HPC per la Fisica Teorica

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INFN Bari

Istituto Nazionale di Fisica Nucleare

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Hotel Ambasciatori, Rimini, 11-15 giugno 2018

Outline

- HPC@INFN-TH: scientific projects
- HPC@INFN-TH: computational resources (2018-2020,…, 2026)
- Conclusions

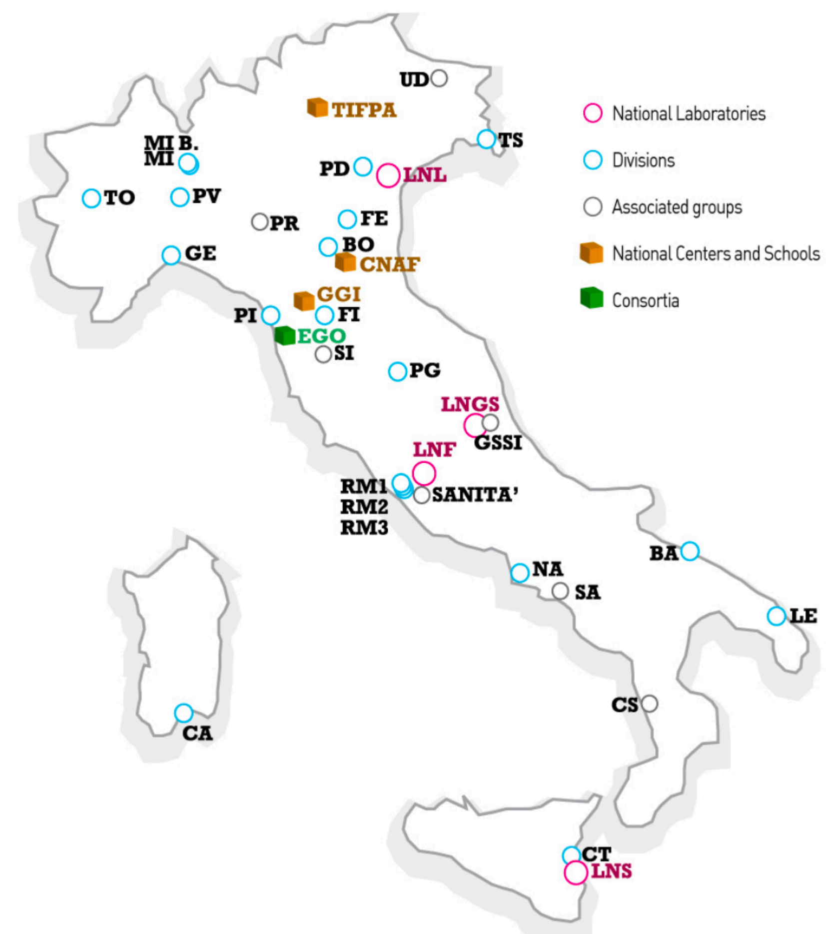
Scientific Projects @ INFN (Th. Physics)

16 scientific projects using HPC resources

***O*(100) researchers (20 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

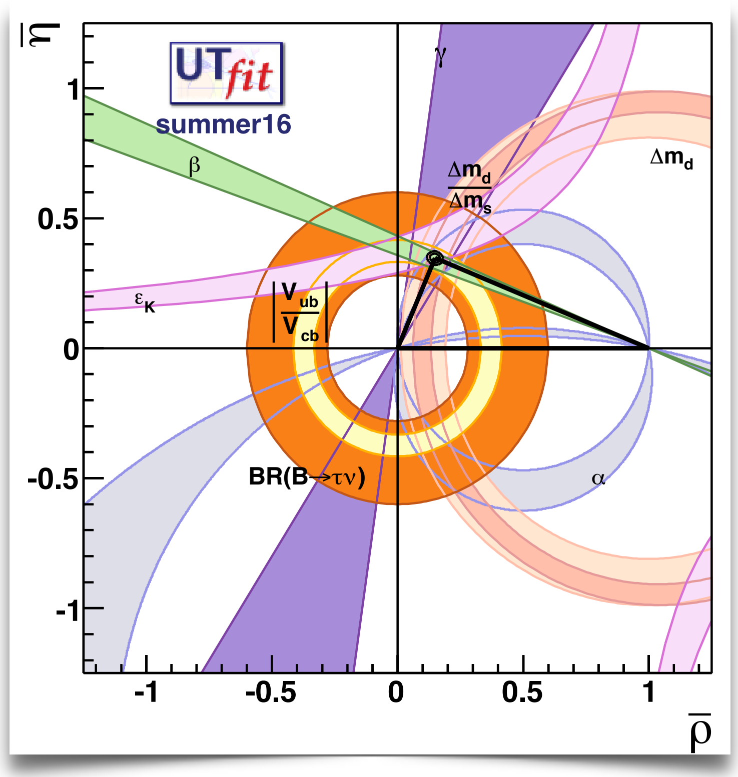
ASSEGNI PROGETTO HPC_HTC PER FISICA TEORICA COMPUTAZIONALE									
Tutor	**Sigla**	**Assegnista**	**Area**	**Sezione**	**Durata**	**Cofinanziatore**	**Tipo di contratto**	**Inizio**	**Fine**
Alessandro Papa	**NPQCD**	**Volodymyr Chelnokov**	**Lattice QCD**	Cosenza/LNF	24 mesi		Assegno di ricerca	15 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

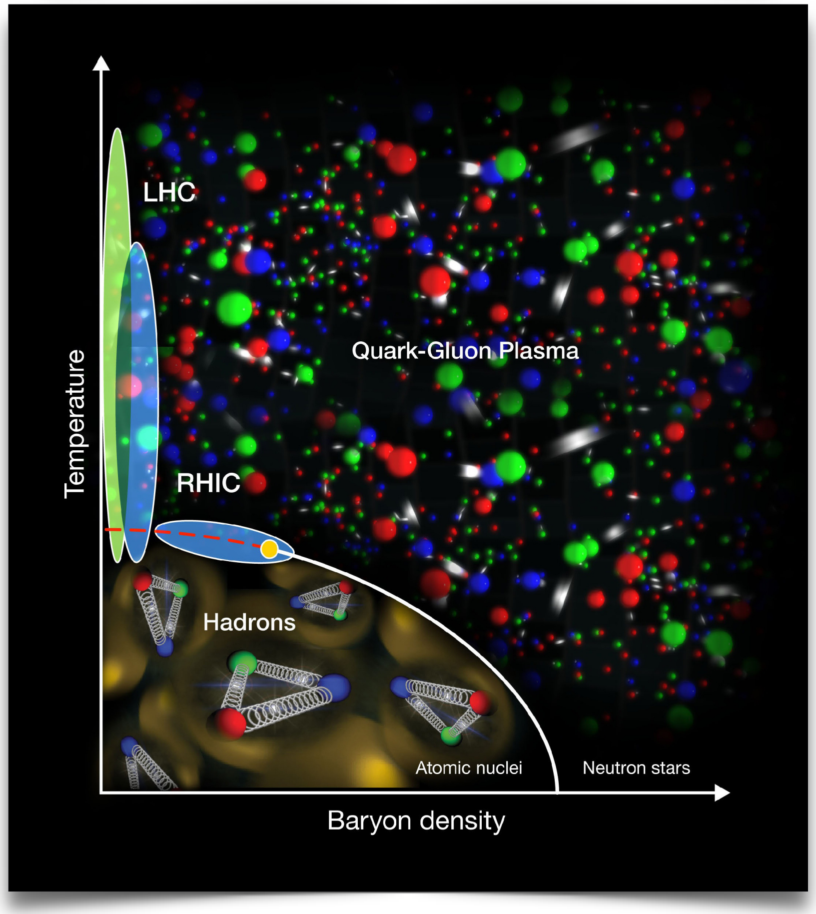
Scientific activity presented at "SM&FT 2017" (Bari, 13-15 December 2017) http://www.ba.infn.it/smft2017

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



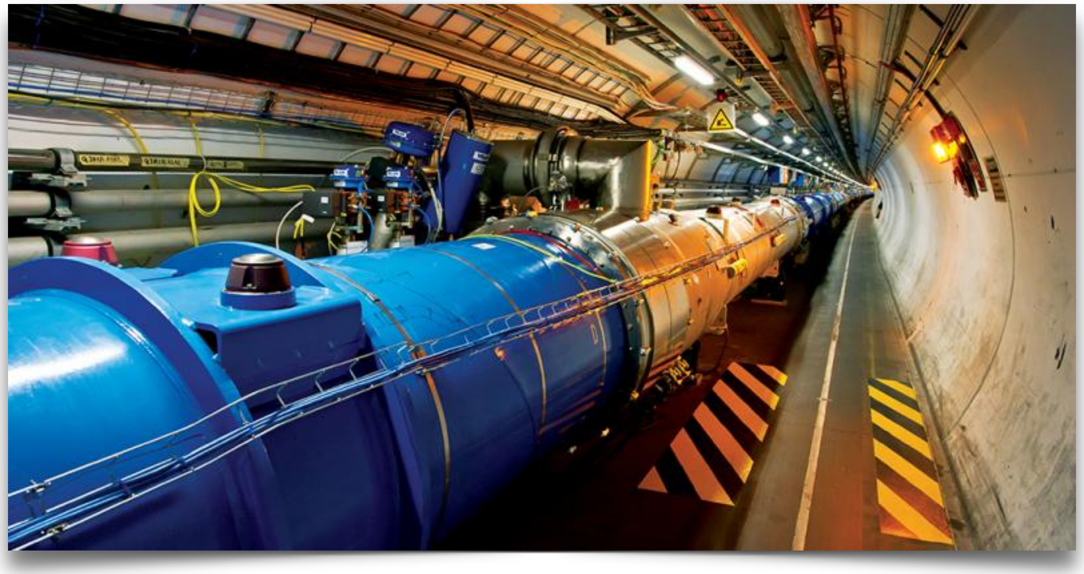


- *In the next years a series of experiments will collect new data that may shed light on the Standard Model and BSM.*
- *The theoretical interpretation of all these data will need non-perturbative calculations with <u>accuracies far beyond the state of the art</u> .*

