Fisica Computazionale Teorica nell'INFN: stato e prospettive

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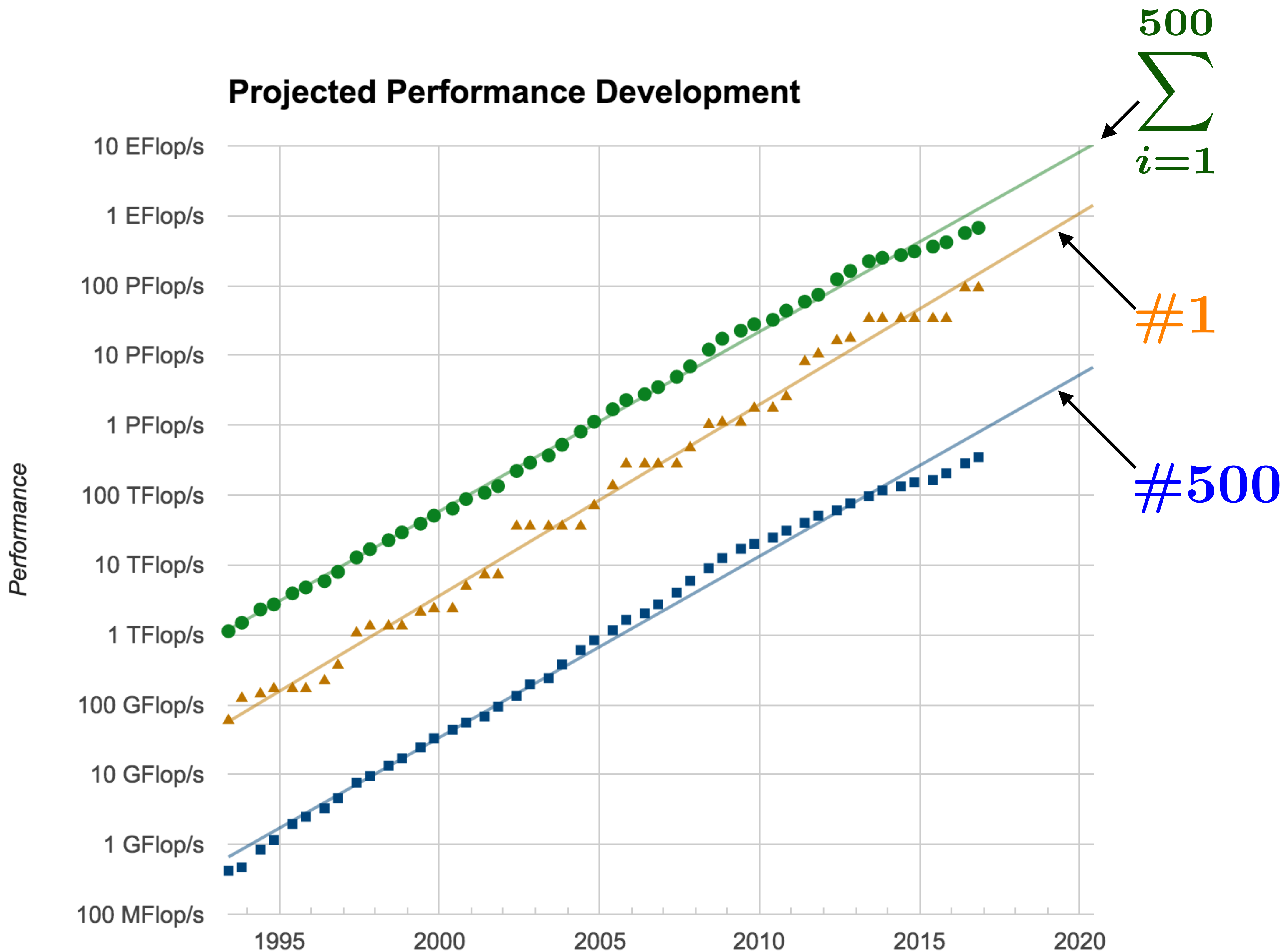
Istituto Nazionale
di Fisica Nucleare

Workshop della CCR
L.N.G.S., 24 maggio 2017

Sommario

- Breve storia del calcolo HPC nel Gruppo Teorico
- Stato attuale e prospettive
- Conclusioni

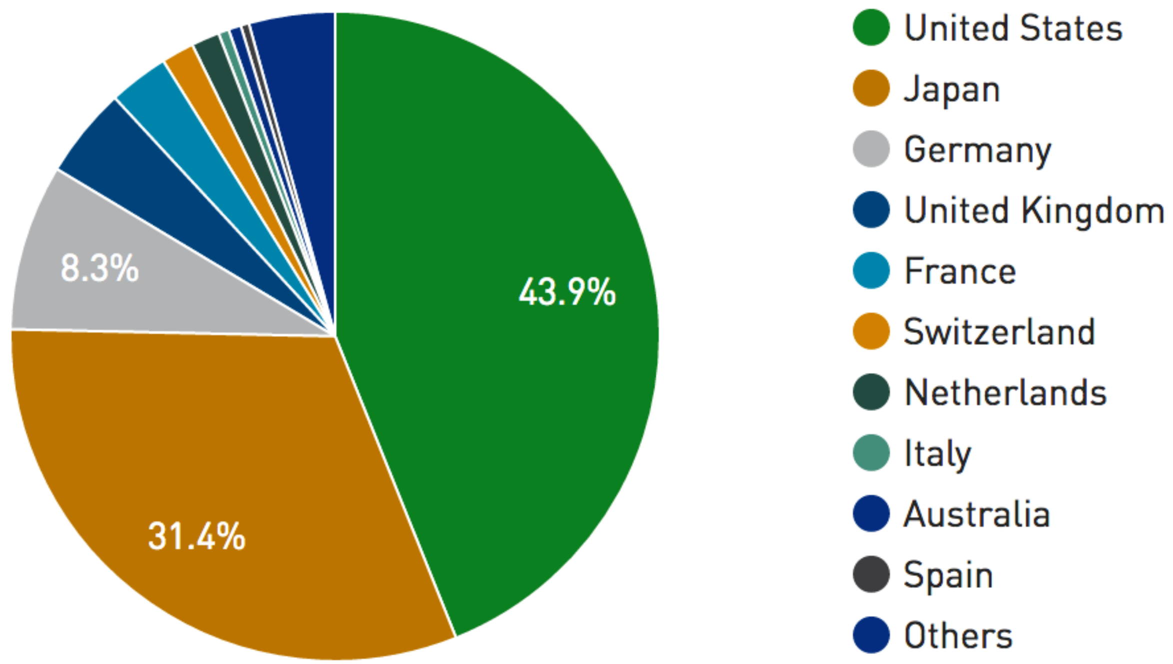
Fisica Teorica e calcolo HPC: ~1980 - 2016



https://www.top500.org/statistics/perfdevel/

TOP 500 (Nov 1996)

Countries Performance Share



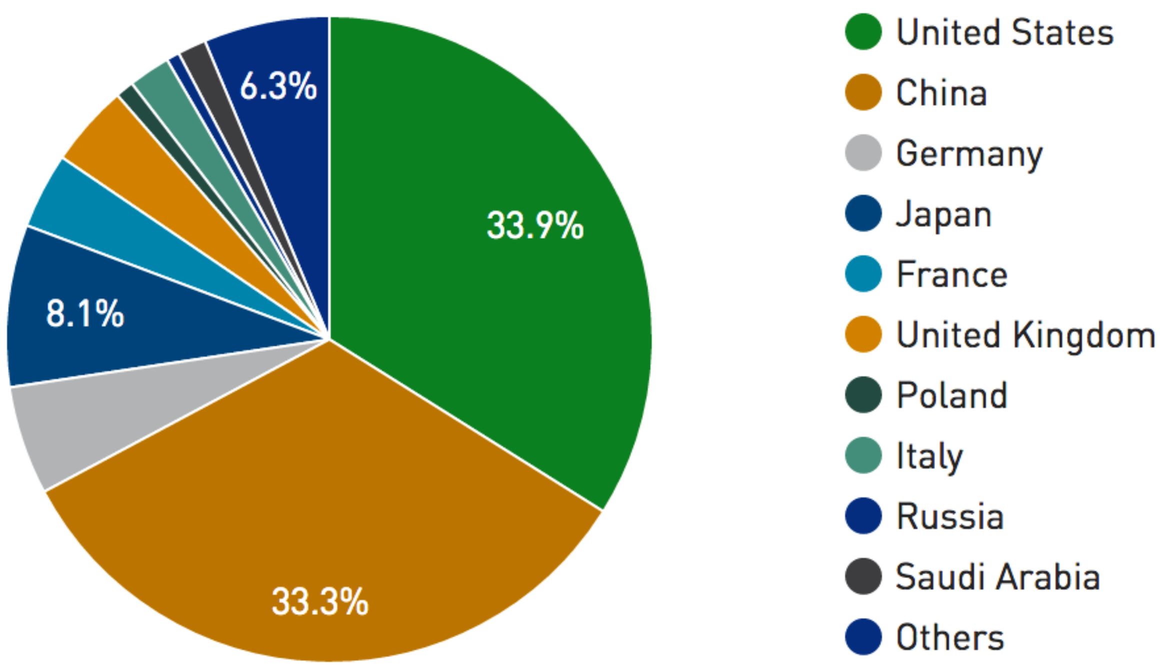
Countries	Count	System Share (%)	Rmax (GFlops)	Rpeak (GFlops)	Cores
United States	267	53.4	3,506	5,281	41,298
Japan	80	16	2,507	3,250	8,534
Germany	51	10.2	660	912	2,585
United Kingdom	18	3.6	360	472	1,488
France	17	3.4	239	357	1,402
Switzerland	9	1.8	130	182	1,015
Netherlands	9	1.8	112	144	363
Italy	6	1.2	42	59	302
China	1	0.2	7	9	32

6 entries found.

Rank	Site	System	Cores	Rmax (GFlop/s)	Rpeak (GFlop/s)	Power (kW)
155	CINECA (/site/47495) Italy	T3D MC128-8 (/system /170950) Cray Inc.	128	12.8	19.2	
299	CINECA (/site/47495) Italy	SP2/32 (/system /169570) IBM	32	6.6	8.5	
307	Centro Di Calcolo Interuniversiatrio Dell Italia (/site/47538) Italy	T3D MCA64-8 (/system /170995) Cray Inc.	64	6.4	9.6	
327	CRS4 (/site/47506) Italy	SP2/30 (/system /169553) IBM	30	6.2	8.0	
407	CILEA (/site/47494) Italy	SPP1600/XA-32 (/system /170723) HPE	32	5.5	7.7	
466	Centro Italiano Ricerche Aerospaziali (CIRA) (/site /47540) Italy	POWER CHALLENGE 10000 (/system/168538) HPE/SGI	16	4.9	6.2	

TOP 500 (Nov 2016)

Countries Performance Share



Countries	Count	System Share (%)	Rmax (GFlops)	Rpeak (GFlops)	Cores
United States	171	34.2	228,032,809	327,303,955	11,660,816
China	171	34.2	223,571,136	394,013,392	21,546,512
Germany	31	6.2	36,501,435	45,628,388	1,600,240
Japan	27	5.4	54,486,820	77,371,577	3,946,560
France	20	4	25,398,803	31,727,765	1,158,428
United Kingdom	13	2.6	27,602,596	31,682,369	1,148,968
Poland	7	1.4	6,162,214	8,157,370	208,284
Italy	6	1.2	14,062,113	21,140,514	606,312
Russia	5	1	4,411,812	6,515,928	181,070
Saudi Arabia	5	1	9,577,664	12,798,147	376,336
India	5	1	3,092,368	4,456,051	133,172
Sweden	4	0.8	3,378,143	4,291,609	123,992
Korea, South	4	0.8	5,679,725	7,597,851	169,696
Switzerland	4	0.8	12,273,082	18,811,648	328,608

6 entries found.

