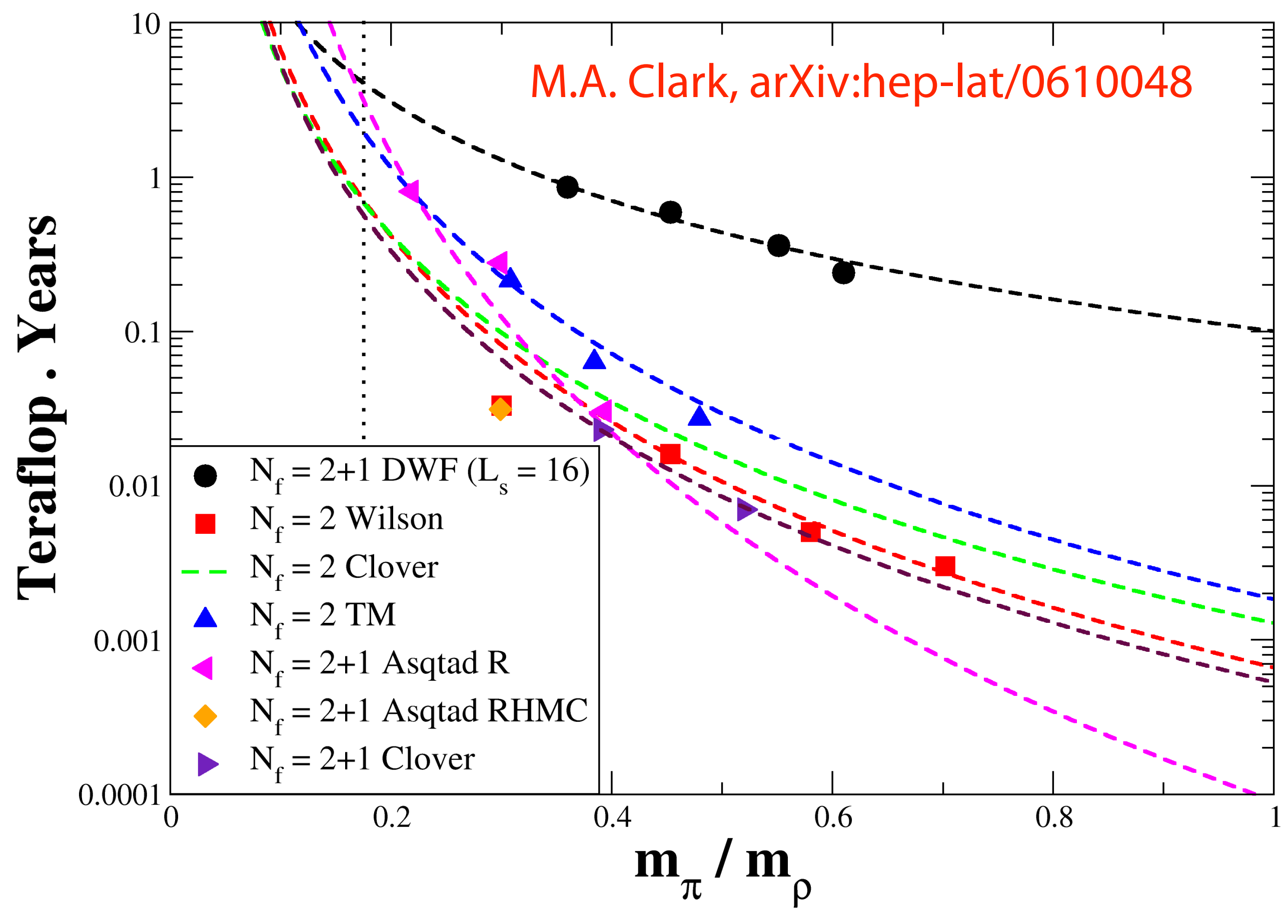


figure from: http://www.int.washington.edu/talks/WorkShops/int_07_2b/People/Joo_B/JooLecture1.pdf

Lattice QCD Simulations as an HPC Challenge

The computational cost of Lattice QCD



the computational cost of numerical simulations can increase dramatically as the lattice spacing decreases

[A. Ukawa, Lattice 2001 Proceedings]

$$C = 1.25 \left(\frac{\#\ \mathrm{confs}}{100}\right) \left(\frac{M_\pi}{400\ \mathrm{MeV}}\right)^{-6} \left(\frac{V^{1/4}}{3\ \mathrm{fm}}\right)^{5} \left(\frac{0.09\ \mathrm{fm}}{a}\right)^{7} \mathrm{Tflops} \times \mathrm{years}$$

(2 flavour)

[M.Bruno et al., arXiv:1411:3982]

$$C = 14 \left(\frac{\#\ \mathrm{confs}}{100}\right) \left(\frac{V^{1/4}}{6\ \mathrm{fm}}\right)^{9/2} \left(\frac{0.065\ \mathrm{fm}}{a}\right)^{7} \mathrm{TFlops} \times \mathrm{years}$$

(2 +1 flavour)

HPC resources for the INFN-TH community (2018)

- CINECA-INFN agreement

MARCONI “A1” (Broadwell)

9 Mcorehours

Model: Lenovo NeXtScale
Architecture: Intel OmniPath Cluster
Nodes: 1.512
Processors: 2 x 18-cores Intel Xeon E5-2697 v4 (Broadwell) at 2.30 GHz
Cores: 36 cores/node, 54.432 cores in total
RAM: 128 GB/node, 3.5 GB/core
Internal Network: Intel OmniPath
Disk Space: 17PB (raw) of local storage
Peak Performance: 2 PFlop/s

MARCONI “A2” (KNL)

120 Mcorehours

Model: Lenovo Adam Pass
Architecture: Intel OmniPath Cluster

Nodes: 3.600
Processors: 1 x 68-cores Intel Xeon Phi 7250 CPU (Knights Landing) at 1.40 GHz
Cores: 68 cores/node (272 with HyperThreading), 244.800 cores in total
RAM: 16 GB/node of MCDRAM and 96 GB/node of DDR4
Internal Network: Intel OmniPath Architecture 2:1
Disk Space: 17PB (raw) of local storage
Peak Performance: 11 PFlop/s

MARCONI “A3” (Skylake)

160 Mcorehours

Model: Lenovo Stark
Racks: 21 +
Nodes: 1.512 +
Processors: 2 x 24-cores Intel Xeon 8160 CPU (Skylake) at 2.10 GHz
Cores: 48 cores/node, 72.576+ 38.016 cores in total
RAM: 192 GB/node of DDR4