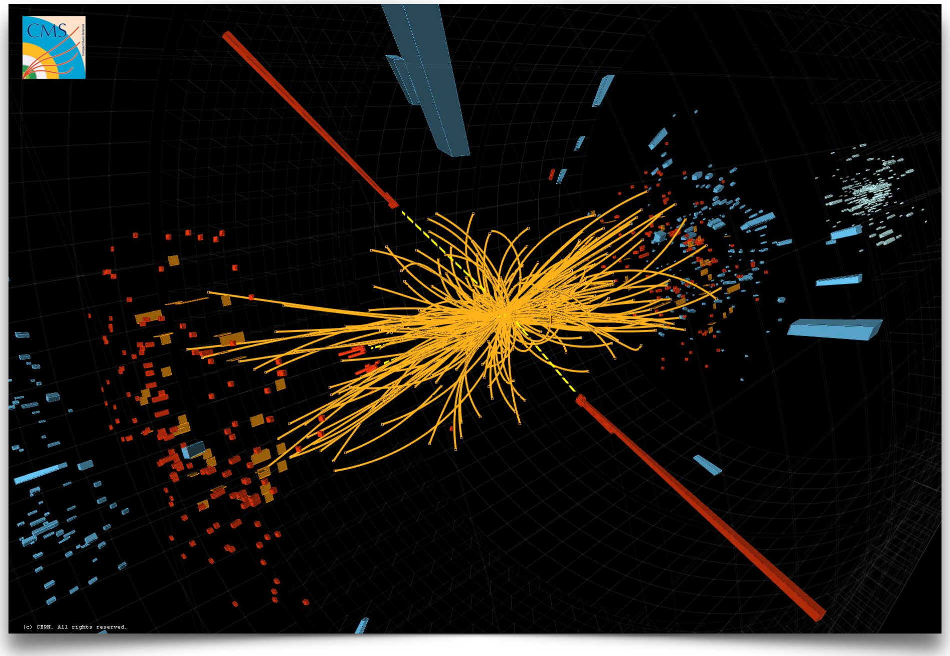
High Energy Physics - Phenomenology

Scientific Projects: QCD@Colliders

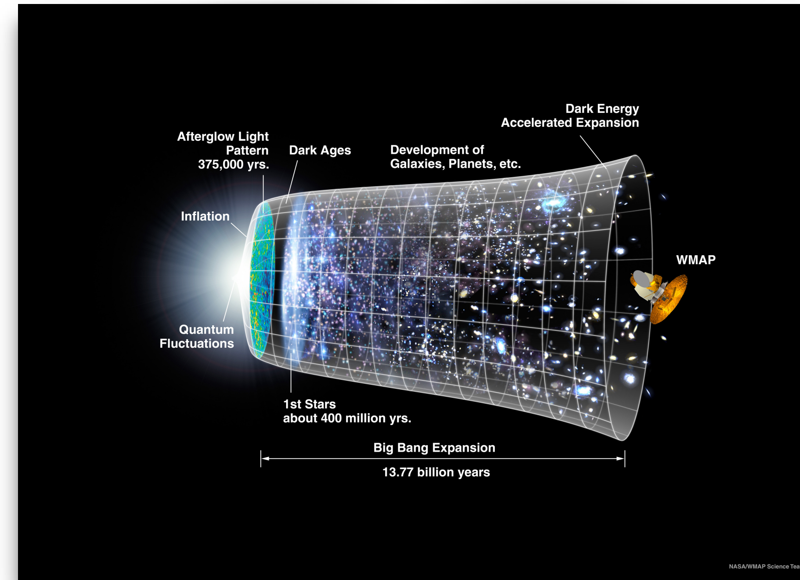
- Monte Carlo event generators to allow a systematic comparison between data and theory at LHC



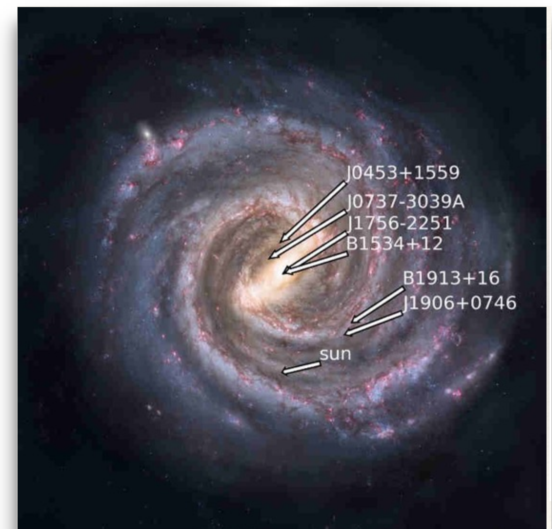
- Higher order QCD corrections and future colliders



General Relativity, Cosmology, Astroparticle Physics

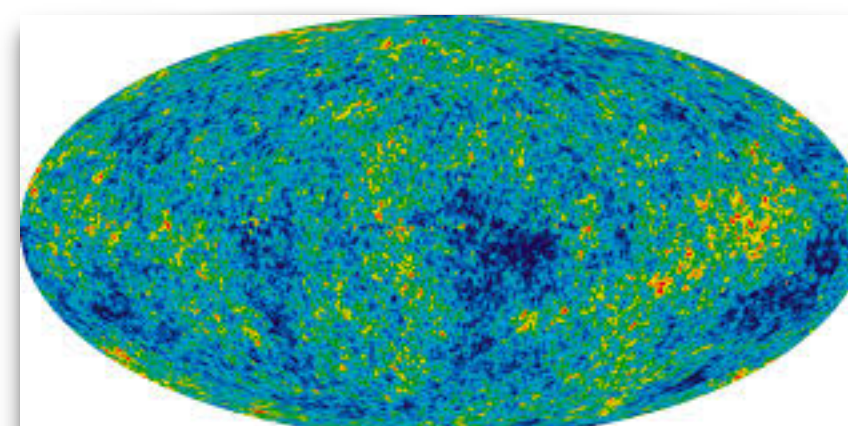


Scientific Projects: INDARK, NEUMATT, TEONGRAV



- 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

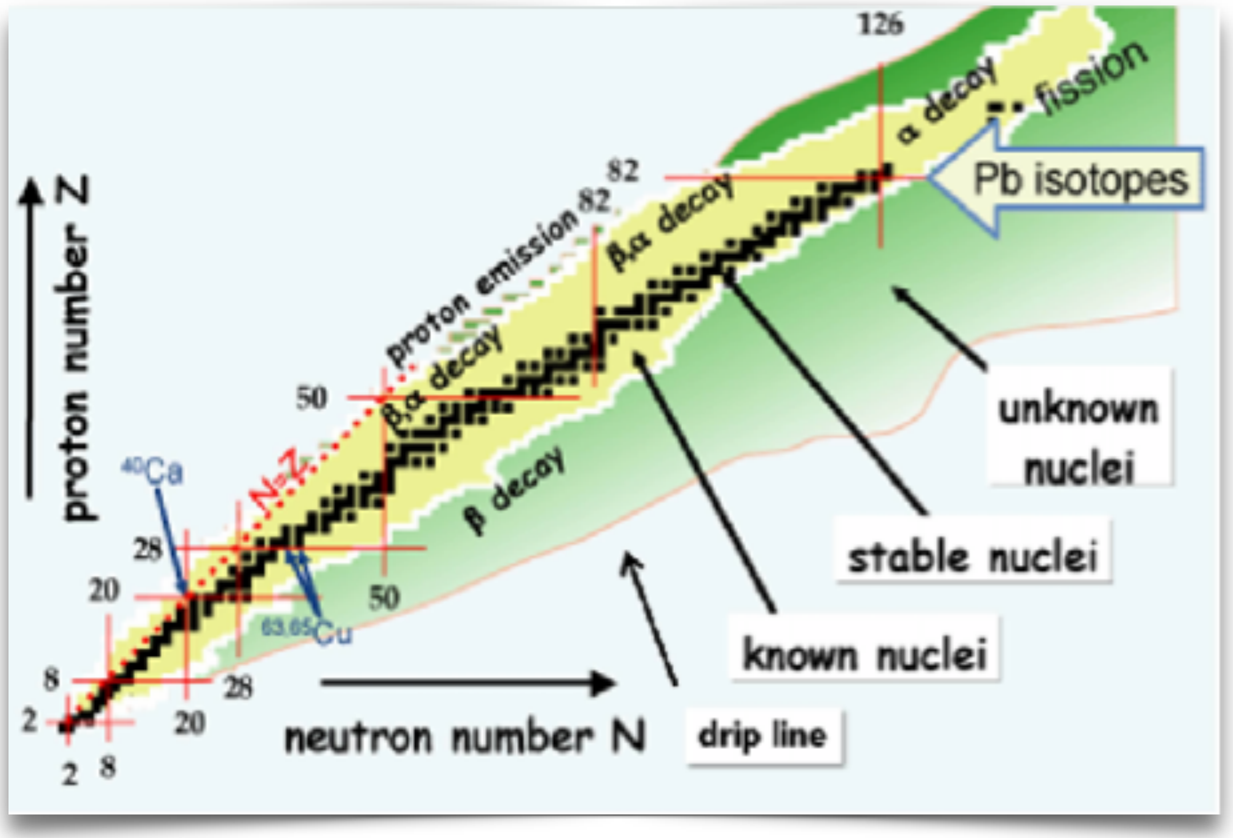
Nuclear Physics

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.