Rank	Site	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
12	CINECA (/site/47495) Italy	**Marconi Intel Xeon Phi** - CINECA Cluster, Intel Xeon Phi 7250 68C 1.4GHz, Intel Omni-Path (/system/178937) Lenovo	241,808	6,223.0	10,833.0	
29	Exploration & Production - Eni S.p.A. (/site/50489) Italy	**HPC2** - iDataPlex DX360M4, Intel Xeon E5-2680v2 10C 2.8GHz, Infiniband FDR, NVIDIA K20x (/system/178425) IBM	72,000	3,188.0	4,605.0	1,227
56	CINECA (/site/47495) Italy	**Fermi** - BlueGene/Q, Power BQC 16C 1.60GHz, Custom (/system/177720) IBM	163,840	1,788.9	2,097.2	821.9
57	CINECA (/site/47495) Italy	**Marconi Intel Xeon** - Lenovo NeXtScale nx360M5, Xeon E5-2697v4 18C 2.3GHz, Omni-Path (/system/178755) Lenovo	54,432	1,723.9	2,003.1	1,360.8
212	CINECA (/site/47495) Italy	**GALILEO** - IBM NeXtScale nx360M4, Xeon E5-2630v3 8C 2.4GHz, Infiniband QDR, Intel Xeon Phi 7120P (/system/178549) IBM/Lenovo	50,232	684.3	1,103.1	2,825.6
371	Exploration & Production - Eni S.p.A. (/site/50489) Italy	**HPCC1** - iDataPlex DX360M4, Xeon E5-2670 8C 2.600GHz, Infiniband FDR14 (/system/178200) IBM	24,000	454.1	499.2	498.5

High Performance Computing nell'INFN

- **~1980 Lattice Gauge Theories**, importanti contributi di teorici italiani

  - 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 da N. Cabibbo "The APE experience" , GGI - Firenze, 8 Feb 2007

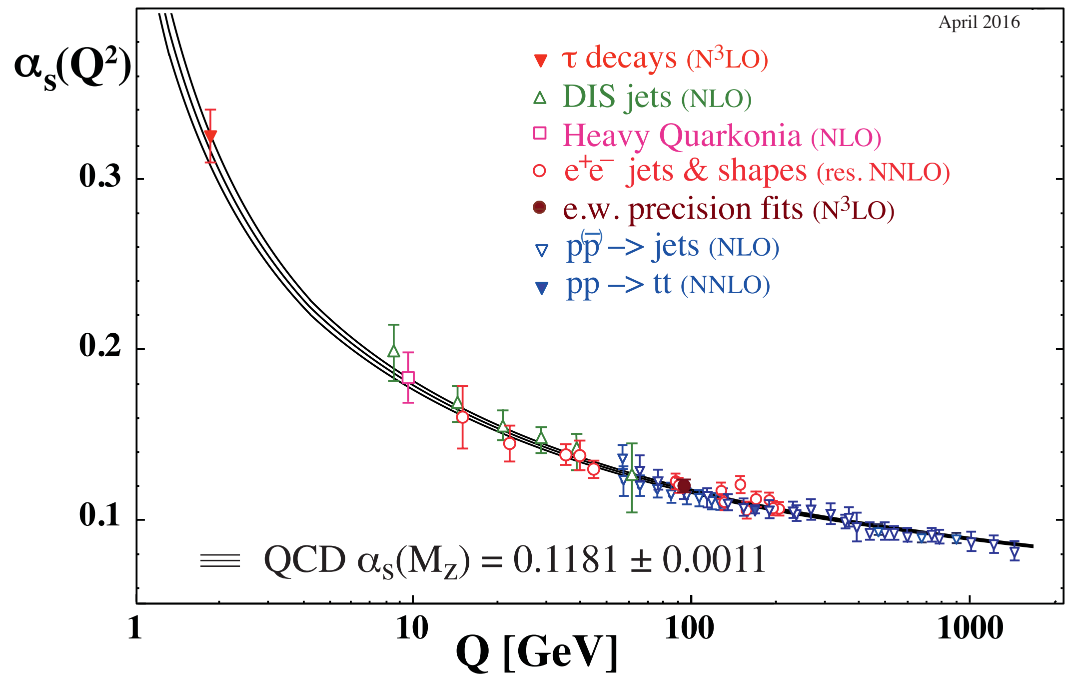
- **~1983-2003 Progetto APE**, sviluppo di calcolatori paralleli dedicati alle LGT (~2 Meuro/anno rivalutati a oggi)

~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 come esempio di intensità computazionale

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

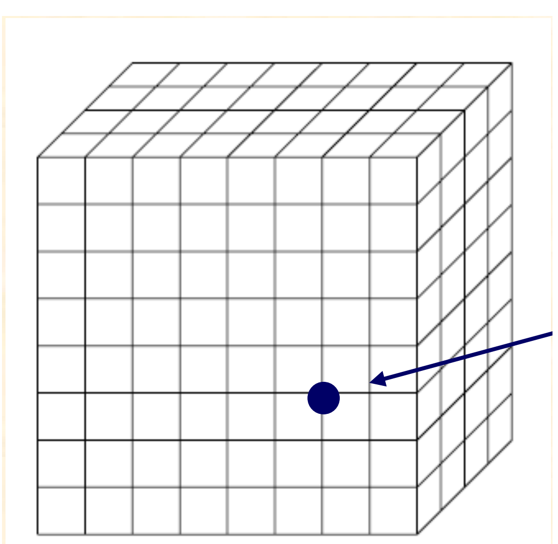
QCD becomes strongly coupled at the hadronic scale 1 GeV or 1 fm (10^{-13} cm)



Asymptotic Freedom

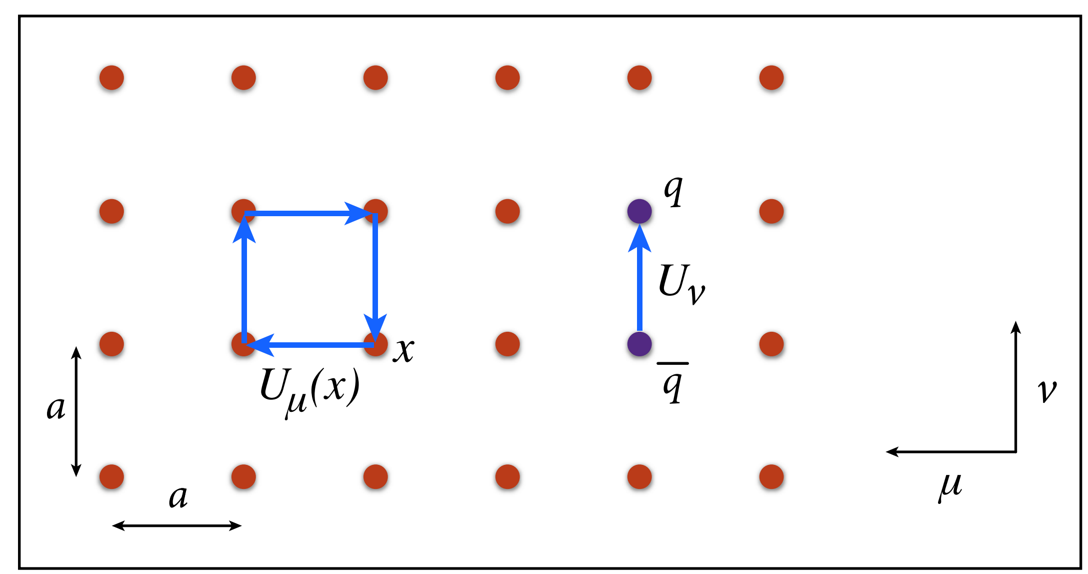
- Discretizzazione dello spazio-tempo

hyper cubic lattice

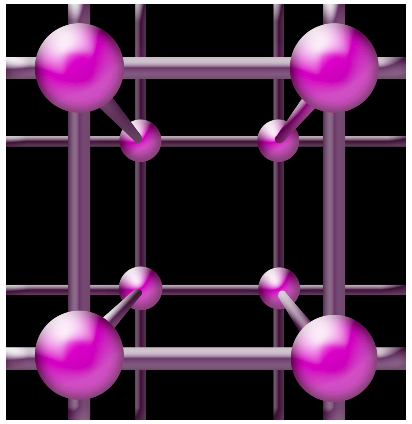


lattice site

$x_\mu = a n_\mu\,, \quad n_\mu \in \mathbf{Z} \quad 1 < x_\mu < L_\mu$



Lattice QCD come esempio di intensità computazionale



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

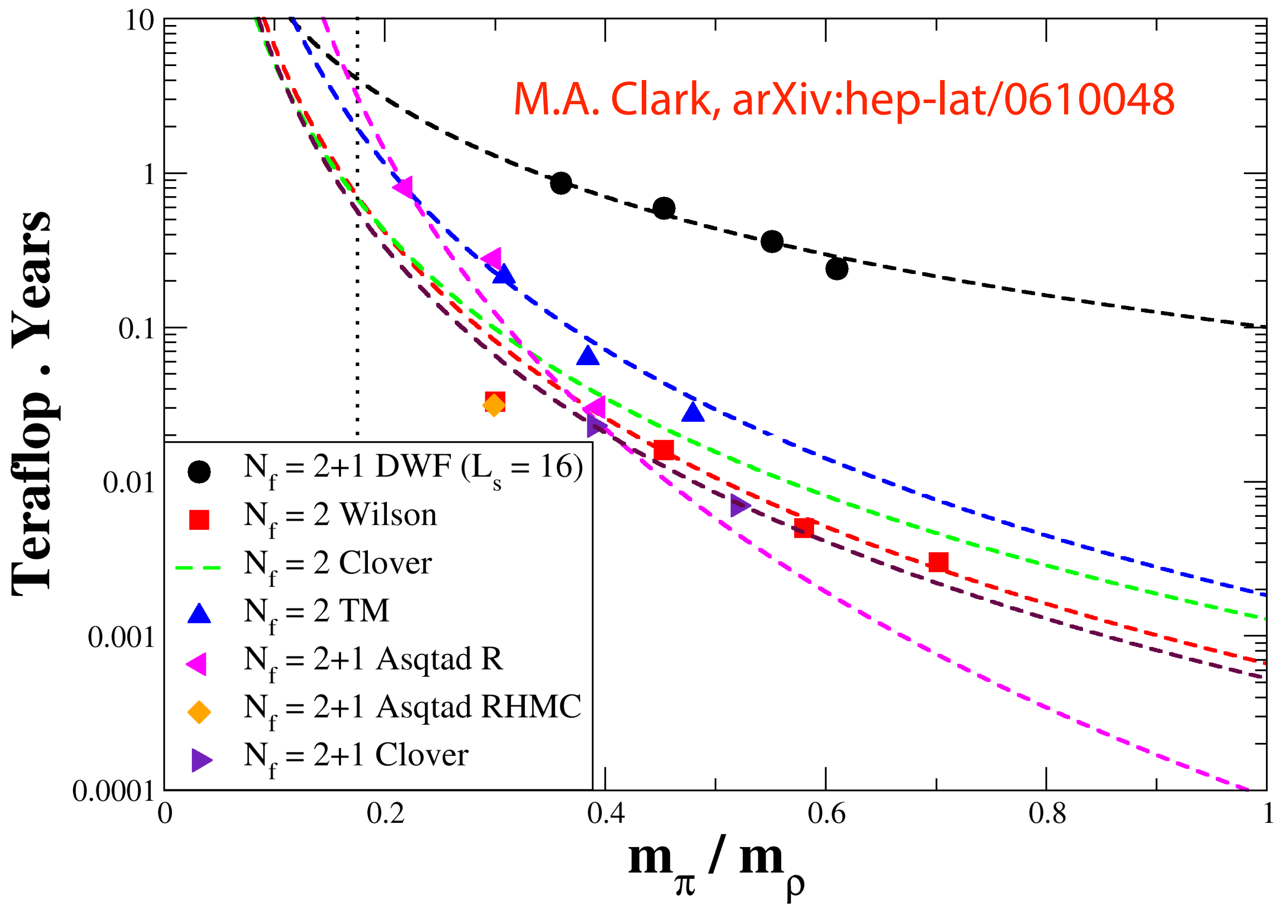
$$Z = \int [dU]e^{-S_g[U]}\prod_f \det(D[U]+m_f)$$

- Numero di variabili di integrazione: $N_s^3 \times N_t \times 4 \times 9 \quad N_s = 48\,, N_t = 12 \ \rightarrow \ \mathcal{O}(10^7)$
- Integrazione numerica diretta non è possibile → ***Metodi Monte Carlo***
- ***"Esperimento" numerico*** → ***Errori statistici (dal Monte Carlo)*** / ***Errori sistematici (dalla discretizzazione)***
- ***Il costo computazionale (e.g. 2 flavour)***

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

[A. Ukawa, Lattice 2001 Proceedings]

Lattice QCD come esempio di intensità computazionale



[A. Ukawa, Lattice 2001 Proceedings]