Peak Performance: about 7.50 PFlop/s

- ISCRA, EU-PRACE

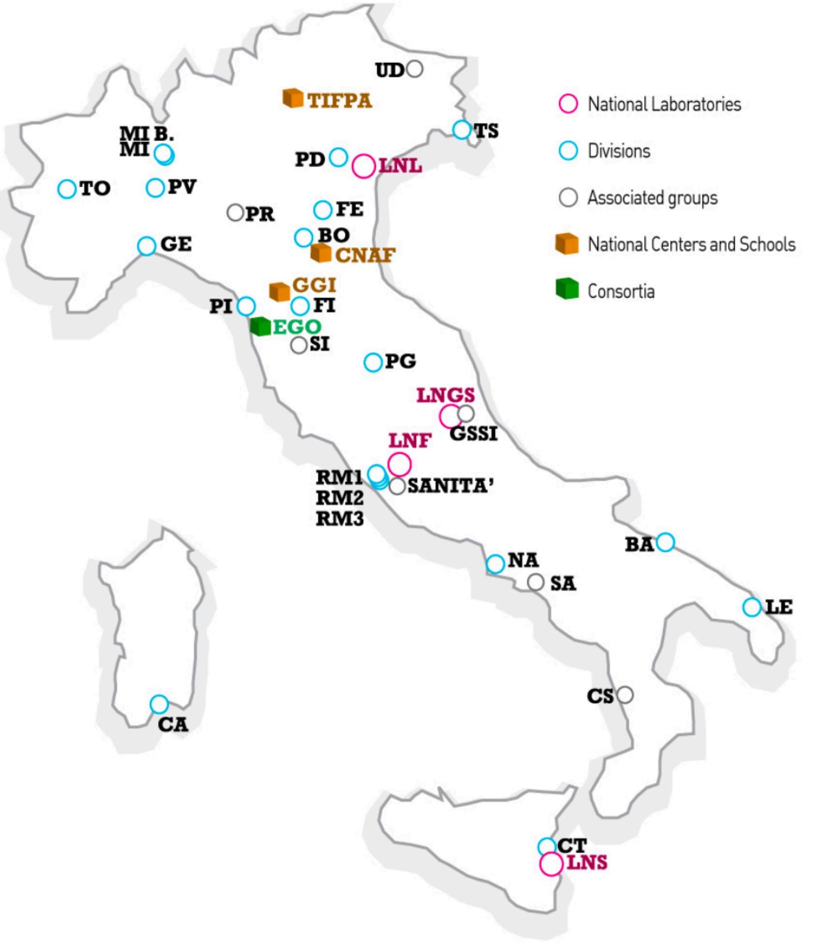
since 2012 ~50 projects: ~1000 Mcorehours (in BG/Q units)

Scientific Projects @ INFN (Th. Physics)

16 scientific projects using HPC resources
~100 researchers (16 fellowships on HPC for Th. Physics)

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



fellowships on HPC for Th. Physics

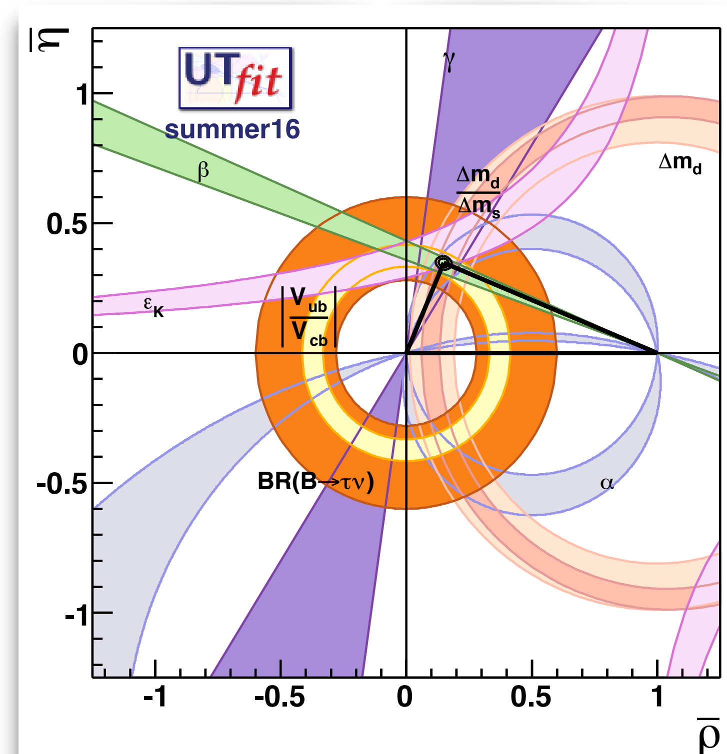
ASSEGNI PROGETTO HPC_HTC PER FISICA TEORICA COMPUTAZIONALE									
Tutor	**Sigla**	**Assegnista**	**Area**	**Sezione**	**Durata**	**Cofinanziatore**	**Tipo di contratto**	**Inizio**	**Fine**
Alessandro Papa	**NPQCD**	**Volodymyr Chelnokov**	**Lattice QCD**	Cosenza/LNF	24 mesi		Assegno di ricerca	15 Febbraio 2018	14 Febbraio 2020
Raffaele Tripiccione	**FIELDTURB**	**Enrico Calore**	**Fluids**	Ferrara	24 mesi	Univ. Ferrara	Contributo di 23K a Dip. Fisica Ferrara	1 Gennaio 2017	31 Dicembre 2018
Luca Del Zanna	**TEONGRAV**	**Antonio Graziano Pili**	**Numerical Relativity**	Firenze	24 mesi	Univ. Firenze	Contributo di 40K a Dip. Fisica/Astronomia FI	1 Febbraio 2017	31 Gennaio 2019
Alessandra Lanotte	**FIELDTURB**	**Gabriella Schirinzi**	**Fluids**	Lecce	12 mesi	INFN – Lecce	Assegno di ricerca	2 Ottobre 2017	30 Settembre 2018
Leonardo Giusti	**QCDLAT**	**Mattia Dalla Brida**	**Lattice QCD**	Milano Bicocca	36 mesi	Univ. Milano Bicocca	RTDA	1 Novembre 2017	31 Ottobre 2020
Leonardo Giusti	**QCDLAT**	**Tim Harris**	**Lattice QCD**	Milano Bicocca	24 mesi	Univ. Milano Bicocca	Assegno di ricerca	1 Novembre 2017	31 Ottobre 2019
Nunzio Itaco	**STRENGTH**	**concorso in svolgimento**	**Nuclear Physics**	Napoli	24 mesi	2a Univ. Napoli	Contributo di 30K a Dip. Fisica 2a Univ. Na		
Sebastiano Bernuzzi	**TEONGRAV**	**Albino Perego**	**Numerical Relativity**	Parma/Milano Bicocca	24 mesi		Assegno di ricerca	1 Luglio 2017	30 Giugno 2019
Alberto Ciampa	**Zefiro Cluster**		**Zefiro Cluster (Pisa)**	Pisa	12 mesi		Rinnovo Assegno in corso INFN Pisa	Ottobre 2016	
Massimo D'Elia	**NPQCD**	**Davide Vadacchino**	**Lattice QCD**	Pisa	24 mesi		Assegno di ricerca	1 Dicembre 2017	30 Novembre 2019
Massimo D'Elia	**NPQCD**	**Francesco Negro**	**Lattice QCD**	Pisa	24 mesi		Assegno di ricerca	2 Dicembre 2016	1 Dicembre 2018
Giorgio Parisi	**DISCOSYNP**	**concorso in svolgimento**	**Disordered Systems**	Roma Sapienza	36 mesi		Contributo di 96K per art. 29	Gennaio 2017	
Mauro Sbragaglia	**FIELDTURB**	**Matteo Lulli**	**Fluids**	Roma TOV	12 mesi	Univ. Roma Tor Vergata	Assegno di Ricerca Universitario bandito dall'Università degli studi di Roma "Tor Vergata"	1 Febbraio 2017	31 Gennaio 2018
Roberto Frezzotti	**LQCD123**	**Marco Garofalo**	**Lattice QCD**	Roma ToV	24 mesi		Assegno di ricerca	1 Ottobre 2017	30 Settembre 2019
Silvia Morante	**BIOPHYS**	**Francesco Stellato**	**Quantitative Biology**	Roma ToV	24 mesi		Assegno di ricerca	1 Gennaio 2017	31 Dicembre 2018
Anastassios Vladikas	**LQCD123**	**Andrew Thompson Lytle**	**Lattice QCD**	Roma ToV	24 mesi		Assegno di ricerca	Giugno 2018 (?)	Maggio 2020 (?)
Silvano Simula	**LQCD123**	**Lorenzo Riggio**	**Lattice QCD**	Roma Tre	24 mesi		Assegno di ricerca	1 Marzo 2017	28 Febbraio 2019
Bruno Giacomazzo	**TEONGRAV**	**Federico Cipolletta**	**Numerical Relativity**	TIFPA	24 mesi		Nuovo assegno bandito da TIFPA	3 Aprile 2018	2 Aprile 2020
Guido Boffetta	**FIELDTURB**	**Alessandro Sozza**	**Fluids**	Torino	12 mesi	Univ. Torino	Assegno di ricerca annuale (costo totale 240599.77 euro)	1 Gennaio 2017	31 Dicembre 2017
Marco Panero	**SFT**	**David Preti**	**Lattice QCD**	Torino	24 mesi		Assegno di ricerca	1 Dicembre 2017	30 Novembre 2019