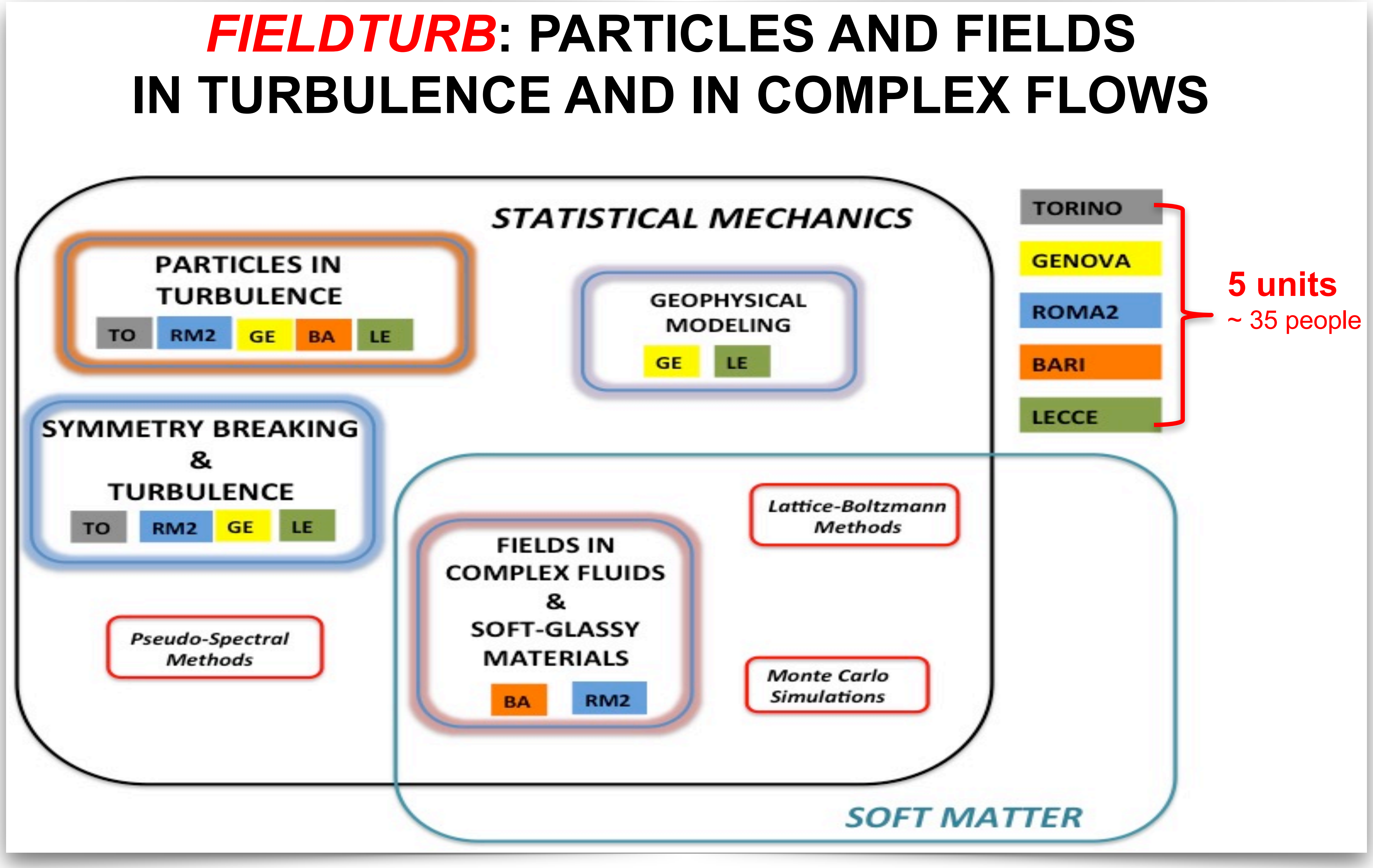
- Development and application of models for nuclear structure studies: Shell Model, Density Functional Theory, Microscopic and algebraic cluster models.

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



Fluid Dynamics

Scientific Projects: FIELDTURB



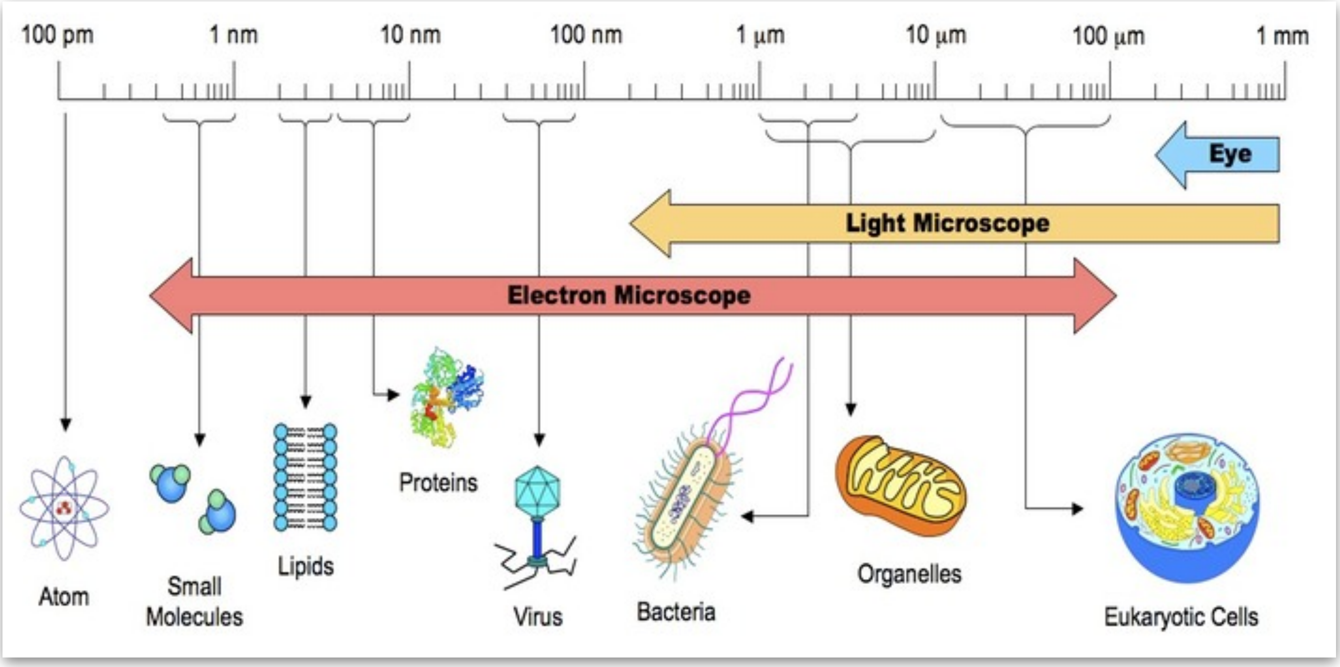
G. Boffetta @ SM&FT 2017, Bari 15 December 2017