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

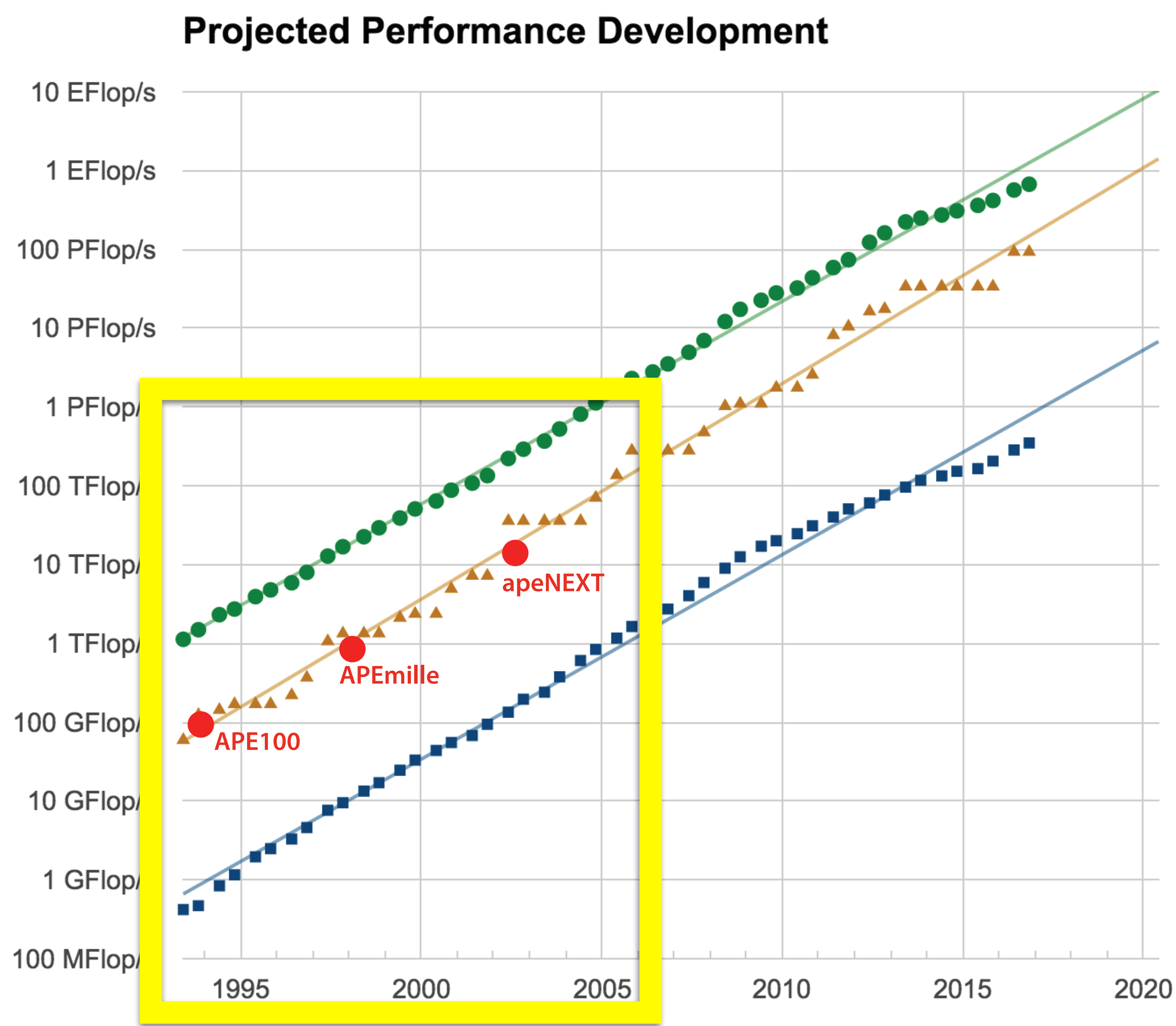
(2 flavour)

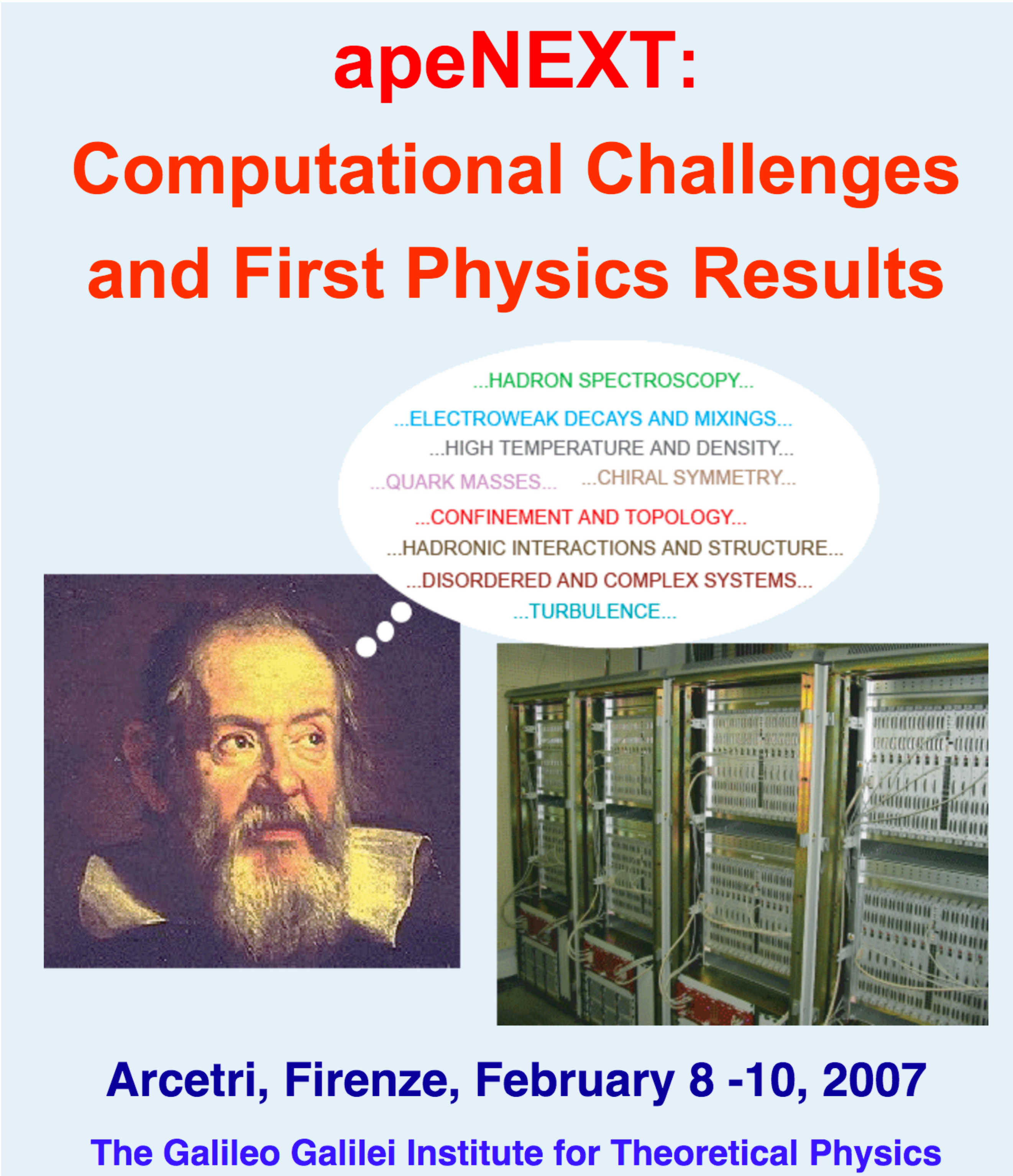
[M.Bruno et al., arXiv:1411:3982]

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

(2 +1 flavour)

APE sulla scala TOP500





Talks

Past

10-02-2007	10:30	**Norman Christ**	Chiral Symmetry, Petaflops and Solving Low Energy QCD
10-02-2007	09:30	**Ulrich H. E. Hansmann**	In Silico Folding of Small Proteins
09-02-2007	16:35	**Alessandro Papa**	Analytic continuation from an imaginary chemical potential
09-02-2007	16:10	**Leonardo Cosmai**	QCD in external fields
09-02-2007	14:50	**Massimo D'Elia**	Vacuum structure and deconfinement
09-02-2007	14:25	**Edwin Laermann**	Bulk QCD thermodynamics at small quark masses
09-02-2007	14:00	**Olaf Kaczmarek**	Heavy quark bindings at high temperature
09-02-2007	11:45	**Maria Paola Lombardo**	Topics in QCD at Finite T and/or mu
09-02-2007	11:00	**Federico Toschi**	Turbulent channel flow on apeNEXT
09-02-2007	10:00	**Francesco Di Renzo**	NSPT@apeNEXT
09-02-2007	09:15	**Hubert Simma**	Fundamental parameters of QCD from the lattice
08-02-2007	17:45	**Nazario Tantalo**	B ---> Dlnu form factors through the Step Scaling Method
08-02-2007	16:45	**Frithjof Karsch**	QCD at finite temperature and density
08-02-2007	15:45	**Gerrit Schierholz**	QCD simulations at realistic quark masses: probing the chiral limit
08-02-2007	15:15	**Dirk Pleiter**	Nucleon structure from lattice QCD
08-02-2007	14:30	**Karl Jansen**	Twisted mass fermions
08-02-2007	12:30	**Giancarlo Rossi**	From theoretical models to simulations: a computational challenge
08-02-2007	12:05	**Vittorio Lubicz**	Lattice QCD and flavor physics (II): Impact of lattice on the Unitarity Triangle Analysis
08-02-2007	11:40	**Silvano Simula**	Lattice QCD and flavor physics (I): Determination of Vus
08-02-2007	10:30	**Olivier Pene**	Physics with the French apeNEXT
08-02-2007	10:00	**Nicola Cabibbo**	The APE experience

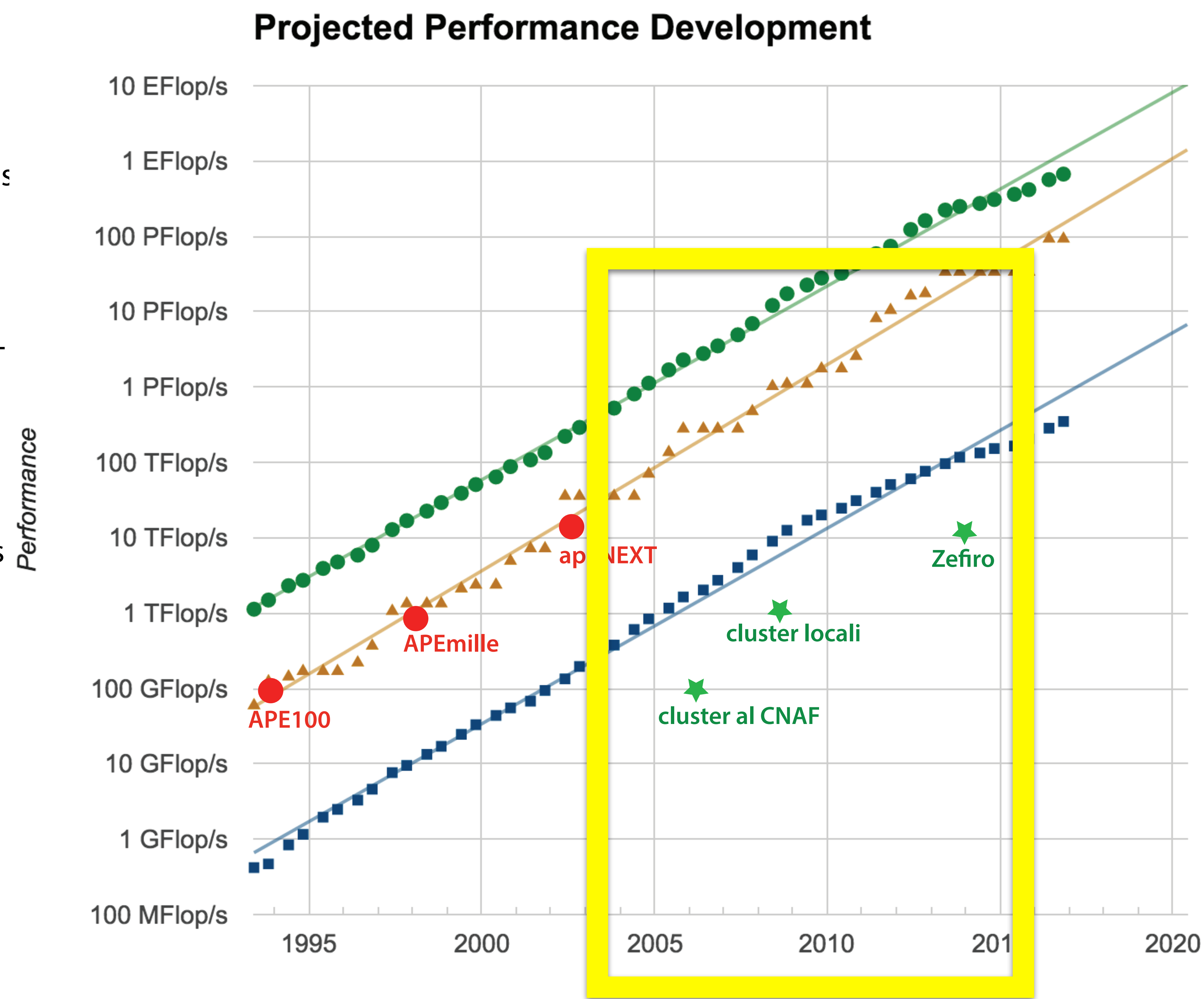
http://www.ggi.fi.infn.it//index.php?page=events.inc&id=10

dopo APE:
i cluster di PC finanziati dalla CSN4

- "Test FARM per HPC" (24 biprocessori Xeon @3.2GHz, Infiniband)
  —> CNAF (~2006) ~100 GFlops di picco

