CSN4 - Risorse di calcolo per il 2024

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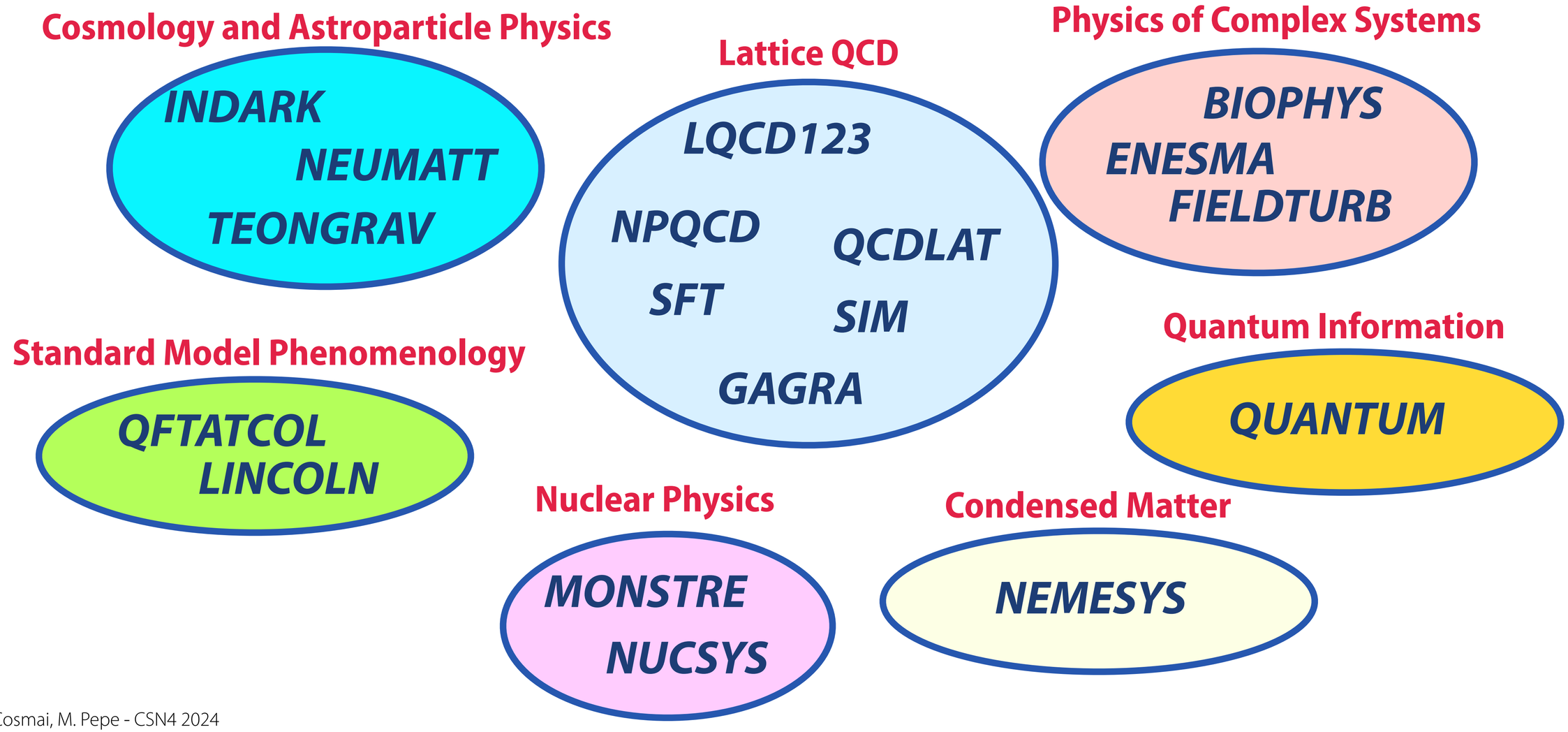
Roma, 7 Settembre 2023