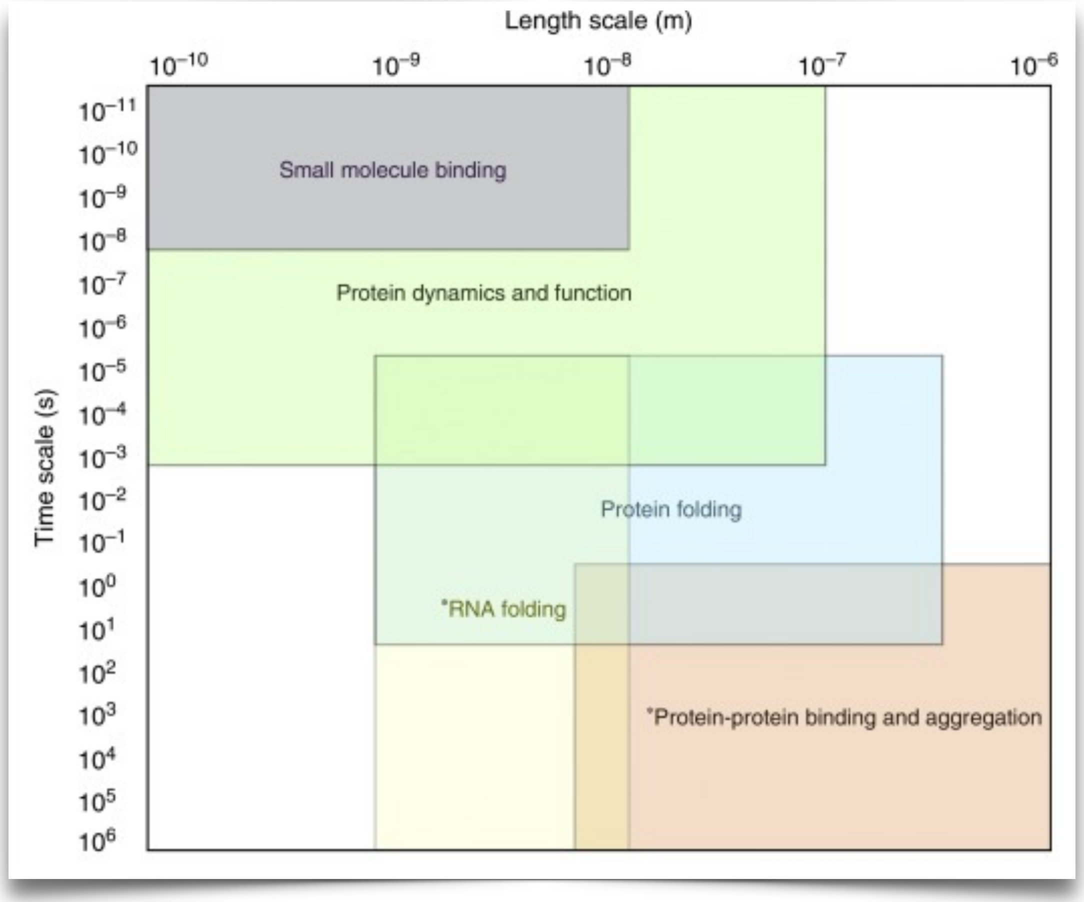
Quantitative Biology

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

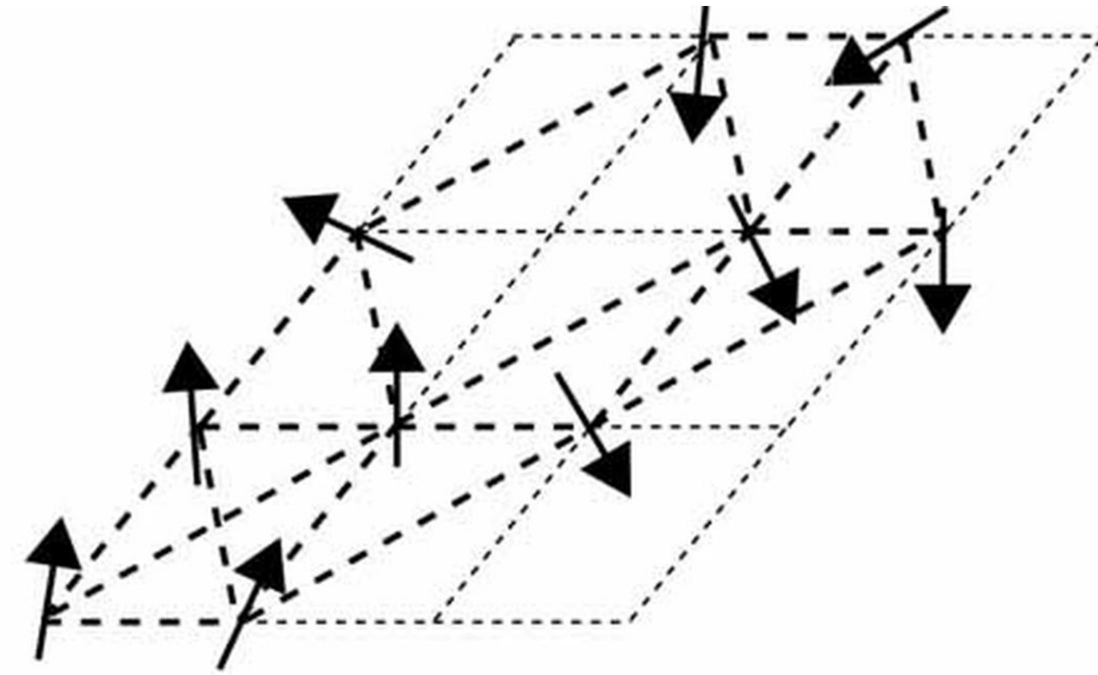
irreversible properties and quantum thermodynamics of ultra cold Fermi and Bose gases, following a change of their trapping potentials

Huge Investments
(H2020 flagships
for graphene
and quantum
information)

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

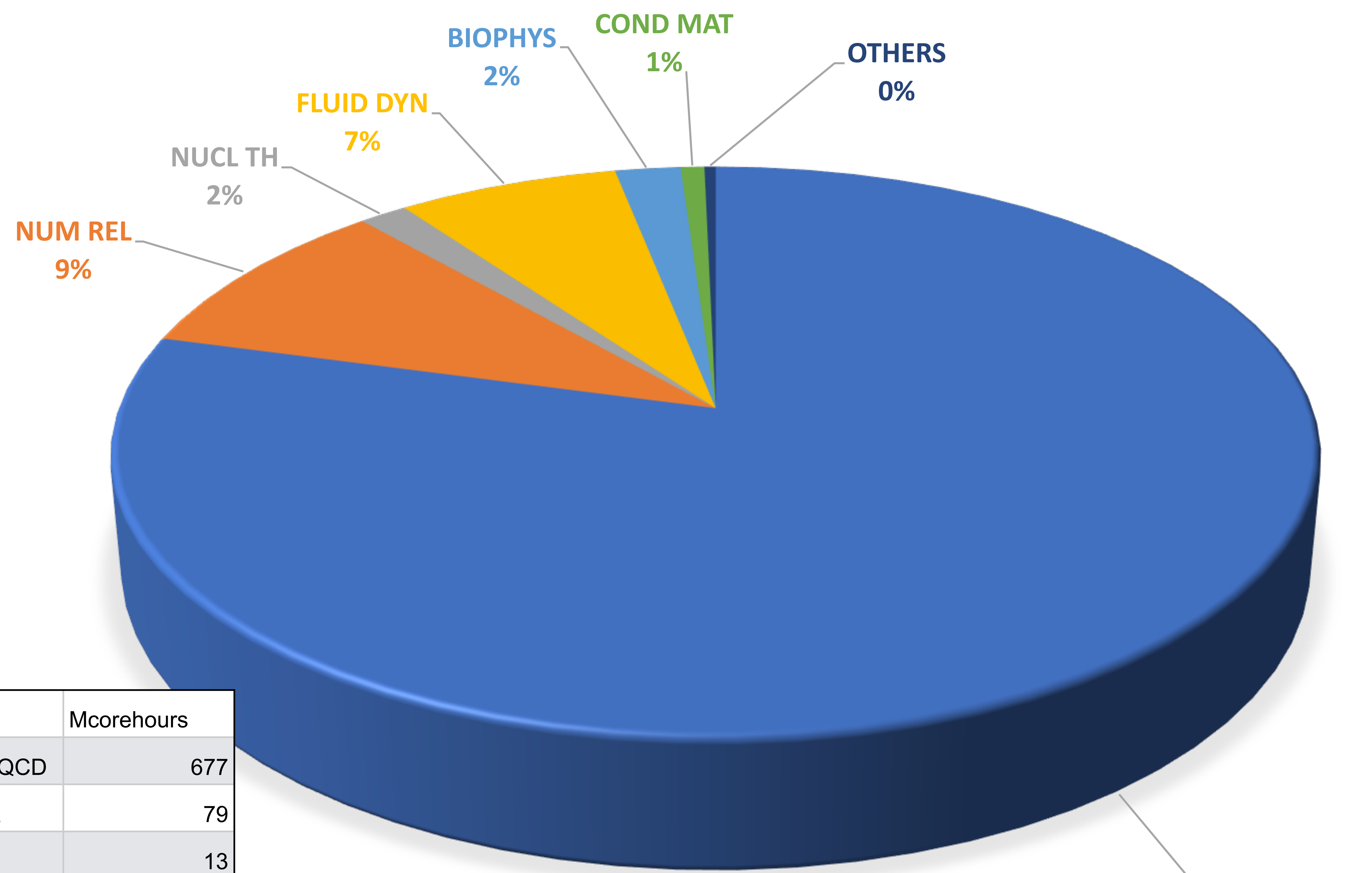
Disordered Systems

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 @CINECA FOR INFN TH-PHYSICS 2012-2017



	Mcorehours
LATTICE QCD	677
NUM REL	79
NUCL TH	13
FLUID DYN	59
BIOPHYS	17
COND MAT	6
OTHERS	3
Total	854

+ *O*(1000) Mcorehours from ISCRA and PRACE

HPC resources for the INFN-TH community (2018)

- CINECA-INFN agreement

INFN CINECA

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)

164 Mcorehours

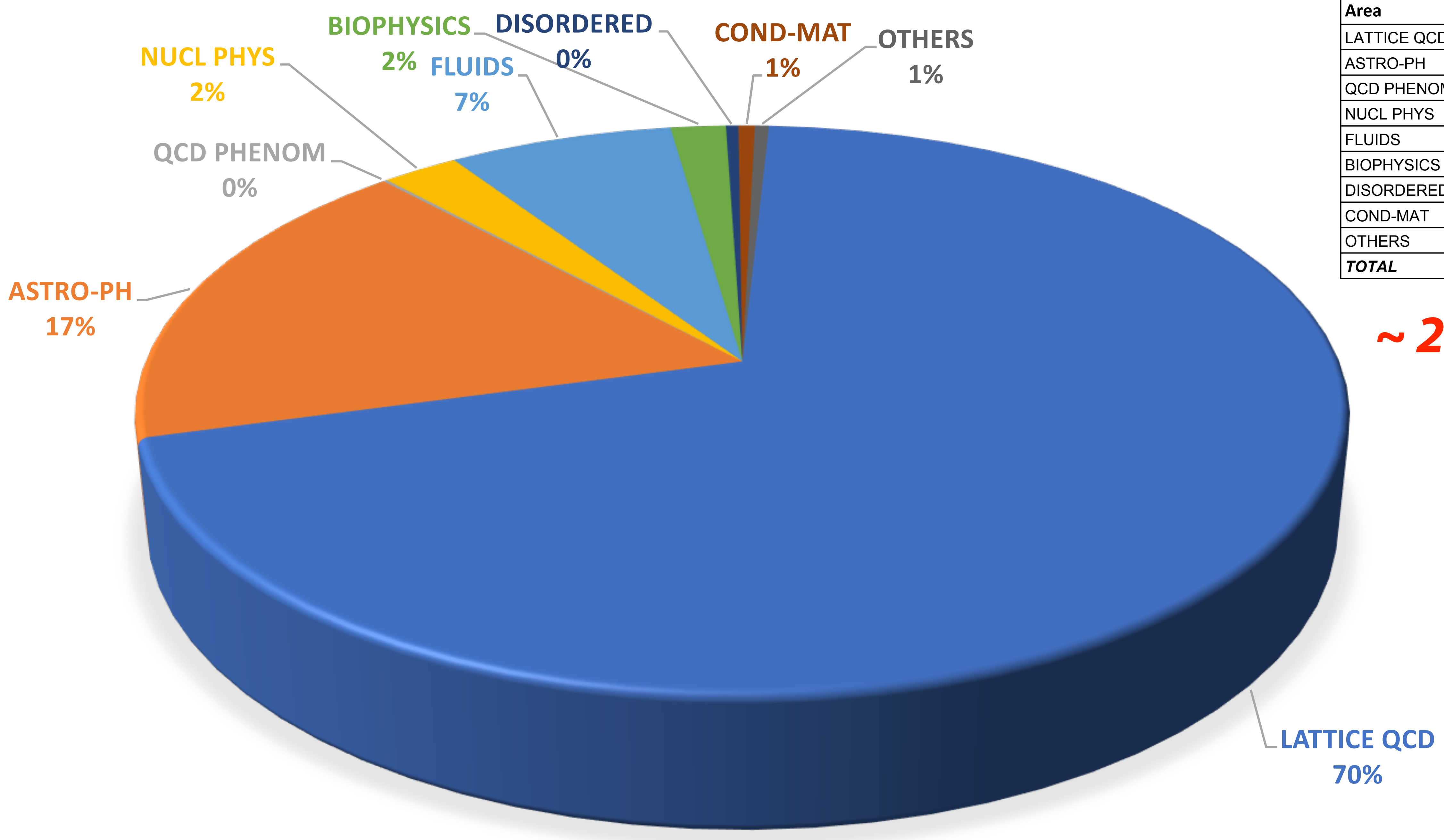
Model: Lenovo Stark
Racks: 21 +
Nodes: 1.512 +
Processors: 2 x 24-cores Intel Xeon 8160 CPU (Skylake) at 2.10 GHz
Cores: 48 cores/node, 72.576+ 38.016 cores in total
RAM: 192 GB/node of DDR4