- I cluster locali (Bari (BA-CS-GE-LE-NA-TO), Catania (CT-PD-LNS-RM1), MilanoBicocca (MIB-PR-RM2-TO), Pisa(PI-MI-RM1)) (~ 2007-2008)
  ~ 500 cores di calcolo ~1 TFlops
  ~ 4 Mcorehours

- cluster CSN4
  "Zefiro" (~2013) O(2000) cores ~10 TFlops
  ~16 Mcorehours



Nuove importanti risorse HPC

~2012: convenzione INFN-CINECA

~2013: progetto premiale SUMA

- SUMA 1900 Keuro, BA / FE / MIB / PI / PR / RM1 / RM2 / RM3

Updated proposal and workplan of the SUMA project

The INFN-SUMA team: R. Alfieri, R. Ammendola, S. Arezzini, D. Badoni, M. Brambilla, R. Benzi, L. Biferale, A. Carboni, A. Ciampa, L. Cosmai, R. Covati, G. De Divitiis M. D' Elia, R. De Pietri, C. Destri, F. Di Renzo, A. Feo, R. Frezzotti P. Giannozzi, L. Giusti, G. La Penna, V. Lubicz, A. Lonardo, E. Mazzoni, V. Minicozzi, S. Morante, P. S. Paolucci, A. Papa M. Papinutto, M. Pepe, R. Petronzio M. Pivanti, S. Piras, F. Rapuano, D. Rossetti, G. C. Rossi, A. Salamon, G. Salina, M. Sbragaglia, S. F. Schifano, S. Simula, N. Tantalo C. Tarantino, R. Tripiccione, E. Vicari, P. Vicini, A. Vladikas

January 14, 2013

Project meetings and workshops

Meetings

April 1-2, 2014 (Ferrara): Agenda

November 8, 2013 (Roma, La Sapienza): Agenda

July 26, 2013 (Roma, La Sapienza): Agenda

December 11, 2012 (CINECA) : Agenda

Workshops

February 11-13, 2015 (Trento) : Agenda

~ 22 annualità postdoc
35 journal papers
38 conference papers

cluster Zefiro

GALILEO

Il progetto Premiale SUMA e la nuova convenzione CINECA (~2012)

GALILEO

(~ Feb 2015 - Oct 2017 (?))

Model: IBM NeXtScale

Architecture: Linux Infiniband Cluster

Nodes: 516
Processors: 2 8-cores Intel Haswell 2.40 GHz per node
Cores: 16 cores/node, 8256 cores in total
Accelerators: 2 Intel Phi 7120p per node on 384 nodes (768 in total); 2 NVIDIA K80 per node on 40 nodes (80 in total, 20 available for scientific research)
RAM: 128 GB/node, 8 GB/core
Internal Network: Infiniband with 4x QDR switches
Disk Space: 2.000 TB of local scratch
Peak Performance: 1.000 TFlop/s (to be defined)

~ 70 Mcorehours / anno

FERMI

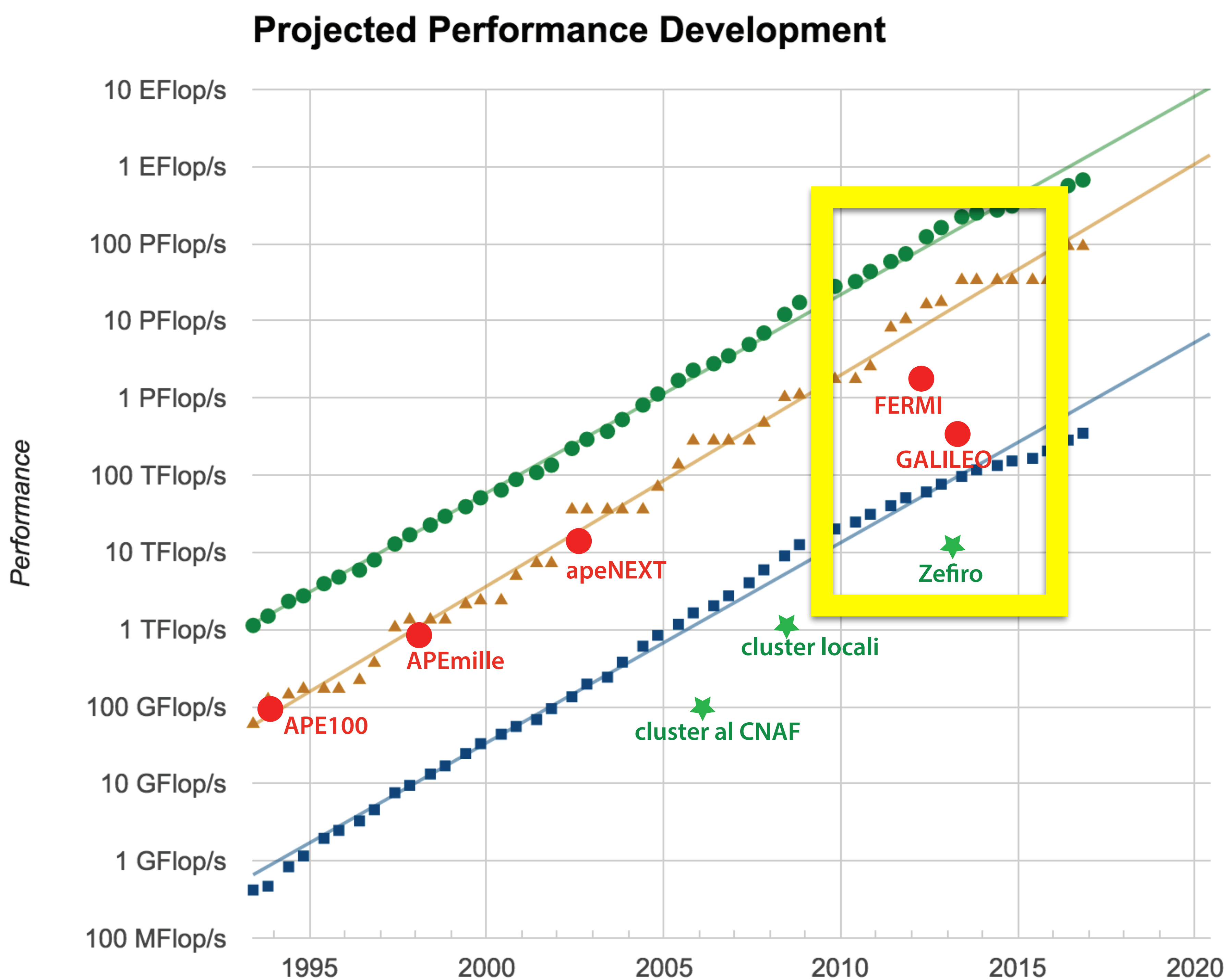
(~ Sep 2012 - Jul 2016)

Architecture: IBM BlueGene/Q
Model: 10 racks
Processor Type: IBM PowerA2, 1.6 GHz
Computing Cores: 163840
Computing Nodes: 10240, 16 core each
RAM: 16 GB/node, 1GB/core
Internal Network: custom with 11 links -> 5D Torus
Disk Space: 2.6 PB of scratch space
Peak Performance: 2PFlop/s

~ 1300 Mcorehours / anno

risorse a disposizione della comunità di fisica computazionale teorica INFN **~10%**

con FERMI & GALILEO…



"The case for a renewed support of computational theoretical physics at INFN"

Large scale computing at INFN?

Tuesday, 9 September 2014 from **10:00** to **16:30** (Europe/Rome)
at **Universita' Roma III (Aula 57)**
via della Vasca Navale 84 - Roma

The case for a renewed support of computational theoretical physics at INFN

S. Arezzini, L. Biferale*, M. Caselle*, A. Cea, A. Ciampa, L. Cosmai, G. de Divitiis, M. D'Elia, R. De Pietri*, C. Destri, P. Dimopoulos, F. Di Renzo, R. Frezzotti, L. Giusti*, G. La Penna, M. P. Lombardo*, V. Lubicz*, E. Marinari, G. Martinelli, V. Minicozzi, S. Morante*, M. Nicodemi*, A. Papa*, M. Papinutto, G. Parisi, F. Pederiva*, A. Pellissetto*, M. Pepe, F. Rapuano, C. Ratti, G. C. Rossi*, G. Salina, F. Schifano, S. Simula, N. Tantalo, C. Tarantino, R. Tripiccione*, E. Vicari, P. Vicini*, M. Viviani*, T. Vladikas

* *Conveners*

(Dated: February 18, 2015)

We outline a proposal for a strong and renewed support by INFN to its research groups active in theoretical computational physics. We argue that theoretical computational physics is important *per se* but it is also an important tool to understand in full the results and implications of present and future experiments. We describe a consistent line of action, review the physics area that would benefit from this line of support, and assess the level of resources needed to put this proposal in practice. We discuss several important advantages that this initiative would bring to all of INFN.

	2014	2016	2017
LGT: hadron physics	100	200	300
LGT: QGP and BSM	90	300	360
LGT: flavor physics	120	240	360
General relativity	60	140	170
Quantitative Biology	5	12	15
Fluid Dynamics	60	120	160
Nuclear Physics	10	15	20
Grand Total (Mcore-h)	**445**	**1027**	**1385**
Grand Total (Eq. Pflops)	**0.640**	**1.49**	**2.00**

~ 2016 fondi da CIPE a INFN per calcolo HPC e HTC

- cofinanziamento per acquisto nuova macchina al CINECA
- finanziamento assegni di ricerca (~ 1 Meuro)

Ministero dell'Istruzione, dell'Università e della Ricerca

Home » Ministero » La Ministra » Comunicati Stampa » 2015 » cs241215

Ministero

Istruzione

Ufficio Stampa

Roma, 23 dicembre 2015

Ricerca, da Cipe ok a 5 progetti per oltre 30 milioni
Dall'infrastruttura di calcolo, agli stage internazionali

Oltre 30 milioni di euro per finanziare progetti di ricerca. Il Cipe (Comitato interministeriale di programmazione economica) ha ammesso al finanziamento, a valere sul Fondo integrativo speciale per la ricerca (Fisr), cinque iniziative, dall'infrastruttura di calcolo agli stage per studenti universitari e ricercatori in aziende italiane all'estero.

"High performance data network"

Proposto dall'Istituto Nazionale di Fisica Nucleare (INFN), il progetto vuole contribuire a realizzare un'infrastruttura di calcolo innovativa di punta a livello nazionale, dove fare anche formazione a giovani laureati e dottori di ricerca. Valore complessivo: **€ 13.500.000**.