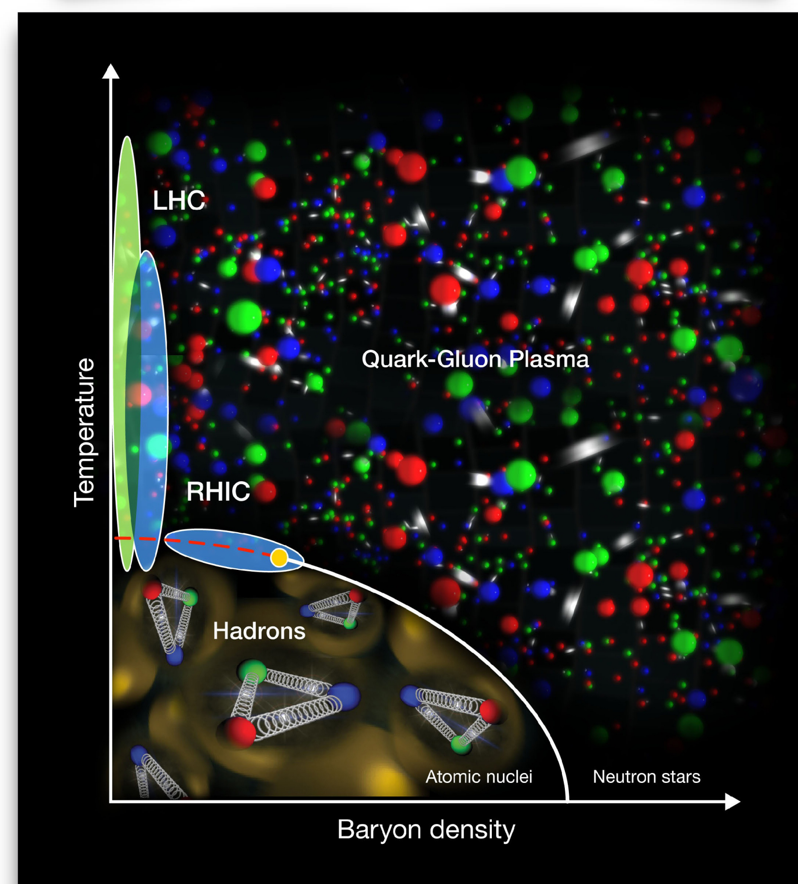
Scientific activity presented at "SM&FT 2017" (Bari, 13-15 December 2017) http://www.ba.infn.it/smft2017

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

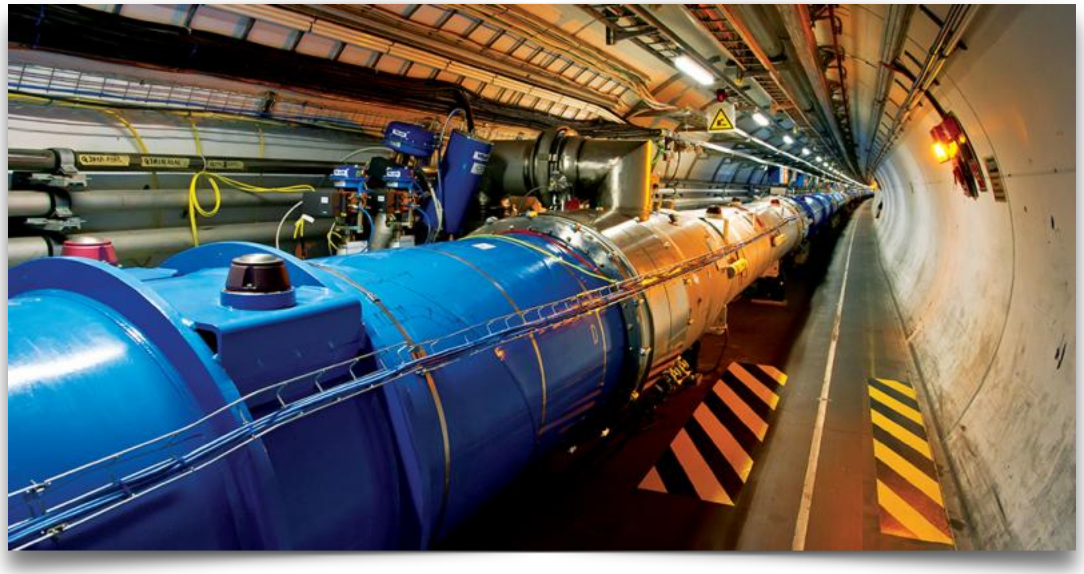




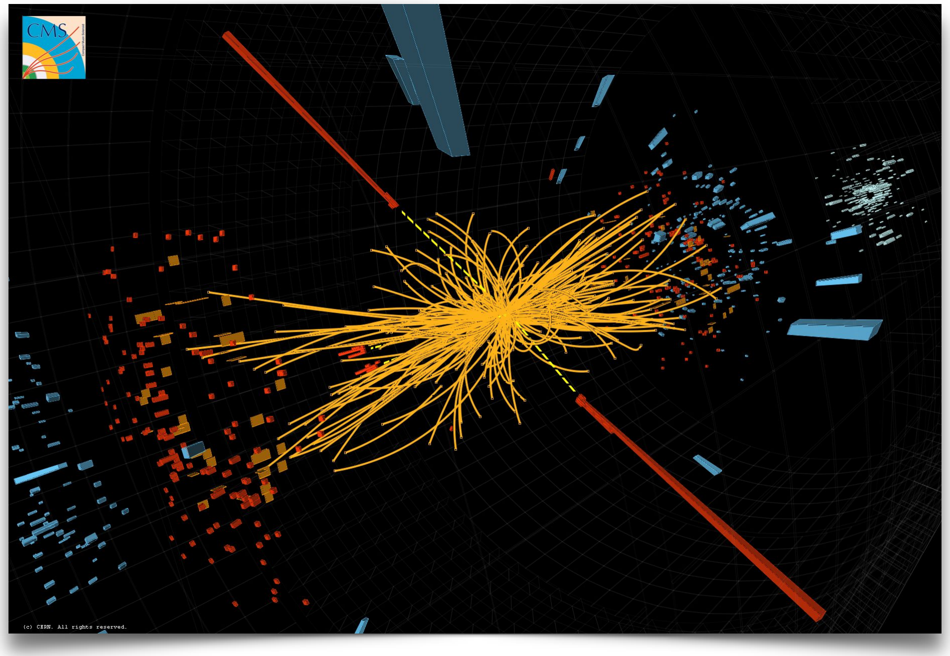
- *In the next years a series of experiments will collect new data that may shed light on the Standard Model and BSM.*
- *The theoretical interpretation of all these data will need non-perturbative calculations with <u>accuracies far beyond the state of the art</u>.*