Computational Theoretical Physics @ INFN

~200 researchers

Many research groups are involved in the activities of ICSC (Centro Nazionale di ricerca in HPC, Big Data and Quantum Computing)

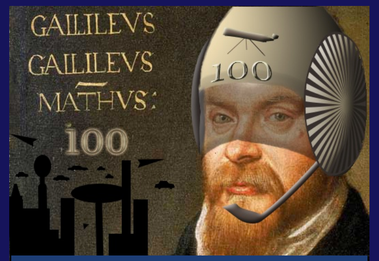


Computing Resources

Cineca-INFN agreement

Cineca-INFN agreement

MARCONI-A3
60 Mcorehours



GALILEO 100
6 Mcorehours

LEONARDO
Booster: 3 Mnodehours

LEONARDO
General purpose

ICSC
Centro Nazionale di Ricerca in HPC
Big Data and Quantum Computing

ISCRA
CINECA

Euro-HPC

EuroHPC JU

EuroHPC
Joint Undertaking

LUMI supercomputer
375 PFlop/s - FINLAND

LEONARDO supercomputer
295 PFlop/s - ITALY

MARENOSTRUM 5
205 PFlop/s - SPAIN

HPC Vega IZUM
6.92 PFlop/s - SLOVENIA

MELUXINA supercomputer
12.81 PFlop/s - LUXEMBOURG

DEUCALION supercomputer
7.22 PFlop/s - PORTUGAL

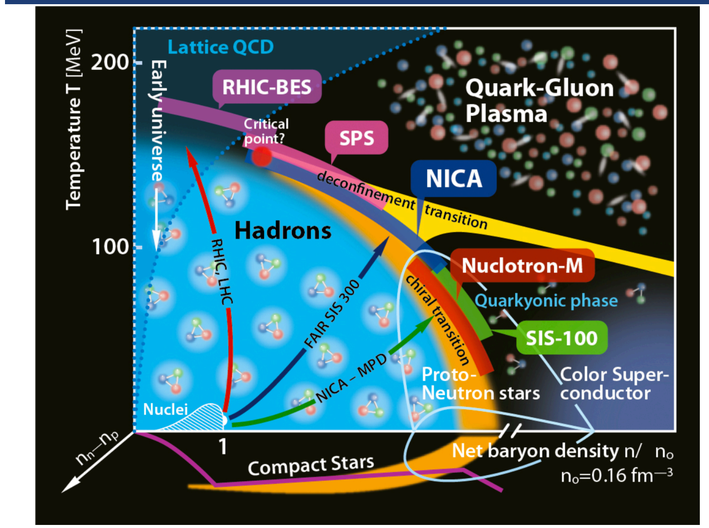
DISCOVERER supercomputer
4.51 PFlop/s - BULGARIA