Lo stato attuale delle risorse HPC per la comunità di Fisica Teorica Computazionale INFN

- **convenzione INFN-CINECA**
  —> 6% MARCONI + 15 Mcorehours GALILEO

- **MARCONI "A1"** **18 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"** **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" (cofinanziamento INFN) (*)**

- 428 nodi di calcolo. Ogni nodo di calcolo comprende:

  Due processori Intel Skylake a 24 core (48 core/nodo) con frequenza di 2.1 GHz;

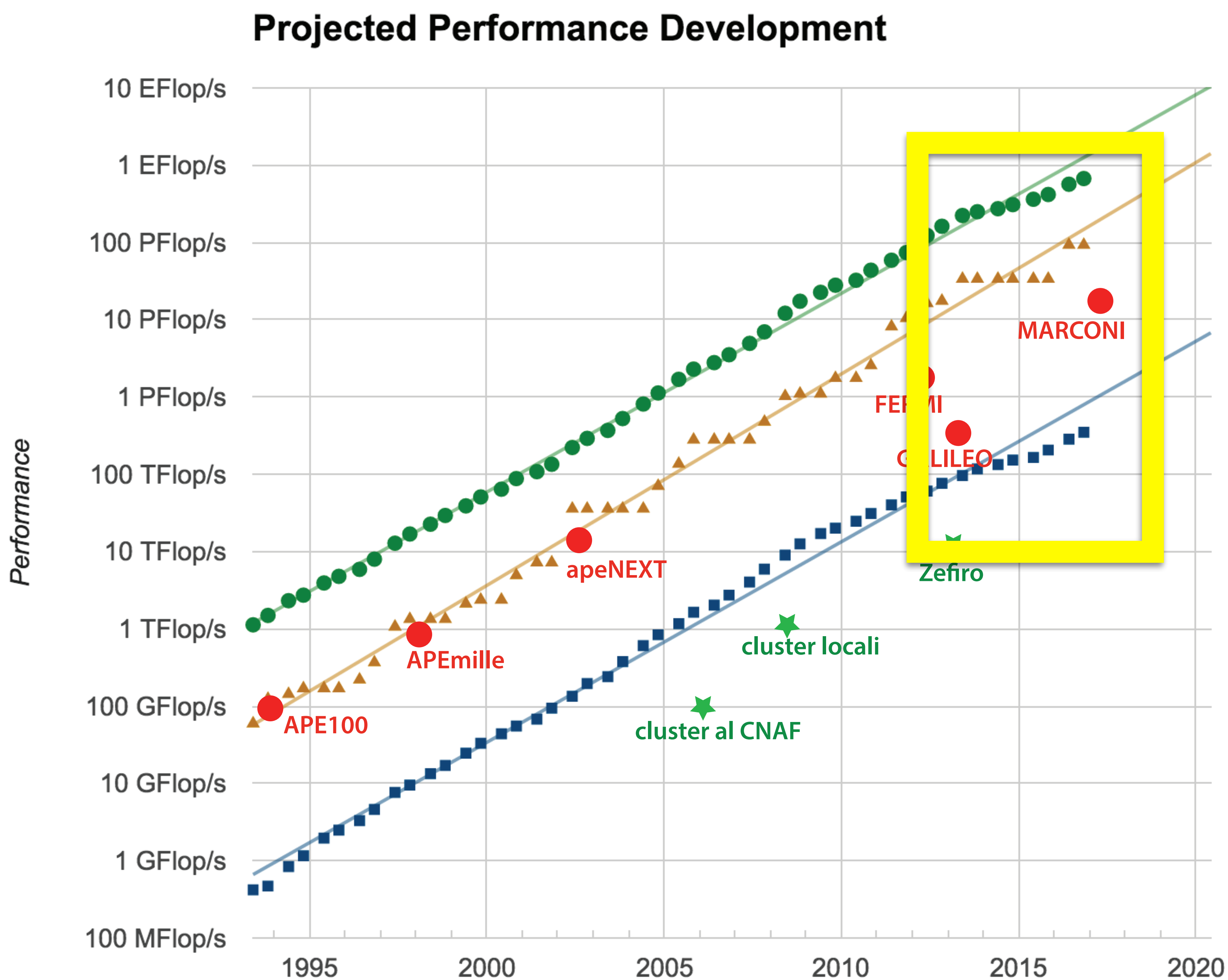
  potenza di picco di ~ 3.22 Tflops/nodode

  Memoria DDR4 @ 2.666 GHz, 192 Gbyte/nodo (4 Gbyte/core)

~1.4 PFlops **~ JUL 2017**

(*) MARCONI "A3" (2500 nodi) ~ 8 PFlops

con GALILEO & MARCONI (A1,A2,A3) ...



Gestione delle risorse HPC dell’INFN al CINECA

Commissione risorse INFN al CINECA (*)

FBS Michele Viviani
BIOPHYS Silvia Morante
FIELDTURB Alessandra Lanotte
LQCD123 Silvano Simula
MANYBODY Francesco Pederiva
NEMESYS Antonello Sindona
NPQCD Leonardo Cosmai
QCDLAT Michele Pepe
QFT_HEP Maria Paola Lombardo
SFT Marco Panero
STRENGTH Nunzio Itaco
TEONGRAV Roberto De Pietri

(*) riunioni periodiche in fonoconferenza per decidere ripartizione risorse

Stato dei consumi di risorse HPC aggiornato (*)

`https://docs.google.com/spreadsheets/d/1saap1WrD1nU9MvMp3mk3Kd9MPJkpZOXqI6pS5E1LRyI/edit?usp=sharing`

(*) a inizio mese

screenshot dal google sheet

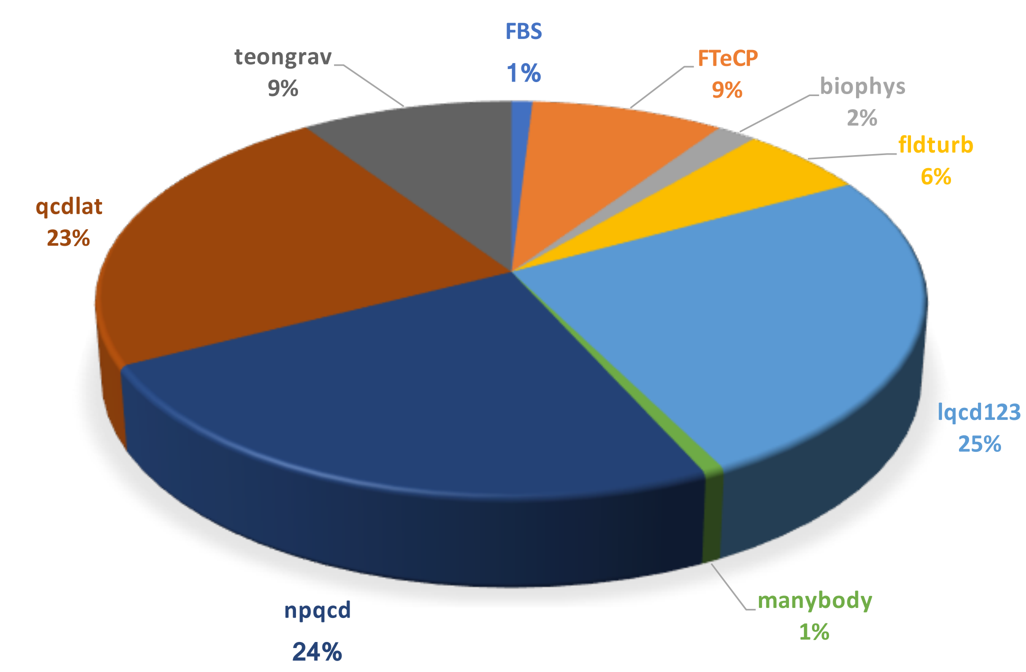
https://docs.google.com/spreadsheets/d/1saap1WrD1nU9MvMp3mk3Kd9MPJkpZOXqI6pS5E1LRyI/edit?usp=sharing

GALILEO stato consumi al 2 Aprile 2017				
account	**assegnazione (corehours)**	**consumo (corehours)**	**consumo/assegnazione (%)**	**consumo/(consumo totale) (%)**
INF17_FBS	250,000	56,479	22.59	2.64
INF17_biophys	1,600,000	419,166	26.20	19.58
INF17_fldturb	2,000,000	224,713	11.24	10.50
INF17_fusion	250,000	177	0.07	0.01
INF17_lqcd123	2,400,000	50,893	2.12	2.38
INF17_manybody	100,000	8,441	8.44	0.39
INF17_nemesys	700,000	75,874	10.84	3.54
INF17_npqcd	2,300,000	586,076	25.48	27.38
INF17_qcdlat	2,600,000	208,775	8.03	9.75
INF17_qfthep	250,000	0	0.00	0.00
INF17_sft	250,000	147,725	59.09	6.90
INF17_strength	150,000	0	0.00	0.00
INF17_teongrav	2,060,000	354,748	17.22	16.57
INF17_test	90,000	7,364	8.18	0.34
TOTALE	***15,000,000***	***2,140,431***	***14.27***	***100.00***

MARCONI "A2" stato consumi al 2 Aprile 2017				
account	**assegnazione (corehours)**	**consumo (corehours)**	**consumo/assegnazione (%)**	**consumo/(consumo totale) (%)**
INF17_FBS_1	1,000,000	23,305	2.33	0.24
INF17_biophys_1	1,500,000	431	0.03	0.00
INF17_fldturb_1	11,500,000	0	0.00	0.00
INF17_lqcd123_1	27,000,000	1,815,821	6.73	18.42
INF17_manybody_1	800,000	379,673	47.46	3.85
INF17_nemesys_1	450,000	0	0.00	0.00
INF17_npqcd_1	27,000,000	7,241,226	26.82	73.46
INF17_qcdlat_1	27,000,000	14,787	0.05	0.15
INF17_qfthep_1	4,500,000	0	0.00	0.00
INF17_sft_1	4,500,000	0	0.00	0.00
INF17_strength_1	250,000	0	0.00	0.00
INF17_teongrav_1	14,000,000	381,676	2.73	3.87
INF17_test_1	500,000	0	0.00	0.00
TOTALE	***120,000,000***	***9,856,919***	***8.21***	***100.00***

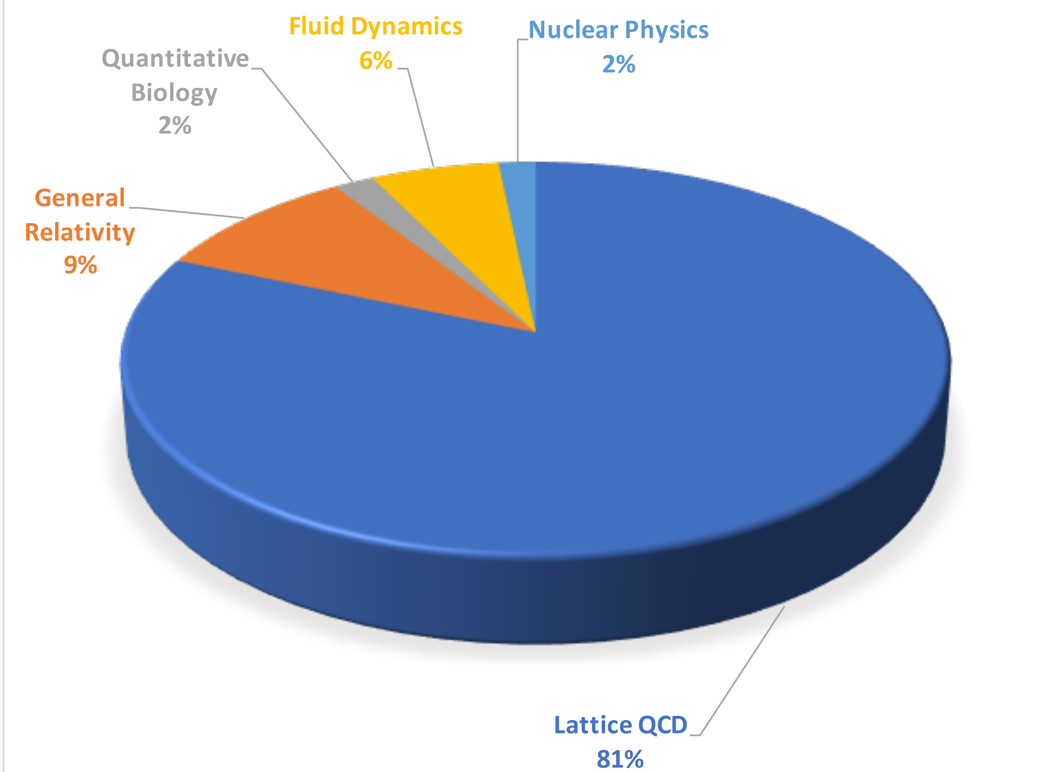
Utilizzo storico delle risorse HPC dell'INFN al CINECA

i.s.	corehours	percentuale
FBS	3,909,987	0.93
FTeCP	36,062,944	8.59
biophys	7,513,439	1.79
fldturb	23,968,009	5.71
lqcd123	106,970,718	25.48
manybody	2,988,883	0.71
npqcd	101,896,796	24.27
qcdlat	96,954,092	23.09
teongrav	39,618,431	9.44
TOTALE	**419,883,299**	**100.00**



FERMI (SET 2012- JUL 2016)