High Energy Physics - Phenomenology

Scientific Projects: QCD@Colliders

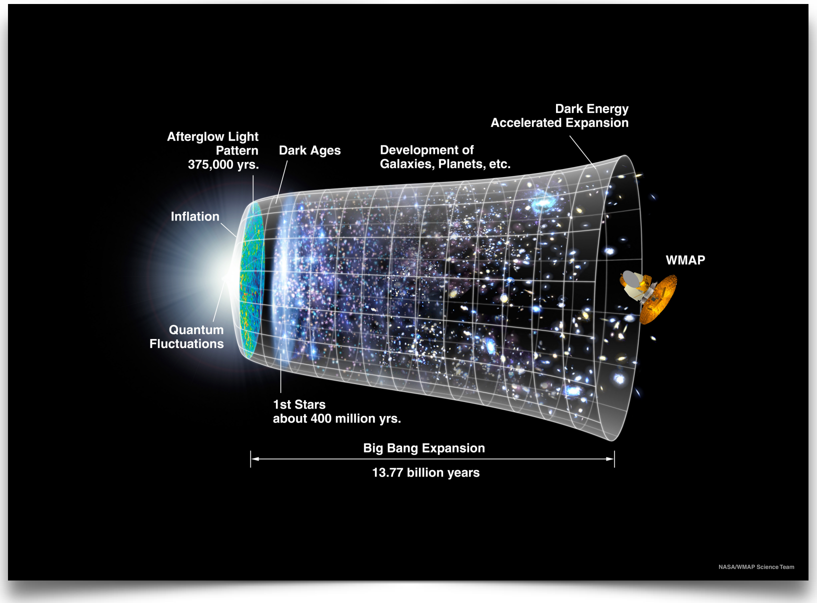


- **Monte Carlo event generators to allow a systematic comparison between data and theory at LHC**

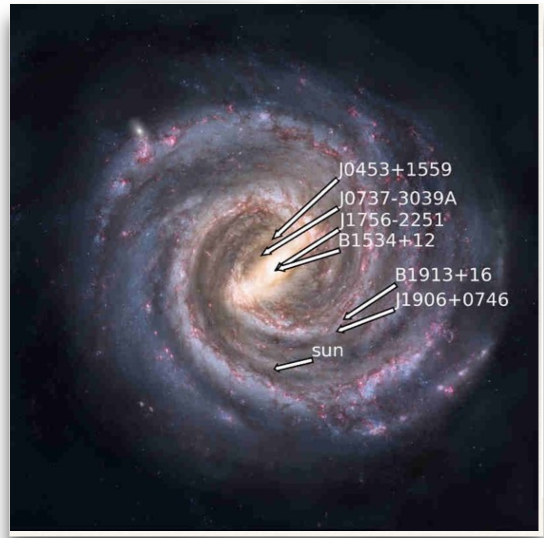


- **Higher order QCD corrections and future colliders**

General Relativity, Cosmology, Astroparticle Physics

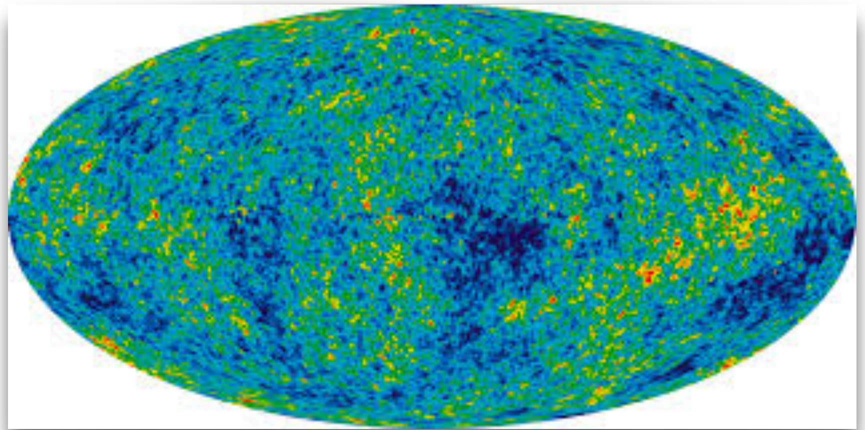


Scientific Projects: INDARK, NEUMATT, TEONGRAV



- 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

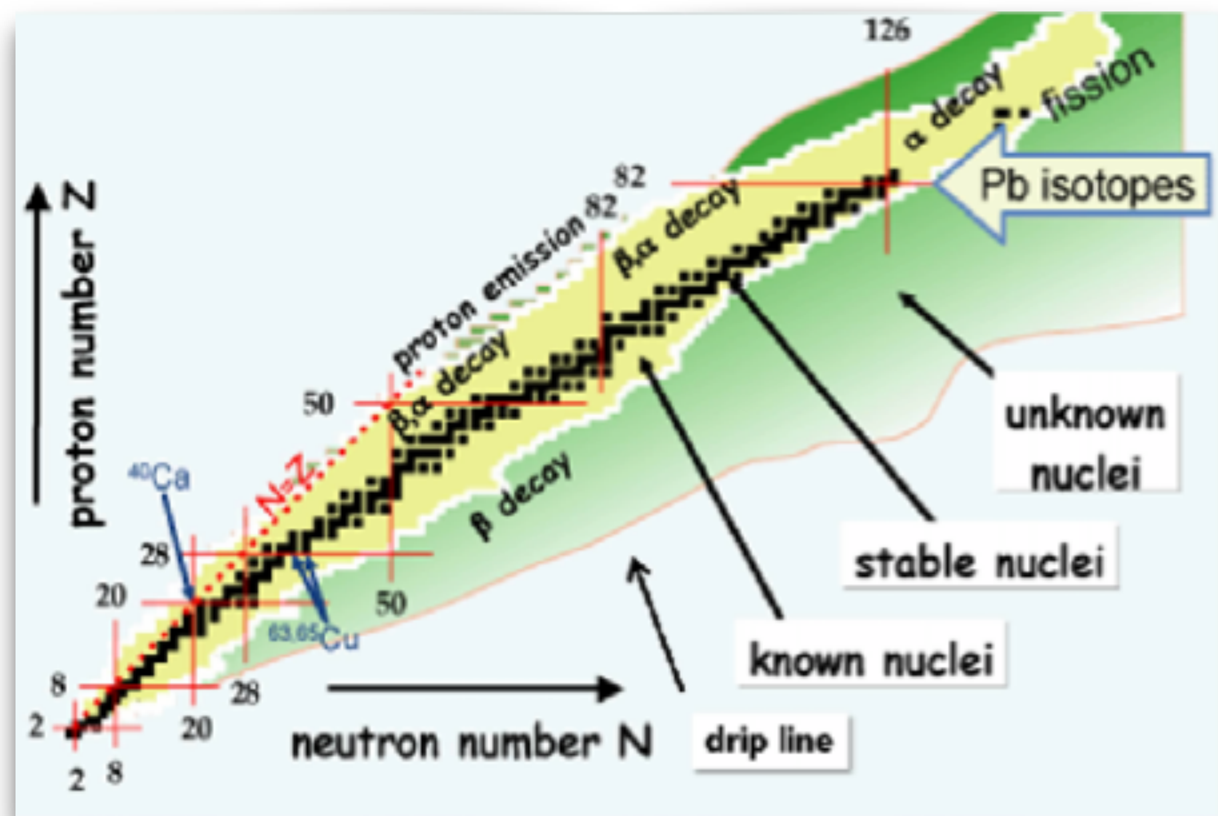
Nuclear Physics

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.