Peak Performance: about 7.50 PFlop/s

- ISCRA, EU-PRACE

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

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



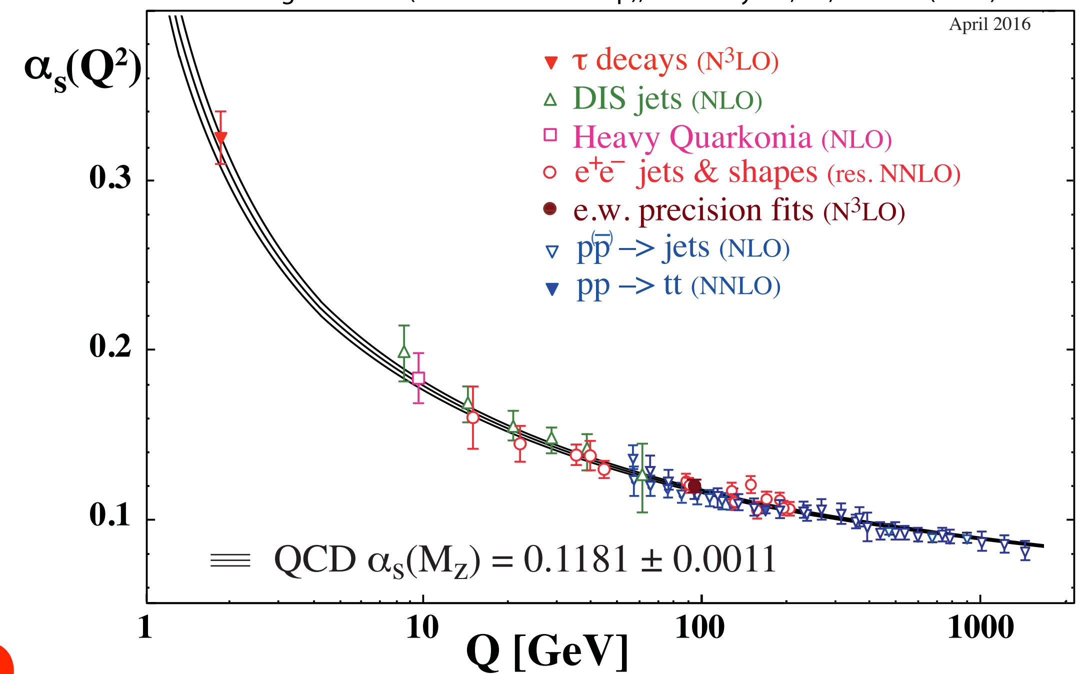
Area	A1+A2+A3 (corehours)
LATTICE QCD	204,800,000
ASTRO-PH	51,000,000
QCD PHENOM	400,800
NUCL PHYS	7,050,000
FLUIDS	20,700,000
BIOPHYSICS	5,100,000
DISORDERED	1,150,000
COND-MAT	1,500,000
OTHERS	1,300,000
TOTAL	*293,000,800*

~ 2 PFlops

Lattice QCD and HPC

strongly coupled at low energies

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

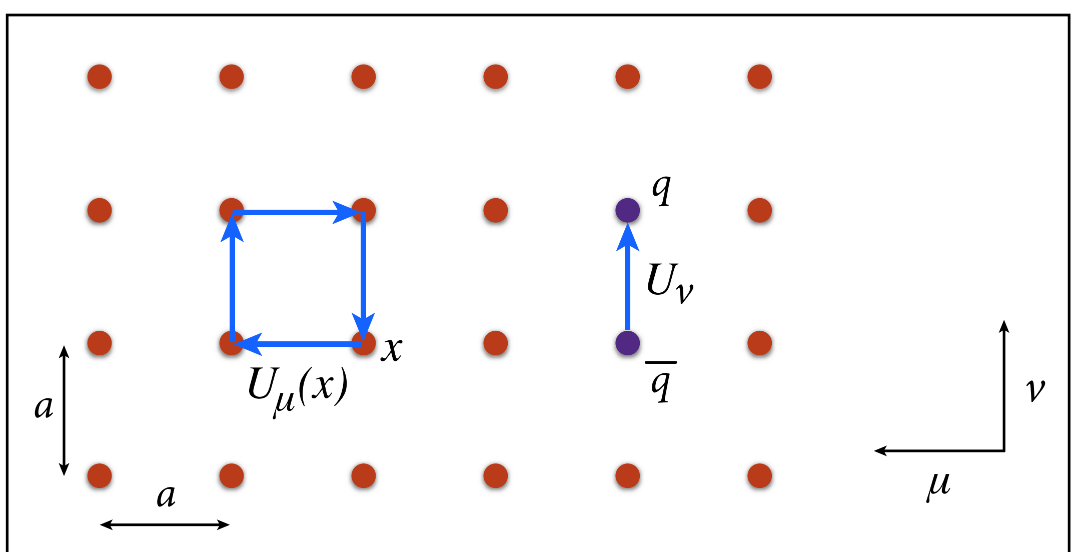


asymptotic freedom at high energies

LATTICE QCD

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

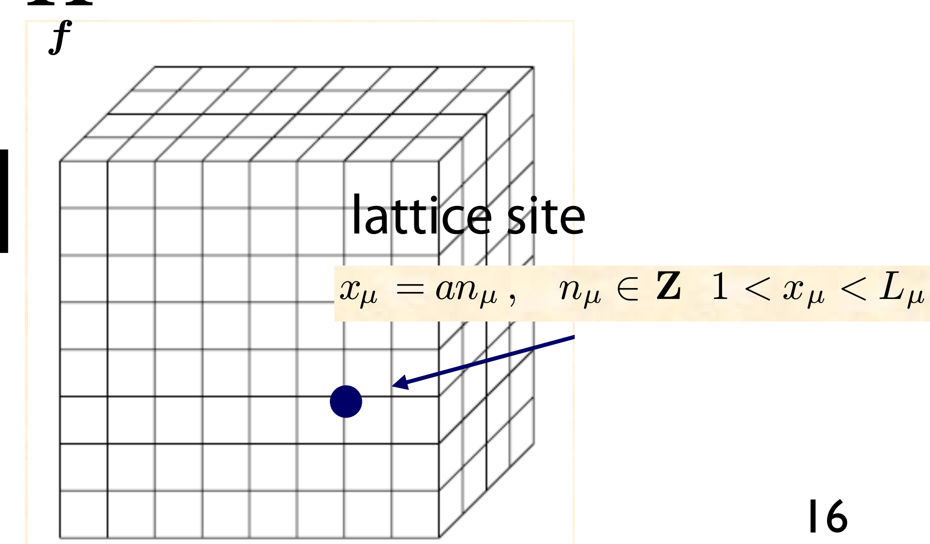
$$\langle \mathcal{O}(U,q,\bar{q})\rangle = (1/Z)\int [dU]\prod_f [dq_f][d\bar{q}_f]\mathcal{O}(U,q,\bar{q})e^{-S_g[U]-\sum_f \bar{q}_f(D[U]+m_f)q_f}$$



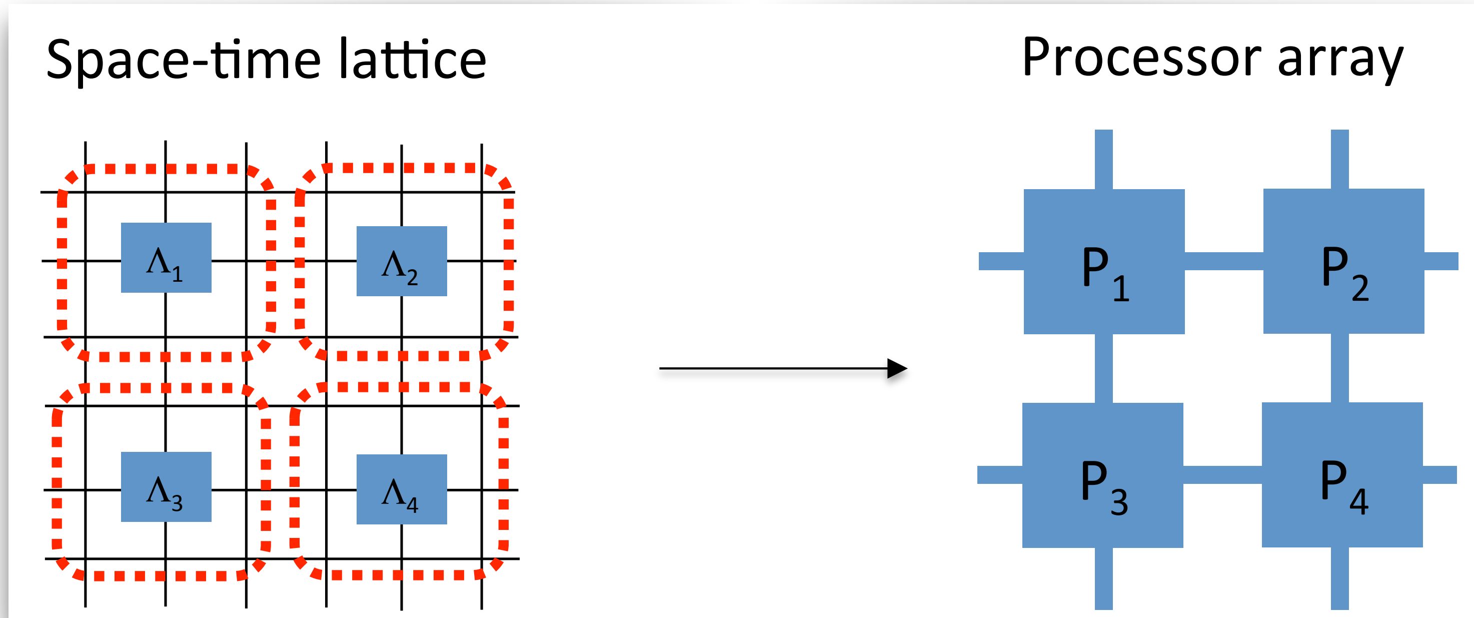
$$Z = \int [dU]e^{-S_g[U]}\prod_f \det(D[U]+m_f)$$

hyper cubic lattice

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



Lattice QCD Simulations as an HPC challenge



courtesy A.Ukawa, arXiv:1501.04215

ideal case of the parallel computation paradigm !