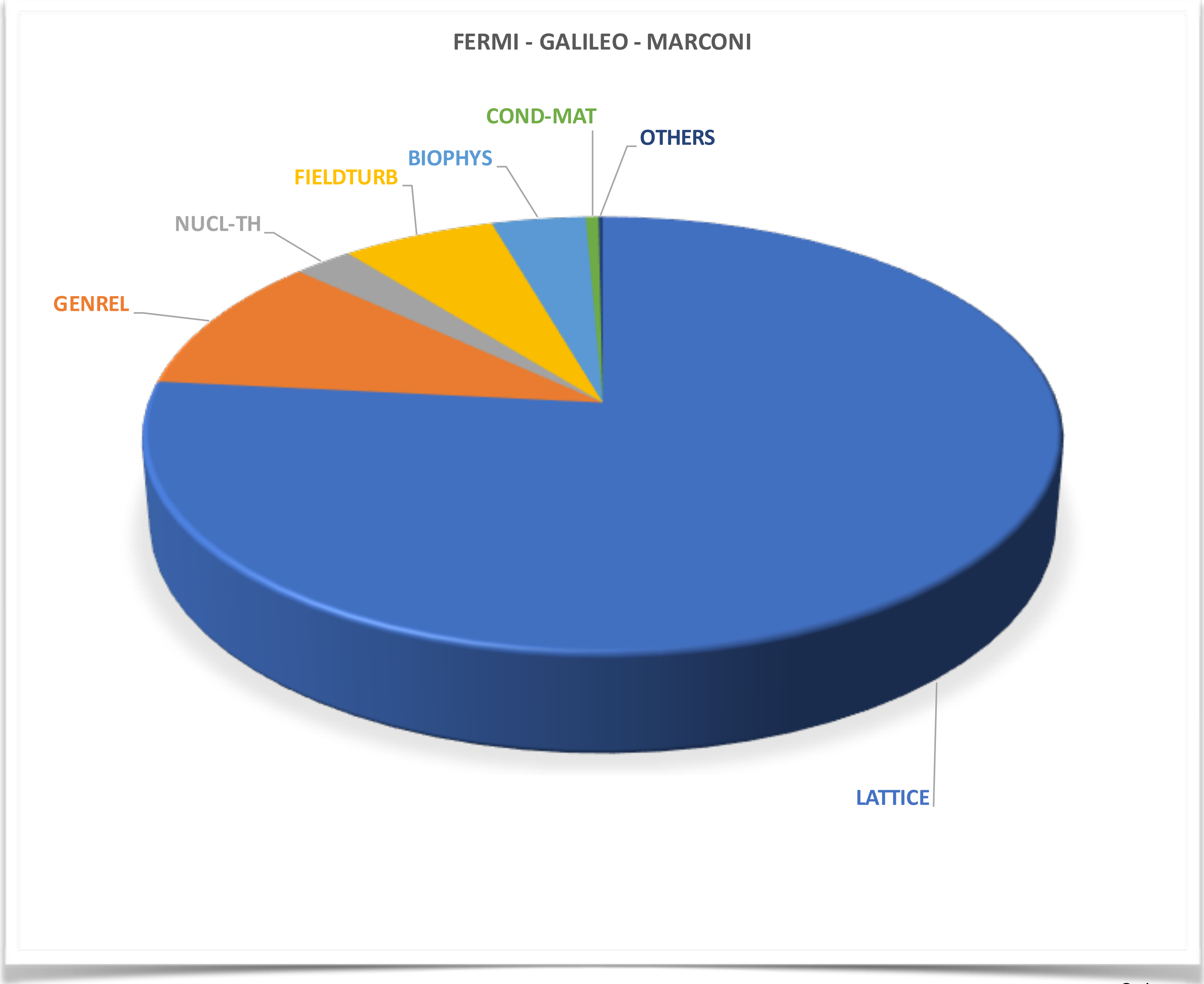
Area	corehours	percentuale
Lattice QCD	341,884,550	81.42
General Relativity	39,618,431	9.44
Quantitative Biology	7,513,439	1.79
Fluid Dynamics	23,968,009	5.71
Nuclear Physics	6,898,870	1.64
Totale	**419,883,299**	**100.00**



Utilizzo risorse HPC dell'INFN al CINECA da Settembre 2012 a oggi (*)

(*) in unità core BG/Q FERMI

AREA	Mcorehours	%
LATTICE	442	76.6
GENREL	59	10.2
NUCL-TH	14	2.4
FIELDTURB	36	6.2
BIOPHYS	22	3.8
COND-MAT	3	0.5
OTHERS	1	0.2
Totale	**577**	**100.0**



Le risorse ISCRA e EU-PRACE (stima dal 2012 a oggi)

- **~30 progetti ISCRA (B-C)**
- **~18 progetti EU-PRACE**
- **~1000 Mcorehours (in unità BG/Q Fermi)**

Fisica Teorica e calcolo HPC: stato e prospettive

Le attività di fisica computazionale con utilizzo di risorse HPC nella CSN4

- High Energy Physics - Lattice
  - LQCD123, NPQCD, QCDLAT, QFT_HEP, SFT
- High Energy Physics - Phenomenology
  - QCD@Colliders
- General Relativity, Cosmology, Astroparticle Physics
  - INDARK, NEUMAT, TEONGRAV
- Nuclear Physics
  - FBS, MANYBODY, STRENGTH
- Fluid Dynamics
  - FIELDTURB
- Disordered Systems
  - DISCOSYNP
- Quantitative Biology
  - BIOPHYS
- Condensed Matter
  - NEMESYS

16 i.s.

O(100) FTE

Roma Tre, 9 Settembre 2014

Large scale computing at INFN?

Tuesday, 9 September 2014 from **10:00** to **16:30** (Europe/Rome)
at **Universita' Roma III (Aula 57)**
via della Vasca Navale 84 - Roma

https://agenda.infn.it/conferenceDisplay.py?confId=8543

Roma Sapienza, 13 Febbraio 2017

Large scale computing at INFN

13 February 2017 *Dipartimento di Fisica Sapienza Univ. di Roma*
Europe/Rome timezone

https://agenda.infn.it/conferenceDisplay.py?confId=12660

~50 partecipanti, 18 presentazioni, sessione di discussione

documento 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.

documento HPC@INFN (2018-2020)

CONTENTS

High Energy Physics - Lattice
(LQCD123, NPQCD, QCDLAT, QFT_HEP, SFT)

Cruciale per la comunità italiana di Lattice QCD per conservare gli attuali livelli di competitività è poter disporre di una adeguata allocazione di risorse computazionale nel medio-lungo termine.
In questo campo i progressi sono fortemente **“HPC-driven”** !

Lattice QCD ed esperimenti

Quantity	Average	σ (%)
$\alpha_{\overline{\rm MS}}^{(5)}(M_Z)$	0.1182(12)	1.0
m_{ud}(MeV)	3.373(80)	2.3
m_s(MeV)	93.9(1.1)	1.2
f_{K^+}/f_{π^+}	1.193(3)	0.3
$f_+^{K\pi}(0)$	0.9704(33)	0.3
$\hat{B}_K$	0.7625(97)	1.3
f_{D_s}(MeV)	248.83(1.27)	0.5
f_{B_s}(MeV)	224(5)	2.2
$f_{B_s}\sqrt{\hat{B}_{B_s}}$(MeV)	270(16)	5.9
ξ	1.239(46)	3.7

FIG. 3: table
Lattice averages and relative accuracy for some of the SM free parameters and hadronic observables in the flavor sector (after Ref. [8]).

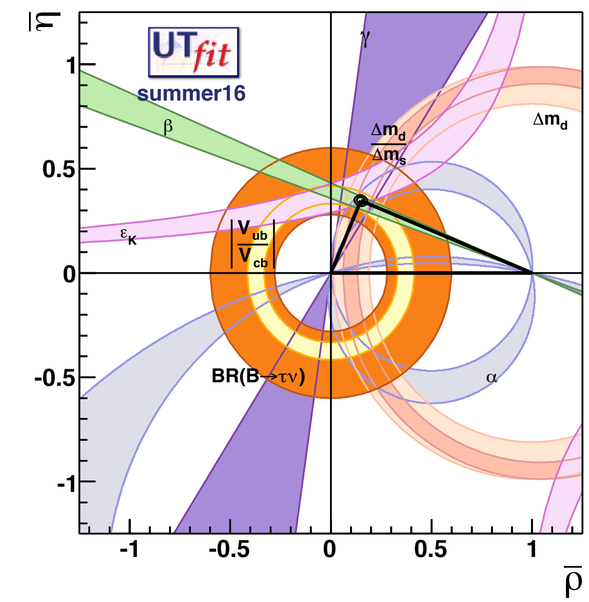


FIG. 4: figure
Results of the UTA unitarity triangle analysis within the SM (see the web page of the UTfit collaboration at http://www.utfit.org).

- Flavor physics
- New Physics
- Strong interactions under extreme environmental conditions
- Dynamical mass-gap generation and other non-perturbative aspects of QCD
- Applications beyond QCD
- Computational strategies and theoretical developments

High Energy Physics - Lattice

(LQCD123, NPQCD, QCDLAT, QFT_HEP, SFT)

LQCD123

production of QCD gauge ensembles at the physical point with $N_f = 2+1+1$ dynamical quarks

production of QCD+QED gauge ensembles with $N_f = 1+1+1$ and C* boundary conditions

QED corrections to hadron observables for flavor physics studies

leptonic and semileptonic decays of mesons, neutral meson oscillations

non-perturbative fermion mass generation

NPQCD

- **Diagramma di fase della QCD a temperatura e densità finita in campi di background (magnetici e cromomagnetici):**
  - *Effetto di campi cromomagnetici sulla linea pseudocritica della QCD con (2+1) flavour*
  - *Fluttuazioni nel numero di quark e possibile localizzazione del punto critico della QCD*
  - *Ordine della transizione di fase della QCD al variare del potenziale chimico e del numero di flavor*
  - *Campi magnetici: Chiral Magnetic Effect; effetti sui mesoni pesanti*

- **Studio della dinamica del confinamento/deconfinamento in QCD:**
  - *Tubi di flusso prodotti da sorgenti statiche al variare di T, potenziale chimico, campi esterni*
  - *Confinamento/deconfinamento indotto da campi magnetici ed altri agenti esterni*

- **Suscettività topologica nella QCD ad alta T e fenomenologia degli assioni**
  - *Studio accurato degli effetti sistematici dovuti al lattice spacing finito ed al volume finito, incluso lo sviluppo di algoritmi e strategie per il freezing della carica topologica, fino a $T \sim$ qualche GeV*

High Energy Physics - Lattice
(LQCD123, NPQCD, QCDLAT, QFT_HEP, SFT)

QCDLAT

- **Theme 1: QCD and flavour physics**
  α_s, m_q, χSB, $\Delta F = 2$ in SM and beyond, g_A, EDM,. . .
- **Theme 2: QCD at high temperature**
  EoS for $N_f = 2 + 1$, transport coefficients, topology (axions),. . .
- **Theme 3: Theoretical developments**
  NP renormalization (SF), $T_{\mu\nu}$, NSPT, improvement, . . .

QFT_HEP

Transport and response properties of strongly interacting systems

heavy quarkonium in a thermalized medium

lattice calculation of spectral functions: issue of systematic errors
interplay with analytic methods (AdS/QCD)

High Energy Physics - Lattice

(LQCD123, NPQCD, QCDLAT, QFT_HEP, SFT)

SFT

- Study of the QCD contribution to the photon production rate in the Quark Gluon Plasma (QGP) following the approach discussed in Phys. Rev. Lett. 112 (2014) 16, 162001: "Lattice Study of the Jet Quenching Parameter"
- Study of the behaviour of QGP in strong external magnetic fields using the non-equilibrium approach discussed in in Phys. Rev. D94 (2016) no.3, 034503 "Jarzynskis theorem for lattice gauge theory".
- Study of the running of the QCD coupling constant with the Schrödinger functional approach, using again the Jarzynski's theorem non-equilibrium approach
- Study of the QCD equation of State
- Extension of non-equilibrium methods to finite density QCD, as a way to overcome the sign problem.
- Study of the thermodynamic Casimir effect in $d = 2$ e $d = 3$ systems near the critical point, and comparison with existing experimental results.
- Study of the lattice discretization of quantum gravity in less than four dimensions.