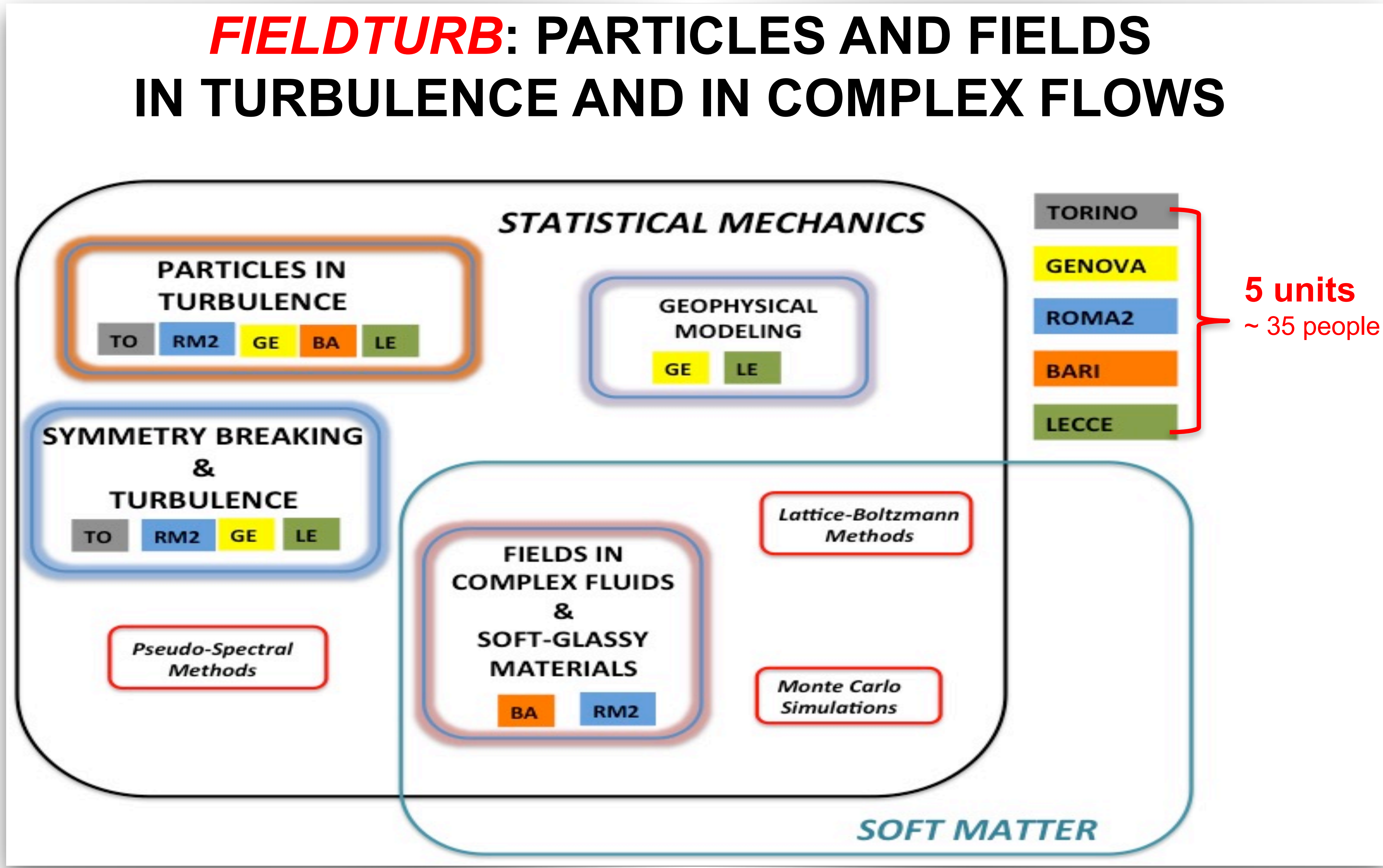
- Development and application of models for nuclear structure studies: Shell Model, Density Functional Theory, Microscopic and algebraic cluster models.

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



Fluid Dynamics

Scientific Projects: FIELDTURB



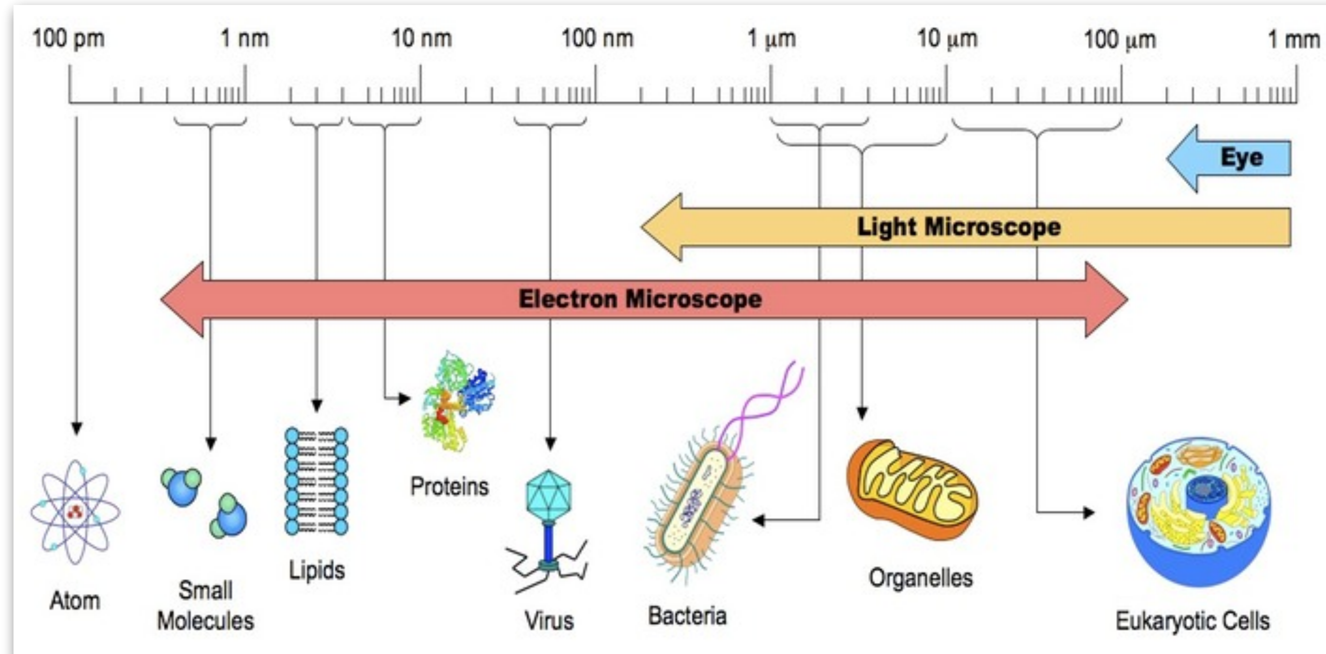
G. Boffetta @ SM&FT 2017, Bari 15 December 2017