KAROLINA supercomputer
9.59 PFlop/s - CZECH Republic

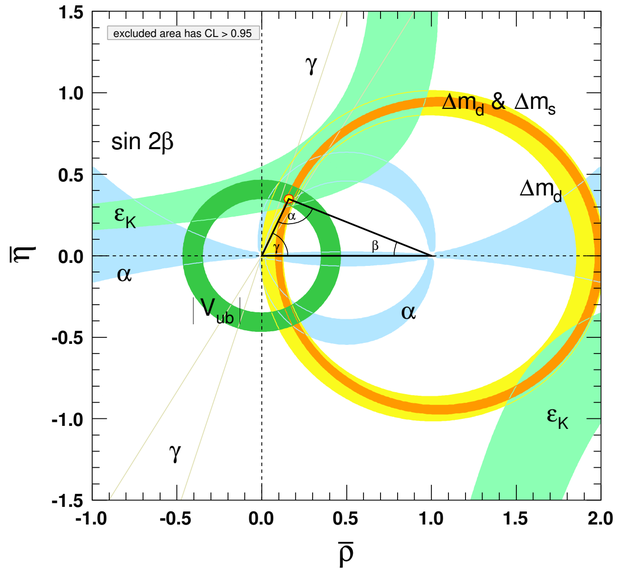
Lattice QCD

LQCD123 NPQCD QCDLAT
GAGRA SFT SIM

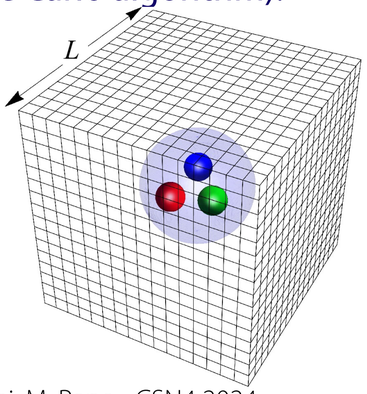
Study of QCD in extreme conditions

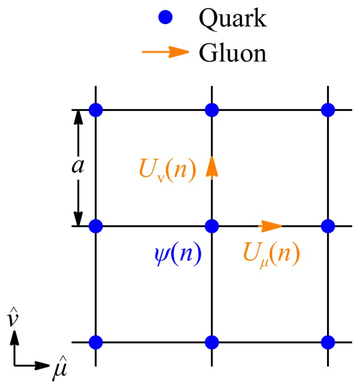


Precision studies of flavor physics, within and beyond the Standard Model



Generates an ensemble of gluon field configurations U distributed according to the QCD action (using the hybrid Monte Carlo algorithm):





A large number of computing nodes is required (up to $\mathcal{O}(10^5)$ cores. On the largest scales the challenge lies in efficiently and effectively exchanging data among the processors or nodes —> MPI, MPI+OpenMP.

Cosmology and Astroparticle Physics

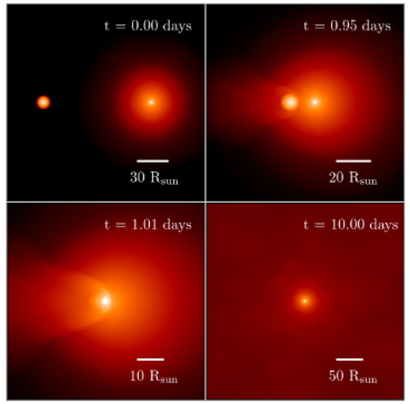
INDARK ***NEUMATT*** ***TEONGRAV***

TEONGRAV

- Modelling of **gravitational wave sources** via both semi-analytical and numerical methods;
- Equation of state of matter in the inner core of **neutron stars**;
- Dynamics of **black hole formation**;
- Electromagnetic counterparts of **gravitational wave signals**;
- Study of strong-field phenomena in modified gravity theories.

Analysis of observational data and numerical simulations of compact objects
(*e.g. Machine learning techniques to analyze gravitational waves from black hole binaries*)

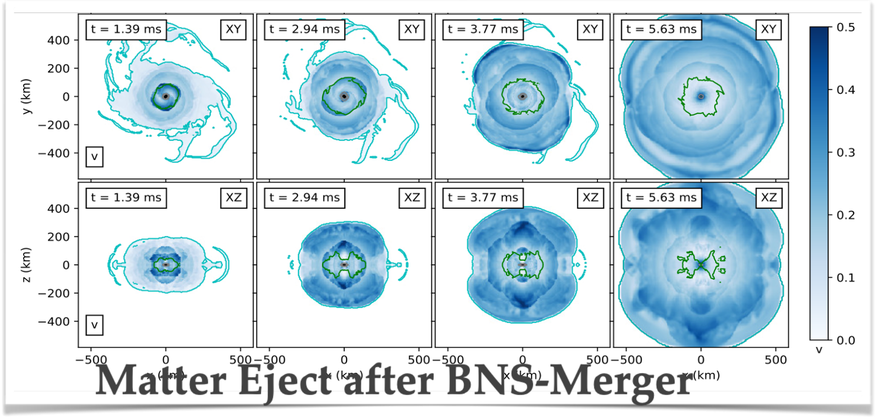
Hydrodynamics and magnetohydrodynamics simulations using state of the art codes in both the Newtonian and the General Relativistic regime
(*e.g. Model dynamical evolution and formation of stellar-mass and supermassive black holes via N-body simulations*)



NEUMATT

GRAVITATIONAL WAVE SIGNAL FROM THE MERGE OF BINARY NEUTRON STARS

Full 3D-simulation of Einstein Equation coupled to matter of the merger. Post-merger signal + study of the the ejected matter. Equation of State effect on the signal.