High Energy Physics - Phenomenology
(QFT@Colliders)

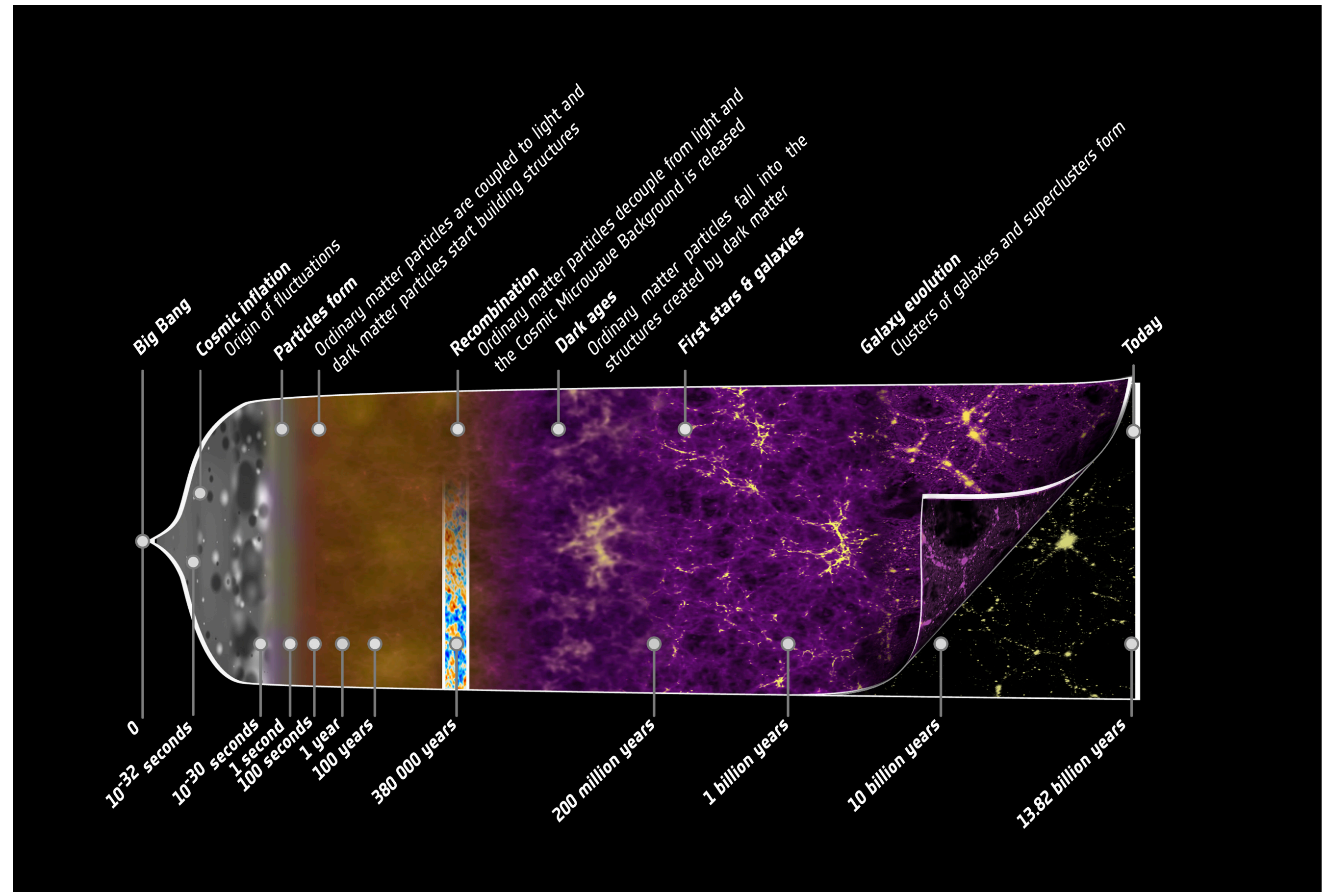
Applicazione di tecniche di Teoria Quantistica dei Campi alla fenomenologia di esperimenti presenti e futuri collider.

Misure sperimentali alla frontiera di intensità ed energia richiedono di calcolare correzioni di QCD next-to-leading-order.

Parallelizzazione di codici per calcolo di ampiezze di loop e integrazione Monte Carlo su stati finali.

General Relativity, Cosmology, Astroparticle Physics

(INDARK, NEUMATT, TEONGRAV)



- CMB (Cosmic Microwave Background)
- LSS (Large Scale Structure)
- Nature of Dark Matter and Dark Energy
- 2015: rivelazione di onde gravitazionali

General Relativity, Cosmology, Astroparticle Physics

(INDARK, NEUMATT, TEONGRAV)

INDARK

- Cosmic Microwave Background. Aim: tests of Inflation, fundamental and astroparticle Physics
  - ✓ CMB simulations: propagation of synthetic data and theoretical signals (e.g. CMB non Gaussianity)
  - ✓ Development of 3-point and 4-point function NG estimators studies.
  - ✓ Parity breaking CMB spectra, bispectra and trispectra
  - ✓ Inflationary parameters, preparation and forecasts for B-mode surveys.
  - ✓ NG tests for CMB spectral distortions.
  - ✓ Development of statistical methods for component separation
  - ✓ Constraints on non standard neutrino interactions
  - ✓ CMB Anomalies and connections to pre-inflationary phases (e.g. string theory motivated scenarios)
- Large Scale Structure. Aims: DM and neutrino studies, tests of Inflation and structure formation.
  - ✓ Production and analysis of N-body simulations
  - ✓ Development for future (Euclid, SKA) analysis beyond power spectrum .
- Cross-correlation of large cosmological and external datasets. Aims: DM , DE/MG studies, Inflation
  - ✓ CMB-LSS (spectroscopic, radio) cross-correlation tests for MG constraints
  - ✓ Development of Einstein-Boltzmann integrators in Effective Field Theory of MG, for cross-correlation forecasts
  - ✓ LSS/CMB-gamma ray cross correlation tests for searches of DM annihilation/decay signal
  - ✓ Predictions of GW from Inflation, combine predictions: interferometers + CMB B-mode.

NEUMATT

- Prepare detailed templates of GW emission by using realistic EoSs
- Investigate the role of:
  - high temperatures,
  - chemical non-equilibrium,
  - production of hyperons and other resonances
- Develop of way to describe the possible transition from hadrons to deconfined quarks during the merger
- Study the formation and the stability of a very strong magnetic field

General Relativity, Cosmology, Astroparticle Physics

(INDARK, NEUMATT, TEONGRAV)

TEONGRAV

- **TEONGRAV** stands for: **TE**oria delle **ON**de **GRAV**itazionali
- Our research is centered on the finding answers to the following questions:
  - Which are the features of the GW signal emitted by the main expected sources (such as, for instance, coalescing compact binaries, rotating non-axisymmetric NSs, oscillating BHs and NSs?
  - Which information on the emitting source could be extracted from a GW detection? For instance, what could we learn on the equation of state of the dense matter in the inner core of a NS?
  - Which information on the nature of gravity could be extracted from a GW detection? For instance, which could be the imprint of modifications or extensions of general relativity (GR) on the GW signal from astrophysical sources?

- **Simulazione della fisica delle sorgenti di onde gravitazionali e degli attesi segnali di onde gravitazionali.**

Nuclear Physics
(FBS, MANYBODY, STRENGTH)

FBS

- Structure and dynamics of few-nucleon systems
- Test of nuclear interaction derived from chiral effective field theory (low energy theory of QCD)
- Study of reactions of astrophysical interest
- Study of fundamental symmetries (parity & time reversal)
- Electroweak reactions (form factors, beta decays,. . .)
- Hypernuclei

MANYBODY

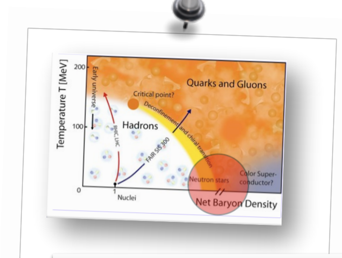
Many-Body theory: projection Monte Carlo

We compute ground state energies of nuclei by means of projection Monte Carlo methods. The ground state of a many-body system is

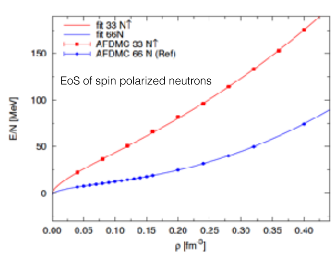
Projection MC many-nucleon systems

Equation of state of dense matter

The *fine tuning* of the hyperon-nucleon interaction is essential to understand the behaviour of matter in extreme conditions.

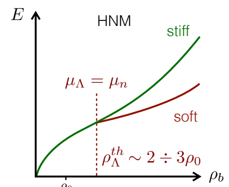


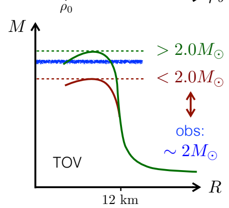
Far away from any possible perturbative treatment..



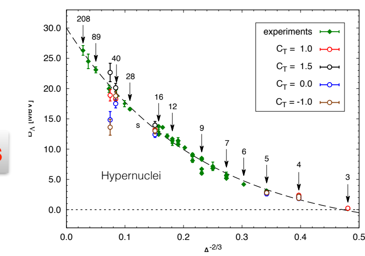
Example: Neutron stars

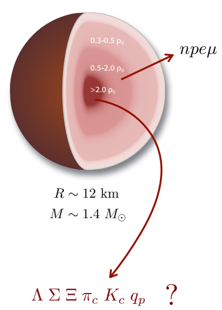
Equation of state





Neutron star structure





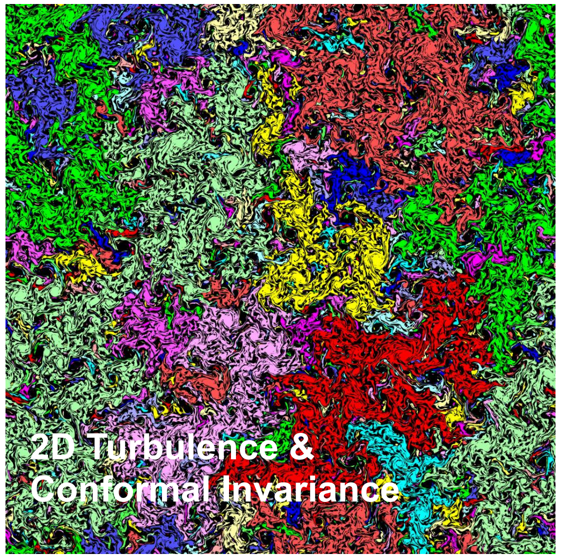
Internal composition still largely unknown

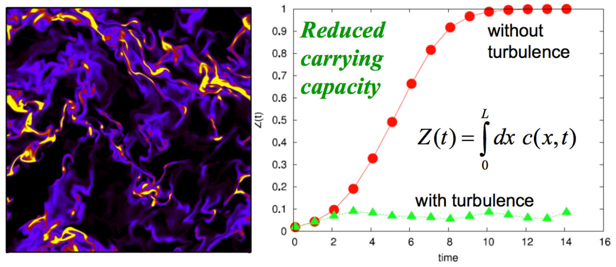
STRENGTH

- correlazioni a molti corpi ⇒ proprietà spettroscopiche dei nuclei
- dinamica delle eccitazioni nucleari & meccanismi di reazione

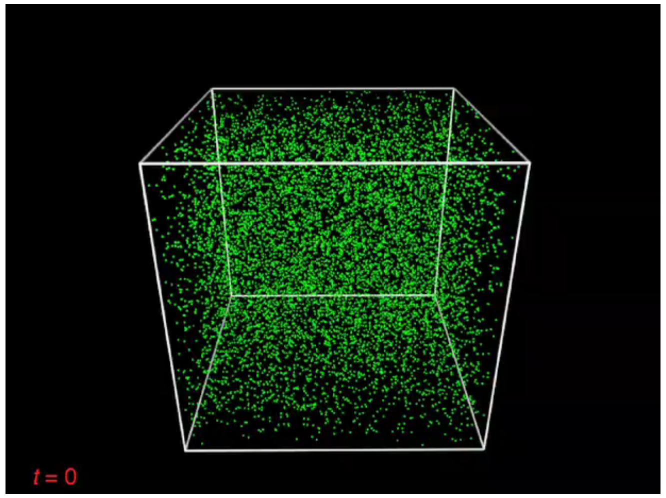
Fluid Dynamics

FIELDTURB





Population dynamics in flows



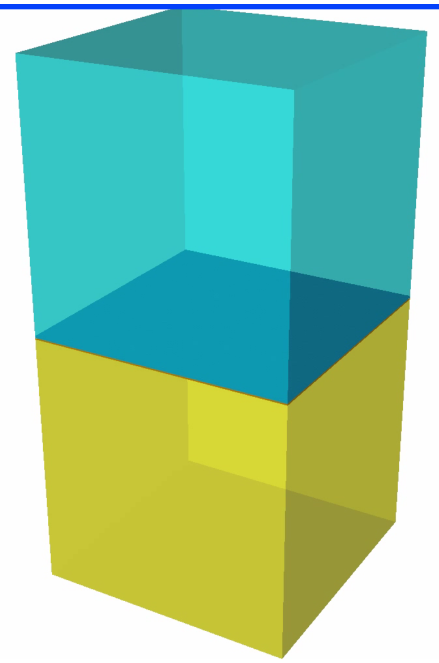
Complex systems far from equilibrium with many dof

Wide range of applications
(from astrophysics to biology)

Theoretically challenging

Computationally and experimentally demanding

Of large impact



Turbulent convection

Recent relevant publications

Phys. Rev. Lett. **112**, 1 (2014); **112**, 18 (2014); **113**, 3 (2014); **113**, 11 (2014); **113**, 25 (2014); **115**, 26 (2015)

Phys. Rev. X **4**, 041006 (2014), **6** 041036 (2016)

Nat. Comm. **4**, 2148 (2013); **5** 5310 (2014)