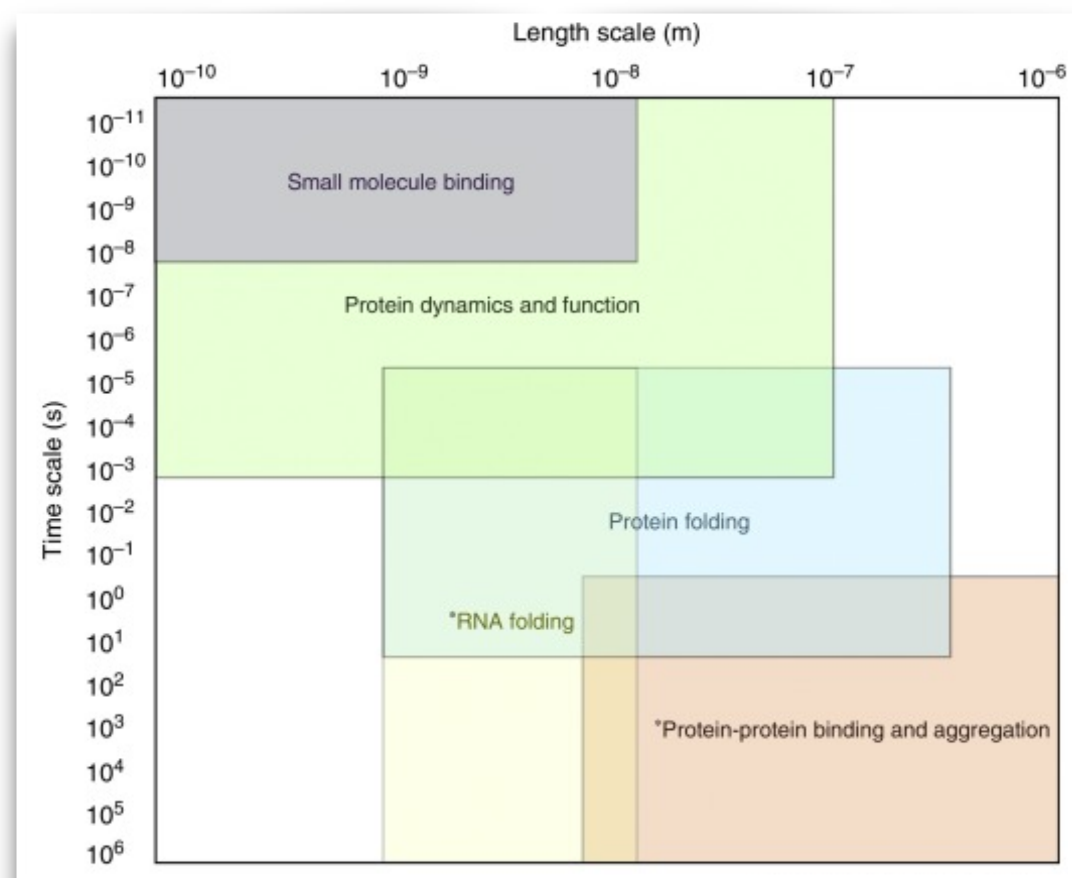
Quantitative Biology

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

technological Interests
(from nano-electronics
To health-care)

Computational methods: Density Functional Theory (DFT), Time Dependent (TD) DFT, Many Body Perturbation Theory (MBPT)

ensembles of ultra-cold atomic gases [atomic gases in mono(bi)-chromatic traps]; magnetic and spin systems

fundamental properties
(High energy physics in solid-state setting!)

topological quantum field theory on space-time (2+1) and (1+1) manifolds; quantum Montecarlo; semi-classical multiscale approaches

NEMESYS
out-of-equilibrium, non-adiabatic and excited-state features of interacting many fermion and boson systems confined to low-dimensions

electrons in honeycomb-like lattice potentials: graphene, graphene related and beyond graphene nanostructures

Huge Computational Costs
(10^6 Coreh
per simulation)

spectral features, dielectric screening, conductivity and electro-mechanical properties of charge-carriers

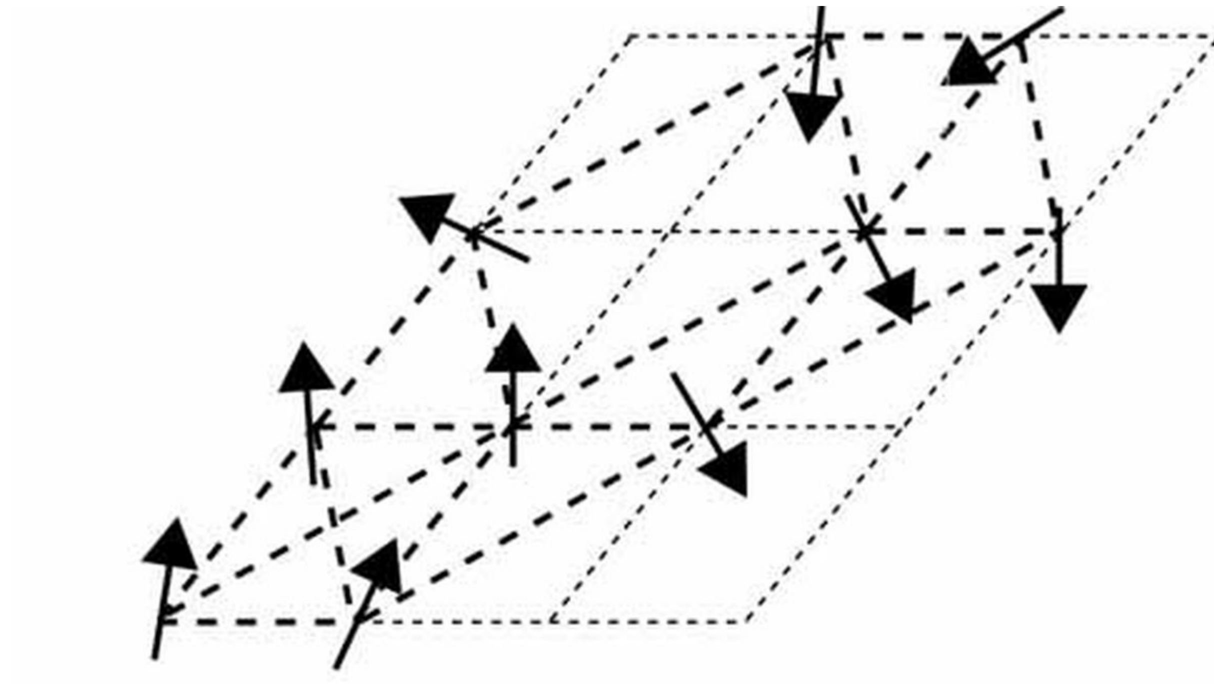
irreversible properties and quantum thermodynamics of ultra cold Fermi and Bose gases, following a change of their trapping potentials

Huge Investments
(H2020 flagships for graphene and quantum information)