Matter Eject after BNS-Merger

INDARK

dark energy and matter, axions, neutrinos, modified gravity

Markov Chain Monte Carlo codes interfaced with Boltzmann codes

InDark è l'IS che si propone di studiare il modello cosmologico standard e le sue estensioni, e le connessioni con la fisica delle particelle. Si occupa di **inflazione**, **materia ed energia oscure**, **neutrini** e altre **relic cosmologiche leggere** (e.g. **assioni**), e **gravità modificata**.

A questo scopo, in InDark si utilizzano risorse HPC per:

- *Produzione di simulazioni di osservabili cosmologiche*
  - Simulazioni del campo di CMB, ideale o come osservato da diversi esperimenti passati e futuri. Utilizzate per es. per validare estimatori o per studiare il potere vincolante di esperimenti futuri rispetto a nuova fisica.
  - Simulazioni N-body della distribuzione di materia per la costruzione di covarianze ed estimatori di nongaussianità.
  - Simulazioni di calibrazione per la formazione delle strutture cosmologiche per modelli di axion dark matter, gravità modificata, interacting dark energy. Post-processing delle simulazioni prodotte per gli stessi modelli.
  - Calibrazione e ottimizzazione di codici N-body.

Physics of Complex Systems

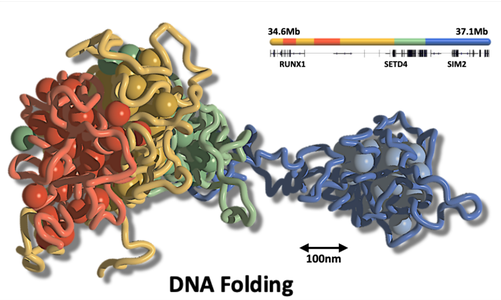
BIOPHYS ***ENESMA*** ***FIELDTURB***

BIOPHYS

Investigation of the three-dimensional structure of the mammalian genome

Structural properties of proteins and protein assemblies

Computational techniques: classical and ab-initio Molecular Dynamics, Monte Carlo and enhanced sampling by molecular dynamics algorithms.

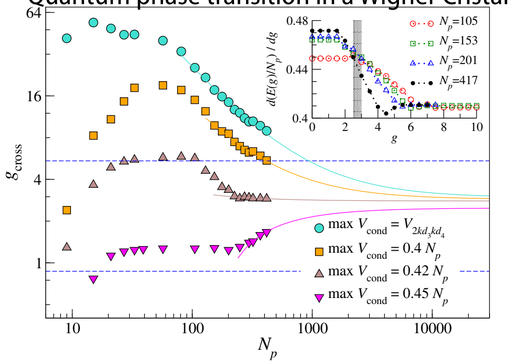


DNA Folding

ENESMA

Simulation of disordered systems (spin glasses, models of structural glasses, hard and soft spheres near the jamming point, optimization and inference problems, models of light propagation in disordered media, ecological models, etc...).