PNAS **111**, 7558 (2014); **112**, 4208 (2015)

SOFT MATTER **10**, 4615 (2014); **11**, 1271 (2015); **12** 514 (2016)

Annu. Rev. Fluid Mech. **49**, 119 (2017)

Quantitative Biology

BIOPHYS

We develop quantitative methods to understand living systems at 3 levels of organization, **strongly relying on high-performance computing**:

1) **The characterization of biomolecules and their interactions** (RM, PI, TR)
2) **The 3D organization and regulation of genomes** (MI,NA, TO)
3) **Regulatory networks of molecules, cells and neurons** (BA,PG,PR,SA)

-- Structural Biology & HPC

- Protein aggregation
  Neurodegenerative diseases
- Antibody-protein interactions
  Tumour theranostic
- *Ab initio* observables calculations
  X-ray spectra
  Diffraction patterns

} **Classical MD**

***Ab initio* calculations**

Disordered Systems

DISCOSYNP

High-Resolution Simulation of Biological Neural Networks

Simulations of Cortical Slow Waves and Transition toward Awake States and of the interplay between sleep and memory consolidation and memory homeostasis in the HBP (- until 2023)

- WaveScalES: models of deep-sleep and transition to awakeness
  - Single-area non-laminar
  - Single-area laminar
  - Multi-area
  - Neuromodulated STDP, LTP/LTD
- Tight collaboration with NEST and NESTML teams for requirements fulfilment
  - New models for neurons, probability kernels functions, stimulus, observables, etc.
- WaveScalES models initially prototyped using the proprietary DPSNN engine, eventually ported to NEST and offered to HBP community

- Simulazione a grande scala di ***spin glasses***
- ***Hard spheres jamming*** e vetri a bassa temperatura (mezzi granulari, liquidi, cellule viventi, vetri…)
- ***High resolution cortical simulation*** nel progetto ***Human Brain***

Condensed Matter

NEMESYS

- **Main theme.** 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,
  - ensembles of ultra-cold atomic gases,
  - magnetic and spin systems.
- **Program.** Massive simulations of
  - spectral features, dielectric screening, conductivity response and electro-mechanical properties of graphene-related and beyond-graphene materials, including their interfaces and contacts with supporting substrates
  - irreversible properties and quantum thermodynamics of ultra cold Fermi and Bose gases, following a change of their trapping potentials
- **Computational methods.**
  - Density Functional Theory (DFT) and Time Dependent (TD) extensions
  - Many Body Perturbation Theory
  - Topological quantum field theory on space-time (2+1) and (1+1) manifolds
  - Quantum Montecarlo
  - Semi classical Multiscale Approaches

- Numero rilevante di progetti con richieste HPC.
- Le attività di fisica computazionale con utilizzo di superalcolo richiedono un accesso stabile e prevedibile a ingenti risorse di calcolo.
- Parte delle risorse può essere ottenuta da grant ISCRA e/o EU-PRACE. Ma, per competere con successo, è fondamentale accedere a proprie (INFN) risorse sicure.
- In alcuni casi è necessario anche accedere con priorità a risorse relativamente piccole (O(400) core) per attività di sviluppo e test di algoritmi.

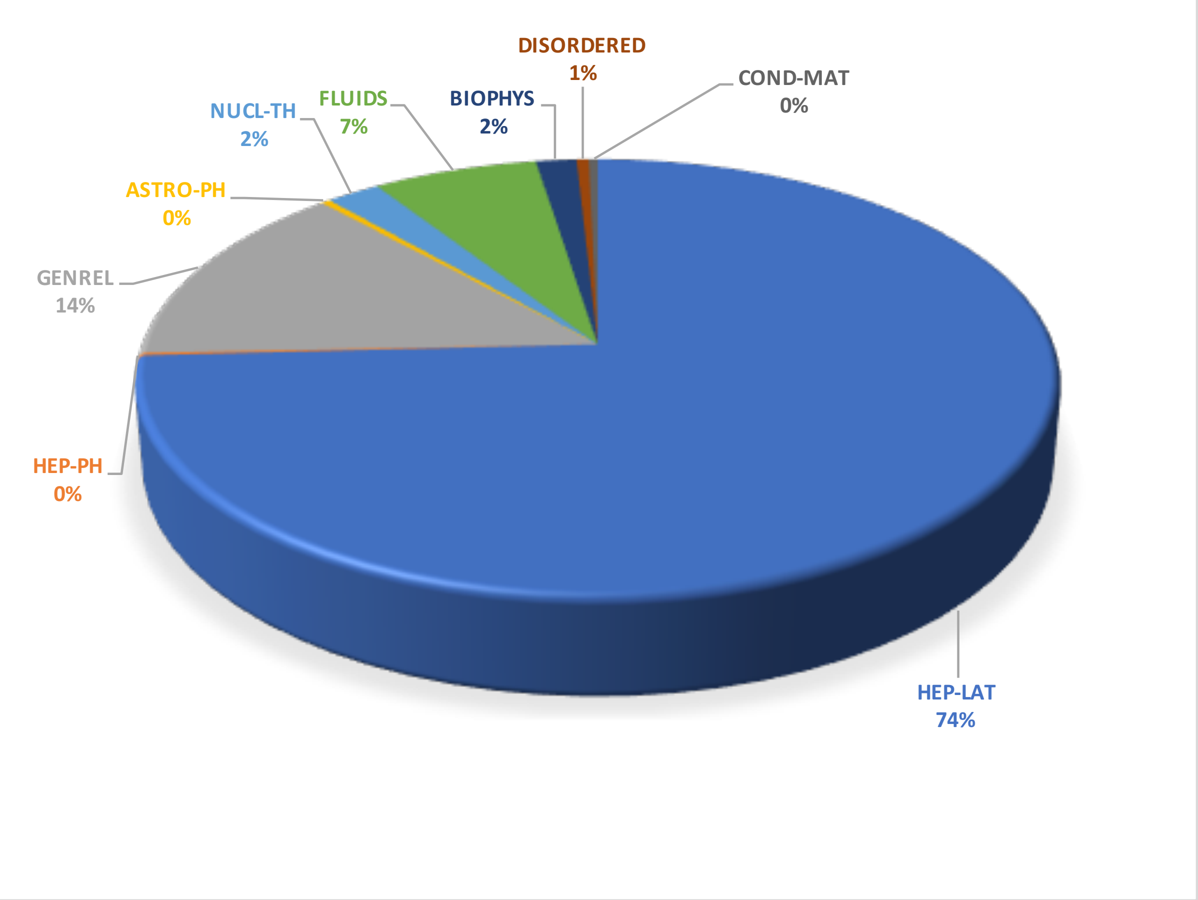
  → coda dedicata con ~20 nodi di MARCONI “A3” ???

- Nell’ambito dei finanziamenti CIPE a HPC e HTC, commissione sperimentali-teorici per “procurement” hardware sperimentale (non per produzione).

Stima delle necessità per la comunità HPC

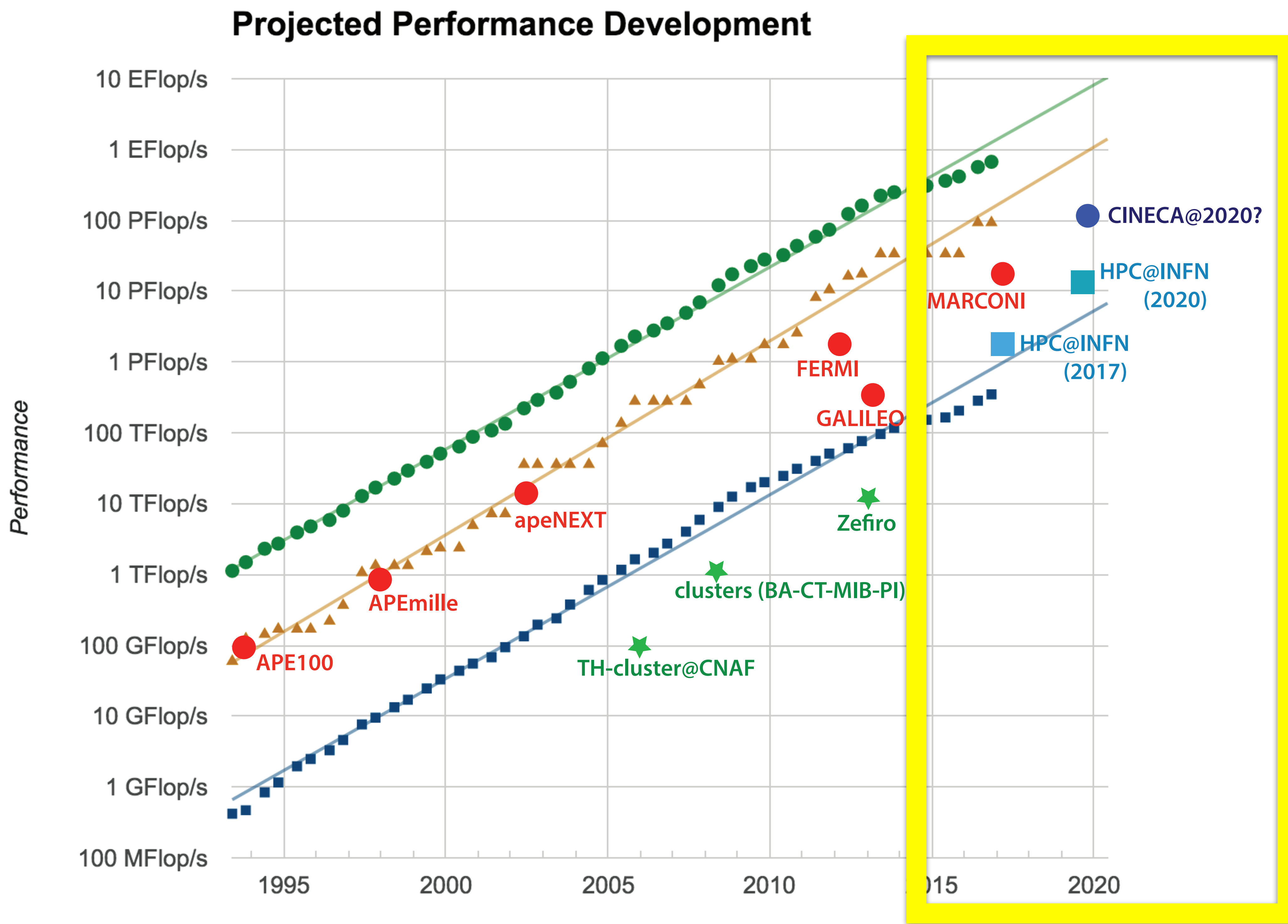
- risorse di calcolo

	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**



- adeguato supporto per postdoc grant e per organizzazione di workshop e meeting

… sulla scala TOP500



...verso Exascale...

European Commission

Europe as a global player in High Performance Computing

Thursday 23 MAR 2017

Ministers from seven European countries (France, Germany, Italy, Luxembourg, Netherlands, Portugal and Spain) have signed a declaration to support the next generation of computing and data infrastructures, a European project of the size of Airbus in the 1990s and of Galileo in the 2000s.

Ministers from seven European countries have signed on to a plan to develop an exascale capability based on technology developed within the EU member states. The goal is to bring up two pre-exascale supercomputers by 2020 and two full exascale systems no later than 2023.

More to the point, the EU wants to position itself a distinct HPC leader on par with that of the US, China, and Japan. The rationale behind this is that these technologies are increasingly seen as catalysts for key industries like manufacturing, healthcare, transportation, and energy, as well as an enabler for things like cloud services, machine learning and the internet of things (IoT).

Conclusioni

- La comunità di Fisica Teorica Computazionale INFN ha una lunga tradizione a partire da ~1980. Forte supporto INFN per il progetto APE a sostegno del calcolo HPC progressivamente venuto a mancare nella prima decade di questo secolo.

- Grazie a un rinnovato supporto dell'INFN (convenzione CINECA, SUMA, CIPE) la comunità computazionale INFN ha riconquistato (a partire da ~2013) competitività rispetto alla comunità internazionale (anche per accesso a EU-PRACE !!!).

- Riteniamo interesse dell'INFN mantenere e sviluppare una comunità con esperienze di calcolo HPC allo stato dell'arte. Questo obiettivo richiede il coinvolgimento di giovani ricercatori.

- Importante promuovere la condivisione di esperienze e competenze fra le comunità HPC e HTC nell'INFN.

- La fisica teorica computazionale dipende in modo cruciale dalla disponibilità di risorse HPC allo stato dell'arte. Per soddisfare queste esigenze e per poter contare su risorse stabili e adeguate è opportuno rafforzare le sinergie e la cooperazione dell'INFN su HPC a livello nazionale ed europeo.