- ***Monte Carlo methods*** to numerically evaluate the functional integrals
- ***Locality:*** (property of the field theoretic description of fundamental interactions)
  - the numerical operations at a site ***n*** can be carried out independently of those at a site ***m*** unless the pair is within the limited neighborhood of each other;
  - calculations by a given processor can be carried out independently of those by the other processors, except that the processors with overlapping boundaries have to exchange values of fields in the boundaries before and/or after the calculations in each sub lattice;
  - for a fixed lattice size, the computation time can be reduced by a factor N_P, and for a fixed sub-lattice size, one can enlarge the total lattice size proportionately to the number of processors N_P without increasing the computation time.

Lattice QCD and parallel computers building

name	year	authors	peak speed
Columbia	1984	Christ-Terrano	–
Columbia-16	1985	Christ et al	0.25 GFlop/s
APE1	**1988**	**Cabibbo-Parisi**	**1 GFlop/s**
Columbia-64	1987	Christ et al	1 GFlop/s
Columbia-256	1989	Christ et al	16 GFlop/s
ACPMAPS	1991	Mackenzie et al	5 GFlop/s
QCDPAX	1991	Iwasaki-Hoshino	14 GFlop/s
GF11	1992	Weingarten	11 GFlop/s
APE100	**1994**	**APE Collab.**	**0.1 TFlop/s**
CP-PACS	1996	Iwasaki et al	0.6 TFlop/s
QCDSP	1998	Christ et al	0.6 TFlop/s
APEmille	**2000**	**APE Collab.**	**0.8 TFlop/s**
apeNEXT	**2004**	**APE Collab.**	**10 TFlop/s**
QCDOC	2005	Christ et al	10 TFlop/s
PACS-CS	2006	Ukawa et al	14 TFlop/s
QCDCQ	2011	Christ et al	500 TFlop/s
QPACE	2012	Wettig et al	200 TFlop/s

parallel computers developed by physicists for lattice QCD which gave rise in some cases to commercial supercomputers

QCDOC → **IBM BlueGene/L**

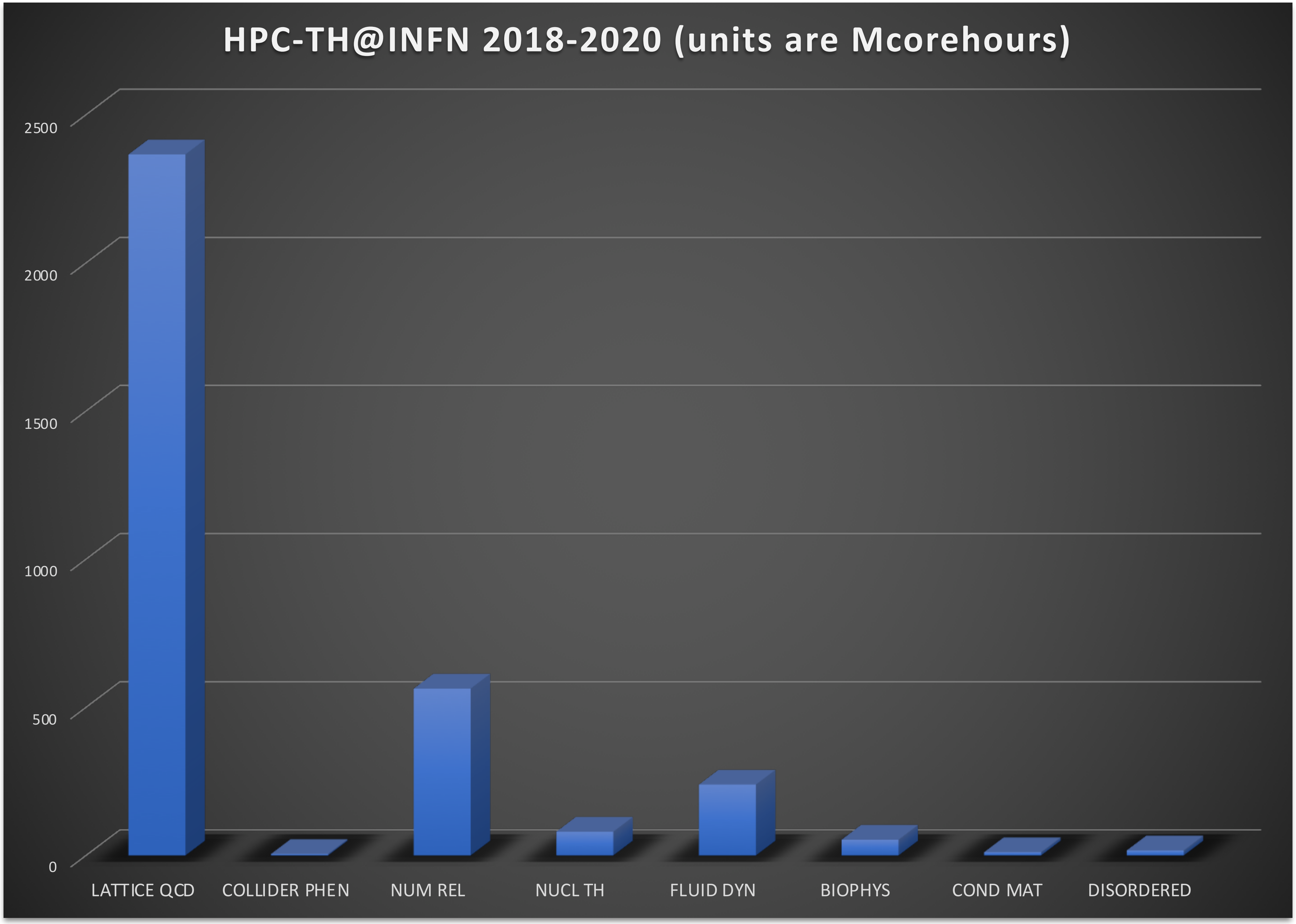
QCDCQ → **IBM BlueGene/Q**

HPC@INFN-Th (2018-2020)

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

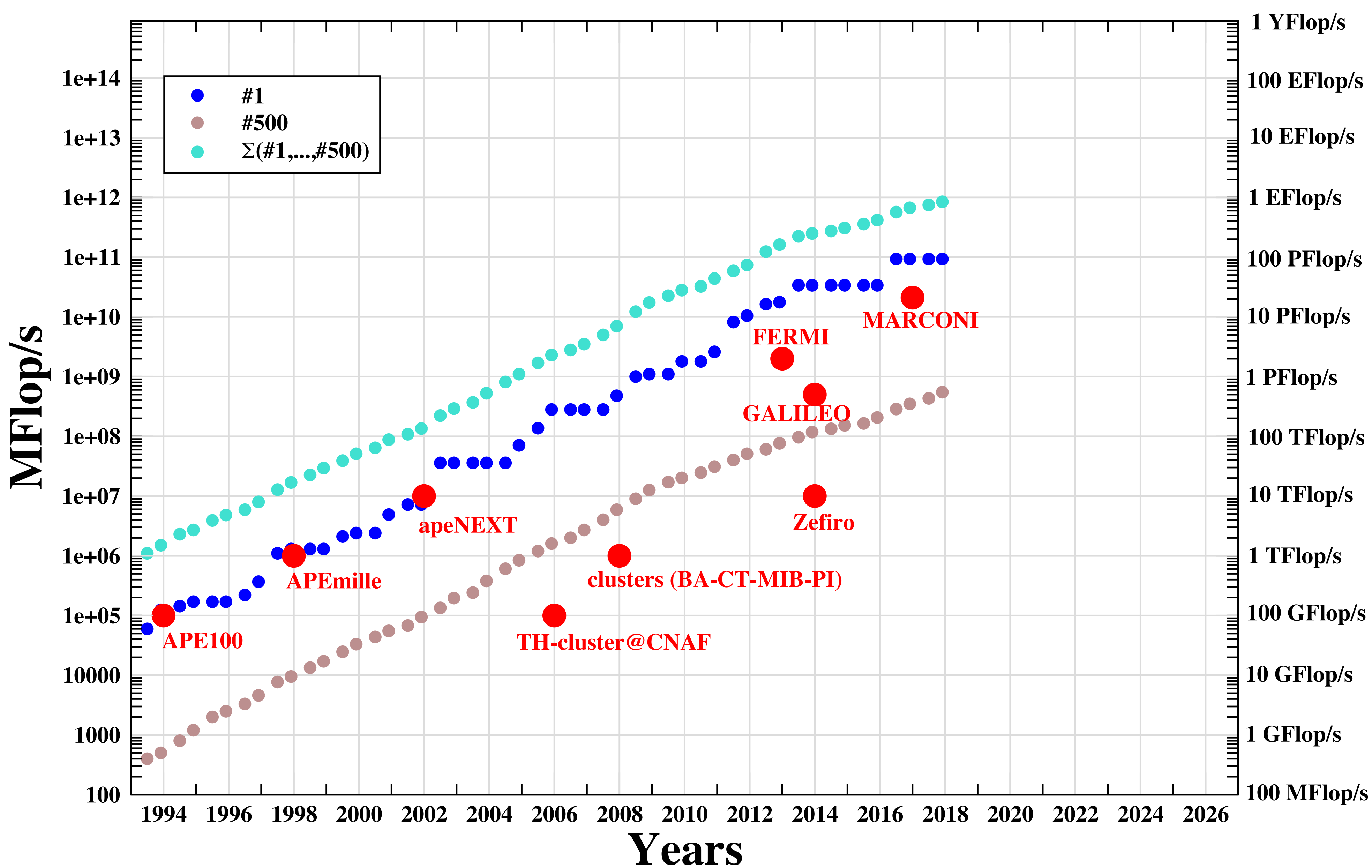
https://drive.google.com/file/d/0BzOFbH1uCRZ1Y09CUHJUdlBJUUU/view?usp=sharing