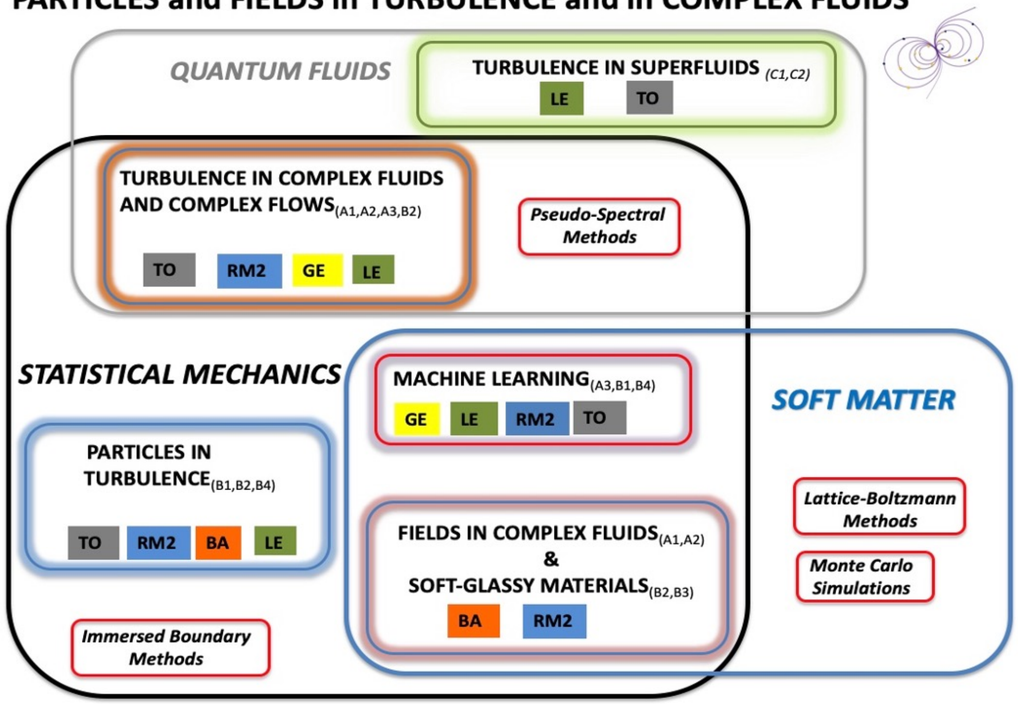
Quantum phase transition in a Wigner Cristal



FIELDTURB

Keywords : Turbulence, Complex fluids, Active matter,
Out-of-equilibrium statistical mechanics, Machine learning

PARTICLES and FIELDS in TURBULENCE and in COMPLEX FLUIDS



Nuclear Physics

MONSTRE

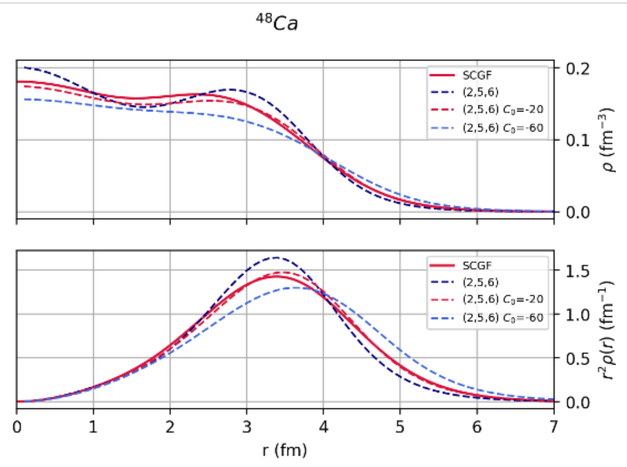
NUCSYS

MONSTRE

Quadro unificato per lo studio dei nuclei atomici, delle reazioni nucleari e della materia fortemente interagente

Keywords

- Struttura Nucleare
- Reazioni Nucleari
- Metodi a Molti-Corpi
- Funzionali Densità



Large Scale Shell-Model Calculations

- **Thick-Restart Lanczos method** - OpenMP-MPI hybrid (dim 10^{11})
- Elementi di matrice di interesse per esperimenti con sonde elettrodeboli (Neutrinoless **double-beta decay**)