A. Sindona @ SM&FT 2017, Bari 15 December 2017

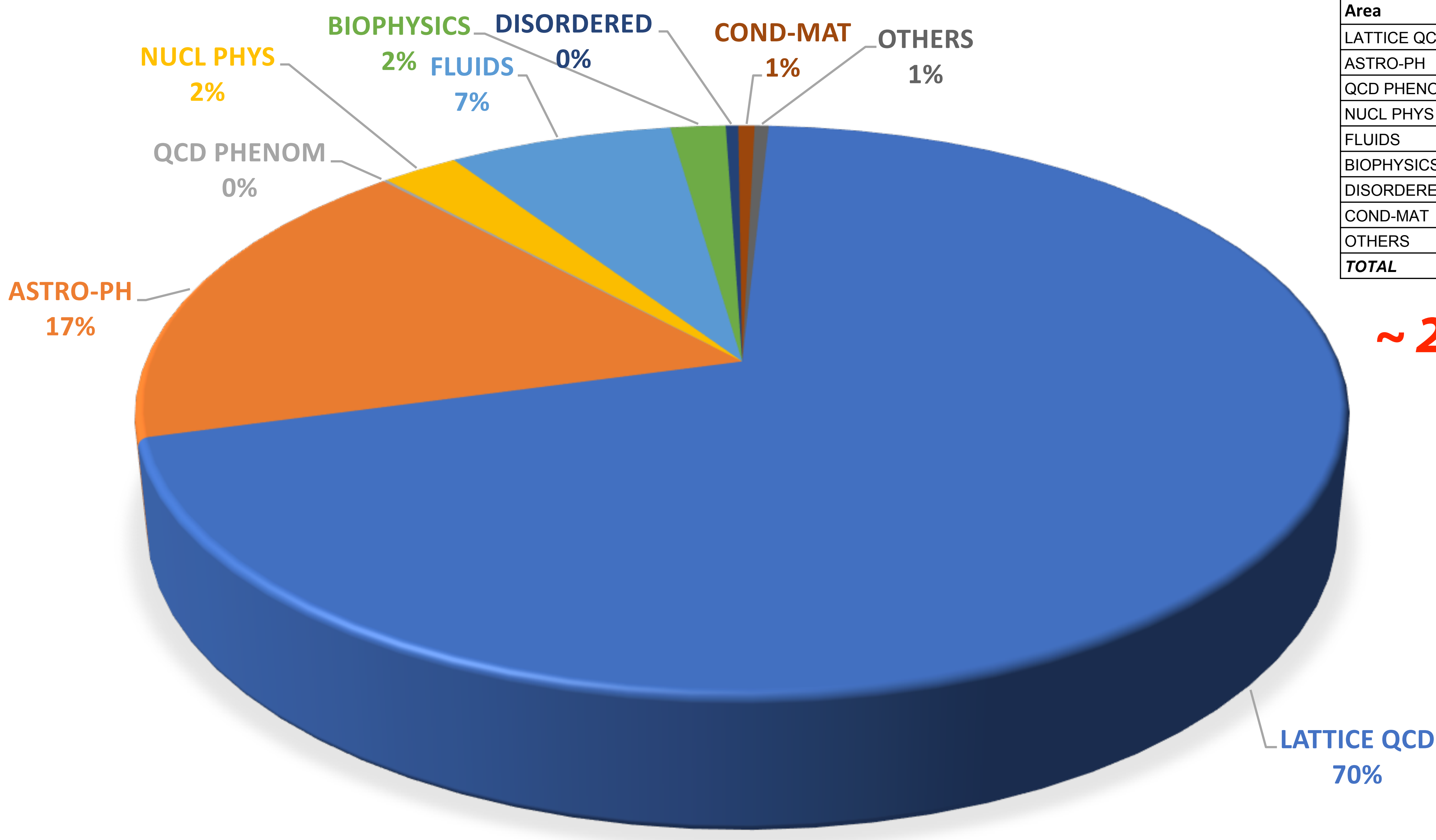
Disordered Systems

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

HPC resources for the INFN-TH community (2018 sharing)



Area	A1+A2+A3 (corehours)
LATTICE QCD	204,800,000
ASTRO-PH	51,000,000
QCD PHENOM	400,800
NUCL PHYS	7,050,000
FLUIDS	20,700,000
BIOPHYSICS	5,100,000
DISORDERED	1,150,000
COND-MAT	1,500,000
OTHERS	1,300,000
TOTAL	***293,000,800***

~ 2 PFlops

HPC@INFN-Th (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.

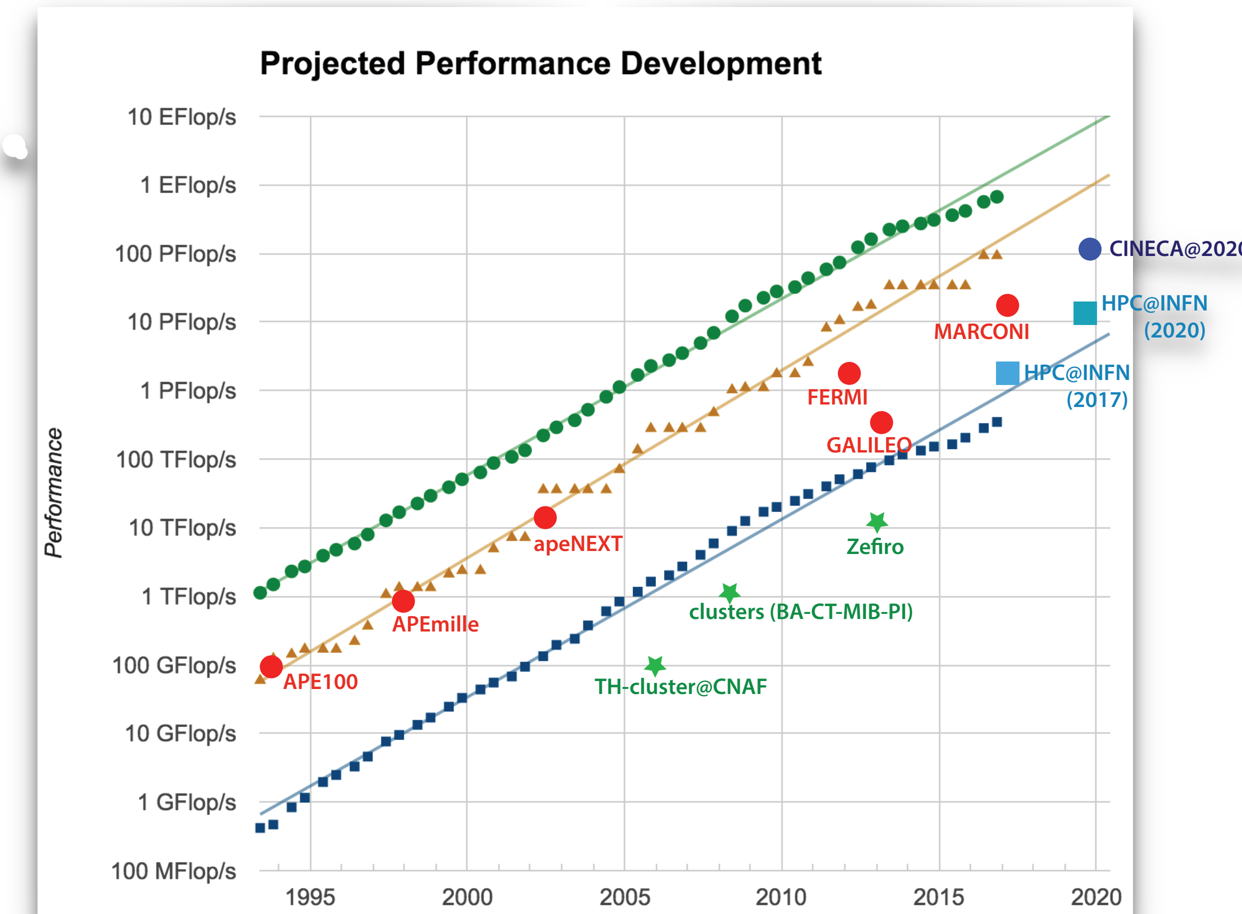
https://drive.google.com/file/d/0BzOFbH1uCRZ1Y09CUHJUdlBJUUU/view?usp=sharing