Year	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
Total (Mcorehours)	**607**	**1097**	**1638**
Total (PFlop/s)	**4.6**	**8.4**	**12.5**

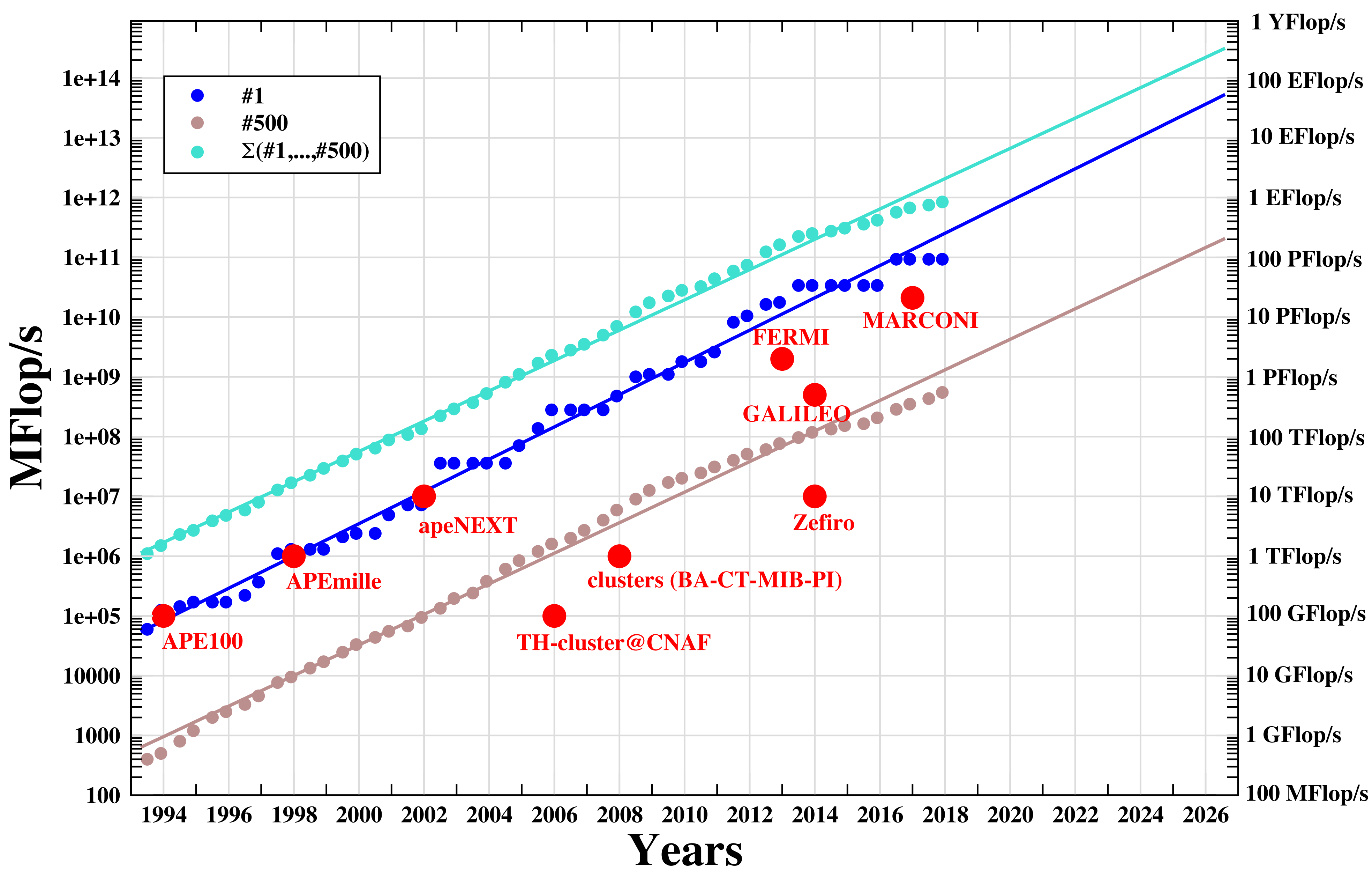


The next 8 years…

The next 8 years…



The next 8 years…



ANNUAL PERFORMANCE INCREASE OF THE TOP500

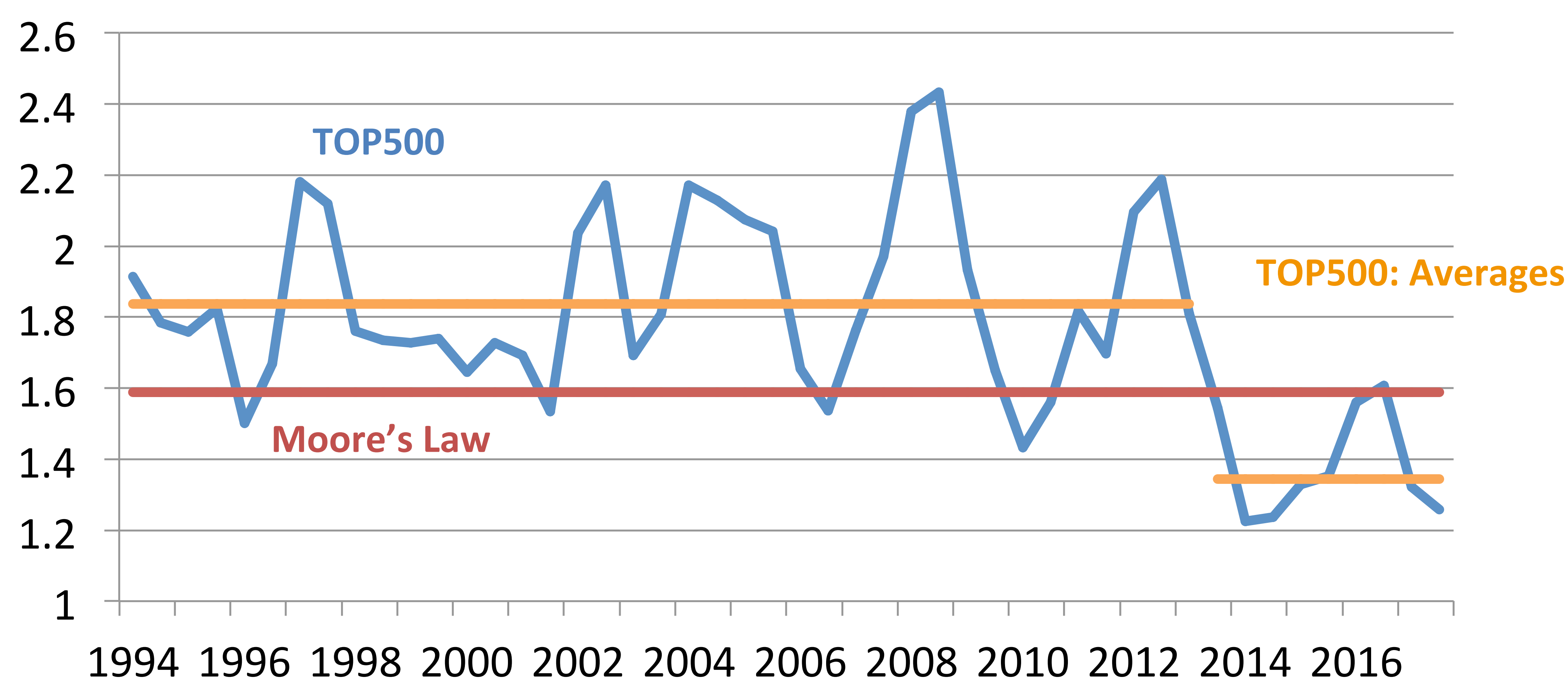
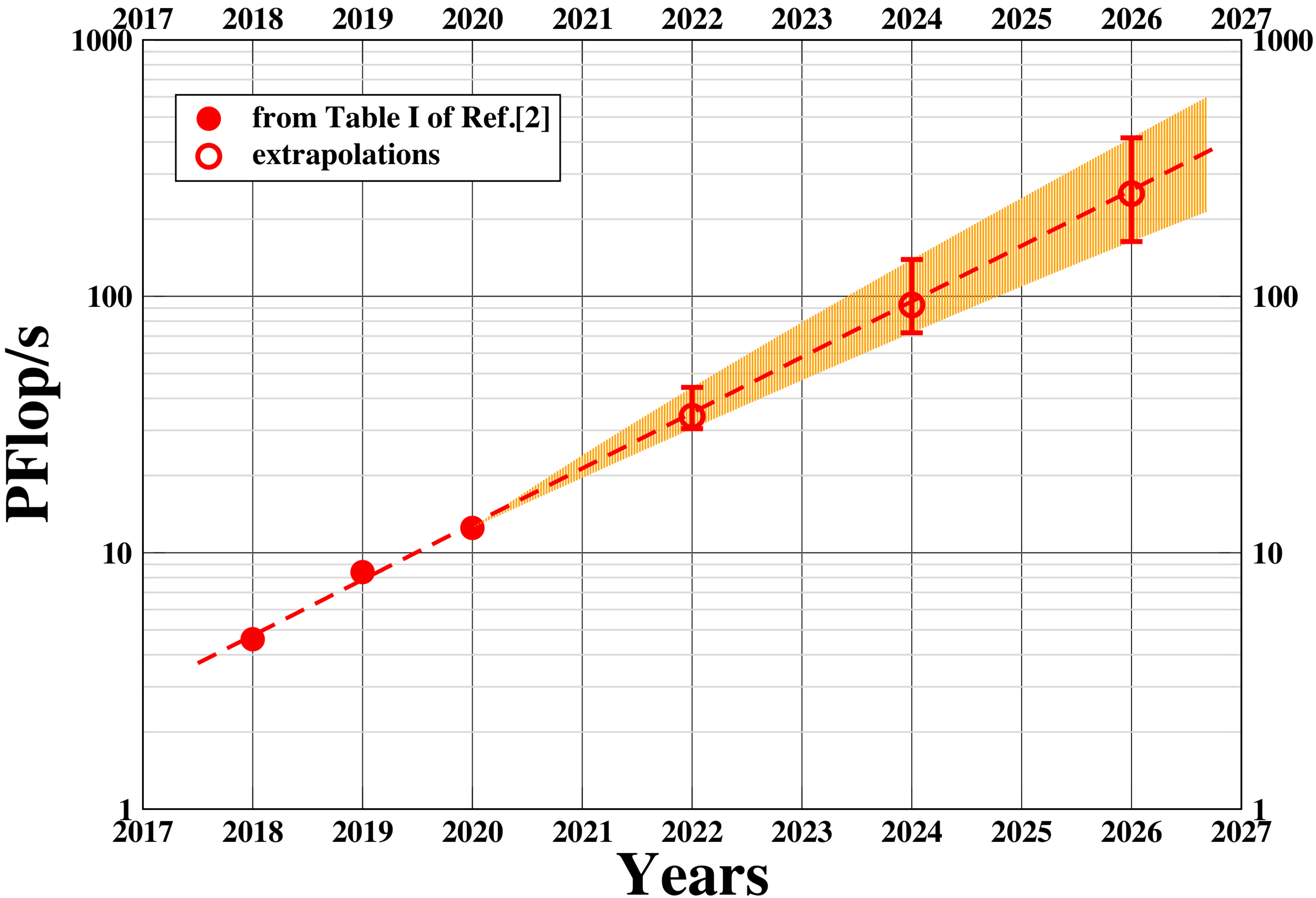
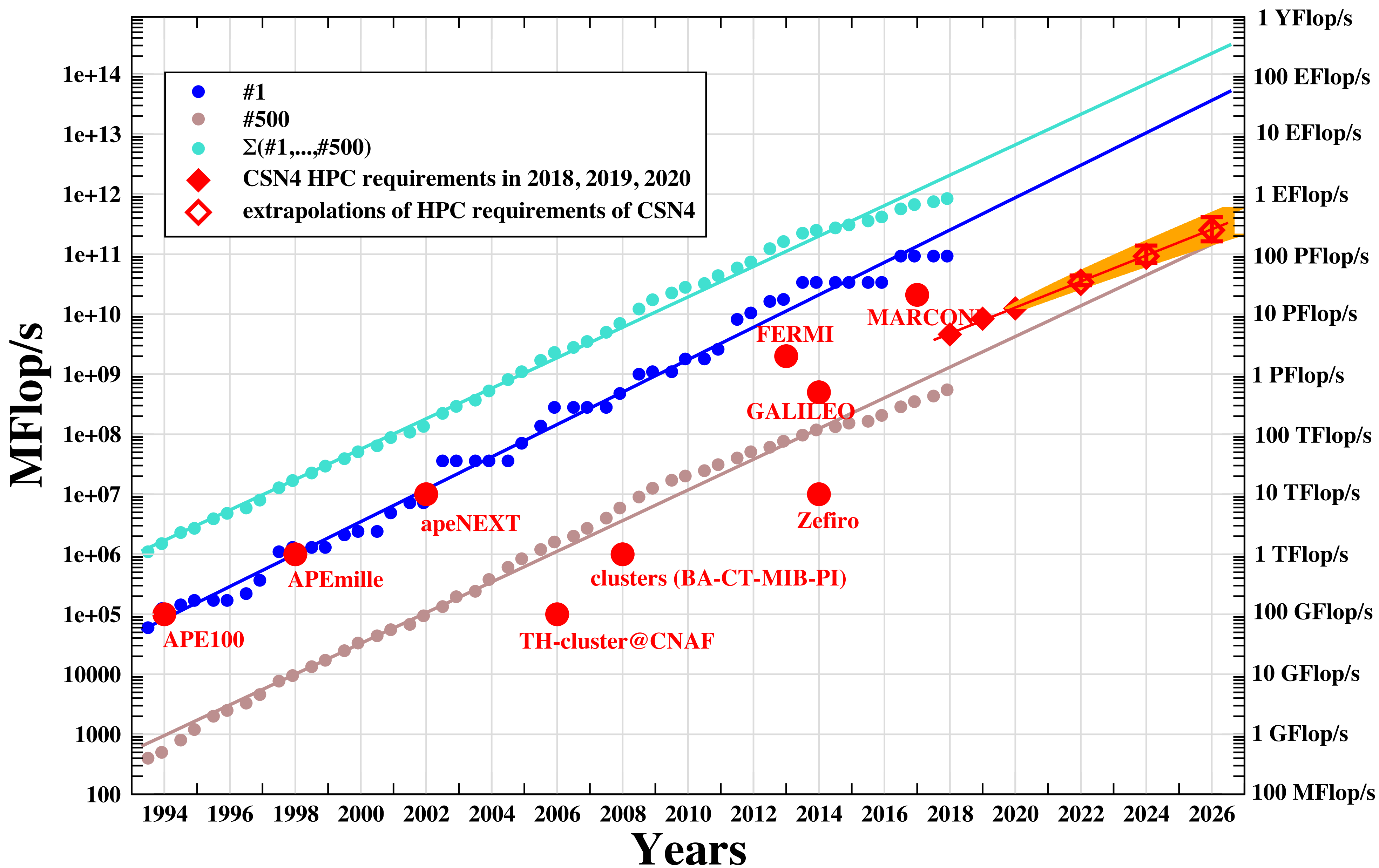


	Table 1 of Ref.[2]			power increase 2.6 every 3 years			power increase 4.5 every 3 years			power increase 5.2 every 3 years		
Year	**2018**	**2019**	**2020**	**2022**	**2024**	**2026**	**2022**	**2024**	**2026**	**2022**	**2024**	**2026**
LGT: hadron physics	54	108	180	344	658	1258	489	1329	3612	540	1623	4873
LGT: QGP and BSM	207	432	648	1239	2368	4527	1761	4785	13003	1946	5843	17544
LGT: flavor physics	117	234	387	740	1414	2704	1052	2858	7765	1162	3489	10478
Colliders Phenomenology	1	2	3	6	11	21	8	22	60	9	27	81
General Relativity	142	182	227	434	830	1586	617	1676	4555	682	2047	6146
Cosmology and Astroparticle Physics	3	4	6	11	22	42	16	44	120	18	54	162
Nuclear Theory	18	27	36	69	132	252	98	266	722	108	325	975
Fluid Dynamics	50	80	110	210	402	768	299	812	2207	330	992	2978
Quantitative Biology	9	18	27	52	99	189	73	199	542	81	243	731
Disordered systems	4	6	8	15	29	56	22	59	161	24	72	217
Condensed matter	2	4	6	11	22	42	16	44	120	18	54	162
Total (Mcorehours)	**607**	**1097**	**1638**	**3131**	**5986**	**11443**	**4451**	**12095**	**32868**	**4918**	**14769**	**44347**