Funzionali dell'energia

- Eq. di stato della materia nucleare

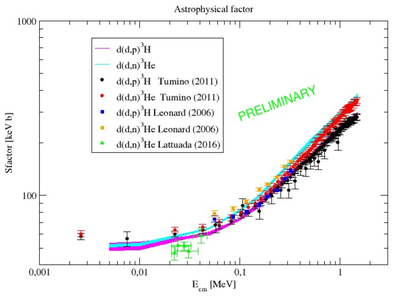
Calcoli *ab initio*

- Quantum Monte Carlo
- Machine Learning

"Quantum Computing applied to Artificial Intelligence" nell'ambito del programma PON R&I 2014-2020

NUCSYS

study of dd fusion



Method of calculation: expansion of the scattering wave functions in a basis
Problem to be solved: linear system M X = T(E)
M=matrix nxn (independent on energy E), T=known vectors, X=solution vector

Calculation of M & T
Tipically n=**300,000**

- 5-dimensional integration
- OpenMP code

Solution of the linear system (Lanczos)
- OpenMP code

Memory intensive calculation: work with 1 node only

- run for different J , energies, interactions,…

- a typical calculation takes 5,000 core hours on 1 Marconi & Galileo100 (48 cores)

NEXT: implementation using GPUs, extension up to A=6

Standard Model Phenomenology

QFTATCOL

QFTATCOL

- Application of Quantum Fiedl Theory to phenomenology of present and future hadron and lepton colliders
- Development of Monte Carlo event generators, for meaningful comparison of Theory predictions vs Experimental measurements
- Simulation of Standard Model and BSM processes, both for backgrounds and signal
- Steadily increasing complexity in theory predictions:
  higher-order radiative corrections (NLO, NNLO, ...), both in QCD and EW theory, to processes with more and more external particles
- CPU intensive computer codes due to multi-loop matrix elements evaluation, Monte Carlo integration and event generation, highly parallelizable

QFT@Colliders [BO, CS, FI, MIB, PV]

- A few examples of CPU intensive phenomenological study

  S. Catani *et al.*, JHEP **08** (2020) 08, 027 [FI]
  "Top-quark pair hadroproduction at NNLO: differential predictions with the $\overline{MS}$ mass"

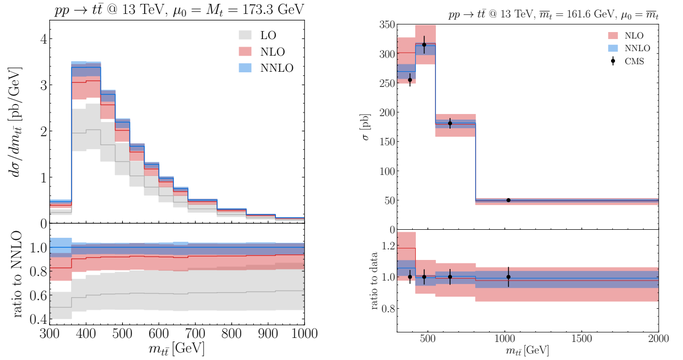


Figure: $m_{t\bar{t}}$ at different accuracies. NNLO greatly improves agreement with CMS data