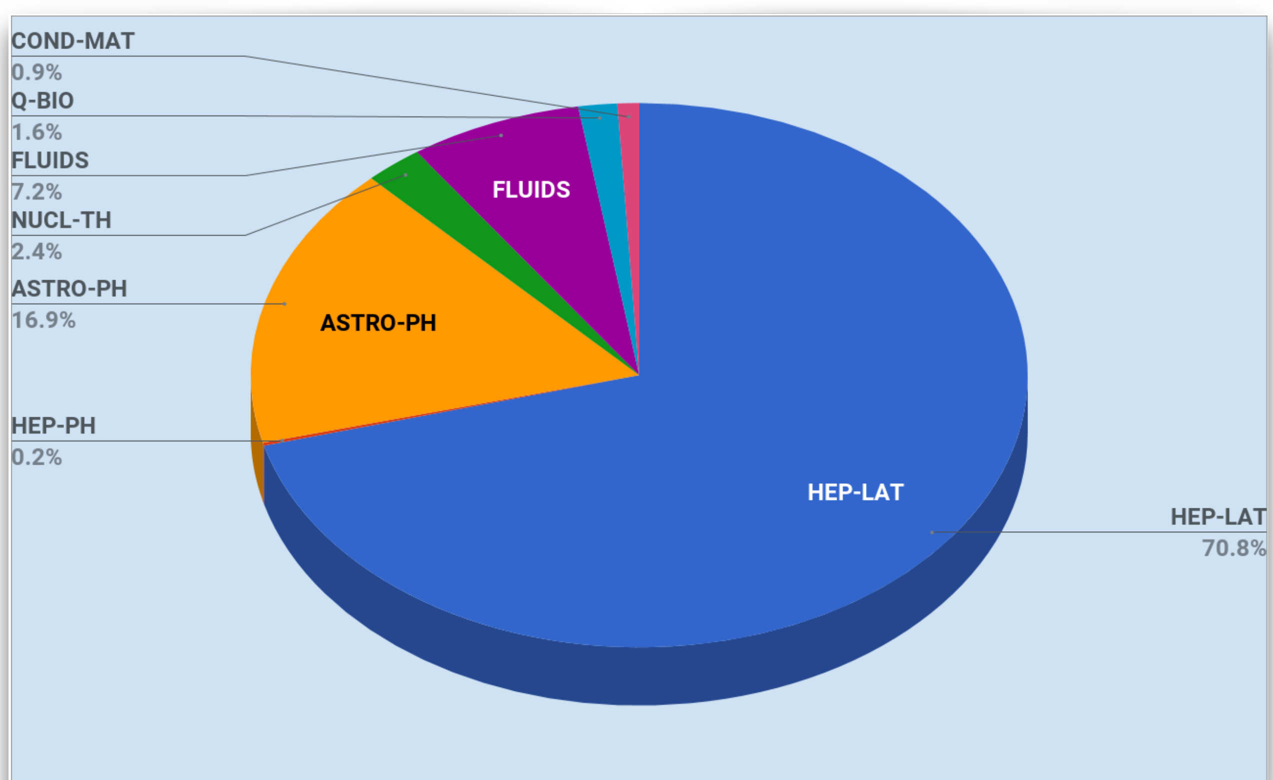
https://agenda.infn.it/internalPage.py?pageId=0&confId=12156

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

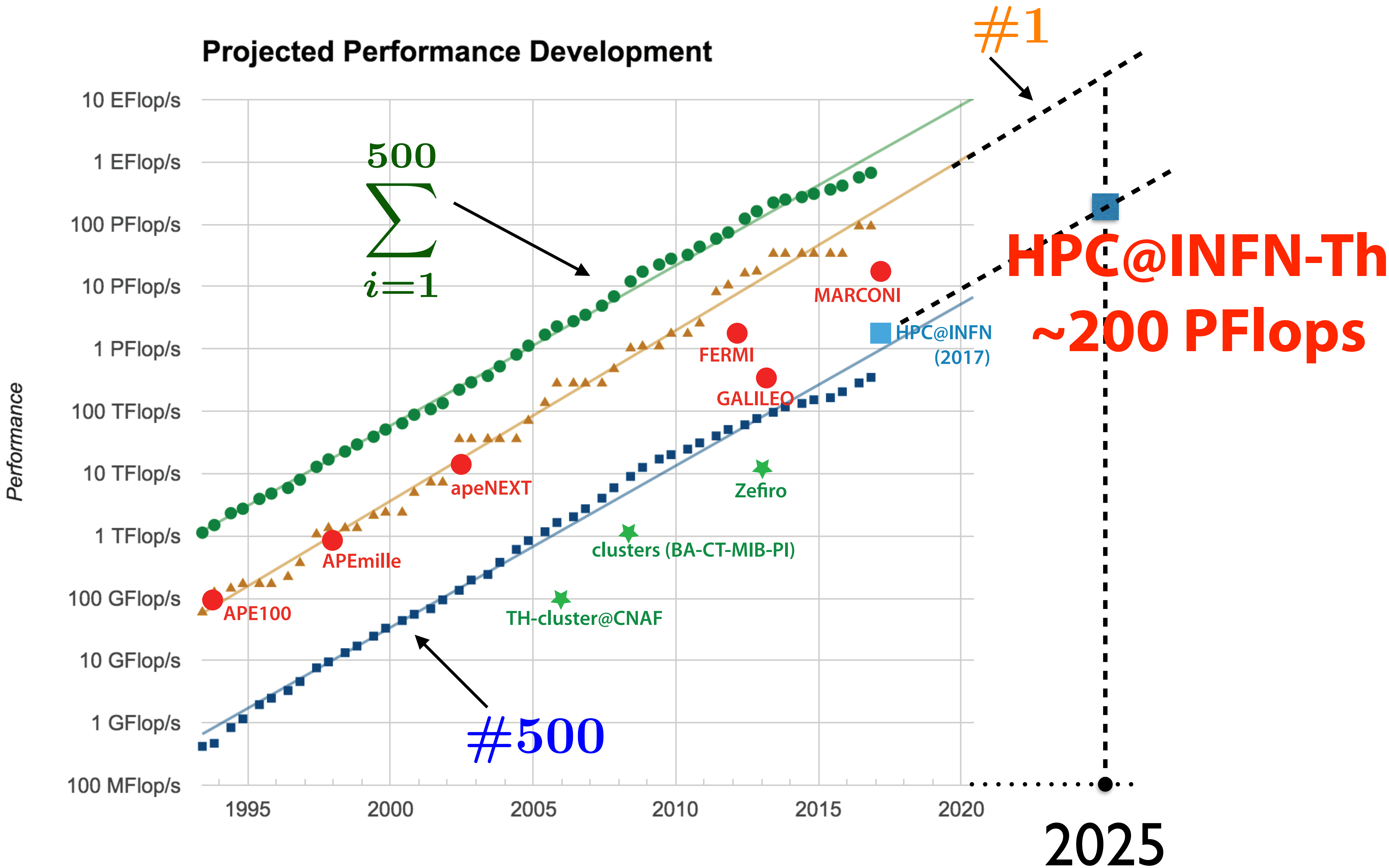
HPC requirements for Th.Physics@INFN

	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-Th (2020–> ...)



Conclusions: 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.

THANK YOU !