Total (PFlop/s)	**4.6**	**8.4**	**12.5**	**23.9**	**45.8**	**87.5**	**34.0**	**92.5**	**251.4**	**37.6**	**113.0**	**339.2**



2017
2018
2019
2020
2021
2022
2023
2024
2025
2026
2027
1000
100
10
1
PFlop/s
from Table I of Ref.[2]
extrapolations
Years



MFlop/s
Years
#1
#500
Σ(#1,...,#500)
CSN4 HPC requirements in 2018, 2019, 2020
extrapolations of HPC requirements of CSN4
APE100
APEmille
apeNEXT
TH-cluster@CNAF
clusters (BA-CT-MIB-PI)
FERMI
GALILEO
Zefiro
MARCONI
1e+14
1e+13
1e+12
1e+11
1e+10
1e+09
1e+08
1e+07
1e+06
1e+05
10000
1000
100
1 YFlop/s
100 EFlop/s
10 EFlop/s
1 EFlop/s
100 PFlop/s
10 PFlop/s
1 PFlop/s
100 TFlop/s
10 TFlop/s
1 TFlop/s
100 GFlop/s
10 GFlop/s
1 GFlop/s
100 MFlop/s
1994 1996 1998 2000 2002 2004 2006 2008 2010 2012 2014 2016 2018 2020 2022 2024 2026

Conclusions

- It is crucial for the theoretical computational physics community to have at disposal in the next years enough computing power to address new and challenging physics problems.

- Estimate of HPC resources to pursue the scientific projects at an international competitive level:

years	CPU (PFlop/s)			Storage (PBytes)		
	min		max	min		max
2018		4.6			1.0	
2019		8.4			1.6	
2020		12.5			2.7	
2022	23.9	34.0	37.6	5.2	7.4	8.2
2024	45.8	92.5	113.0	9.9	20.1	24.5
2026	87.5	251.4	339.2	19.0	54.5	73.6

- 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 supporting a specific programme of post-doc grants.