HPC for CSN4 2 / 3

Risorse di calcolo al CINECA 2023 (consumi al 03/09/2023) —> MARCONI

MARCONI (A3)								
da	*14-Feb-2023*	*a*	*3-September-2023*	*#giorni*	*201*			
account	budget (corehours)	consumo (corehours)	consumo/budget (%)	residuo (corehours)	residuo%	#giorni	consumo linearizzato (su 12 mesi)	consumo/ (consumo linearizzato) %
INF23_biophys	570,000	122,395	21.47	447,605	78.53	201	313,890	*38.99*
INF23_enesma	35,000	0	0.00	35,000	100.00	201	19,274	*0.00*
INF23_euclid	1,000	1,440	144.00	-440	-44.00	201	551	*261.49*
INF23_fldturb	4,280,000	2,309,680	53.96	1,970,320	46.04	201	2,356,932	*98.00*
INF23_gagra	180,000	37,124	20.62	142,876	79.38	201	99,123	*37.45*
INF23_indark	1,070,000	406,858	38.02	663,142	61.98	201	589,233	*69.05*
INF23_lhc	1,000	0	0.00	1,000	100.00	201	551	*0.00*
INF23_lqcd123	8,350,000	3,914,176	46.88	4,435,824	53.12	201	4,598,219	*85.12*
INF23_lspe	1,000	1,004	100.40	-4	-0.40	201	551	*182.32*
INF23_monstre	1,030,000	584,481	56.75	445,519	43.25	201	567,205	*103.05*
INF23_nemesys	290,000	171,975	59.30	118,025	40.70	201	159,699	*107.69*
INF23_neumatt	3,140,000	481,686	15.34	2,658,314	84.66	201	1,729,151	*27.86*
INF23_npqcd	8,360,000	6,412,317	76.70	1,947,683	23.30	201	4,603,726	*139.29*
INF23_nucsys	250,000	177,321	70.93	72,679	29.07	201	137,671	*128.80*
INF23_qcdlat	17,700,000	9,559,847	54.01	8,140,153	45.99	201	9,747,123	*98.08*
INF23_qftatcol	1,280,000	179,831	14.05	1,100,169	85.95	201	704,877	*25.51*
INF23_quantum	215,000	0	0.00	215,000	100.00	201	118,397	*0.00*
INF23_sft	1,970,000	1,067,525	54.19	902,475	45.81	201	1,084,849	*98.40*
INF23_sim	735,000	707,621	96.27	27,379	3.73	201	404,753	*174.83*
INF23_teongrav	6,880,000	3072204	44.65	3,807,796	55.35	201	3,788,712	*81.09*
INF23_test	2,661,000	541,174	20.34	2,119,826	79.66	201	1,465,373	*36.93*
INF23_virgo	1,000	0	0.00	1,000	100.00	201	551	*0.00*
INF23_litebird	1,000,000	356,911	35.69	643,089	64.31	201	550,685	*64.81*
TOTALE	***60,000,000***	***30,105,570***	***50.18***	***29,894,430***	***49.82***	***201***	***33,041,096***	***91.12***

NOTE:

Partizione “accademica” di Marconi 256 nodi

Code di difficile accesso per job grandi

Risorse di calcolo al CINECA 2023 (consumi al 20/07/2023) —> MARCONI100

MARCONI100								
da	*14-Feb-2023*	*a*	*20-Jul-2023*	*#giorni*	*156*			
account	budget (corehours)	consumo (corehours)	consumo/budget (%)	residuo (corehours)	residuo%	#giorni	consumo linearizzato (su 12 mesi)	consumo/ (consumo linearizzato) %
INF23_biophys_0	1,000,000	943,008	94.30	56,992	5.70	156	427,397	*220.64*
INF23_enesma_0	61,000	25,621	42.00	35,379	58.00	156	26,071	*98.27*
INF23_euclid_0	451,000	387,368	85.89	63,632	14.11	156	192,756	*200.96*
INF23_fldturb_0	1,000,000	1,001,927	100.19	-1,927	-0.19	156	427,397	*234.43*
INF23_gagra_0	1,000	8	0.80	992	99.20	156	427	*1.87*
INF23_indark_0	35,000	0	0.00	35,000	100.00	156	14,959	*0.00*
INF23_lhc_0	1,300,000	659,089	50.70	640,911	49.30	156	555,616	*118.62*
INF23_lqcd123_0	4,700,000	5,800,710	123.42	-1,100,710	-23.42	156	2,008,767	*288.77*
INF23_lspe_0	1,000	0	0.00	1,000	100.00	156	427	*0.00*
INF23_monstre_0	130,000	173,822	133.71	-43,822	-33.71	156	55,562	*312.85*
INF23_nemesys_0	130,000	123,192	94.76	6,808	5.24	156	55,562	*221.72*
INF23_neumatt_0	30,000	2,306	7.69	27,694	92.31	156	12,822	*17.98*
INF23_npqcd_0	3,300,000	2,511,399	76.10	788,601	23.90	156	1,410,411	*178.06*
INF23_nucsys_0	20,000	0	0.00	20,000	100.00	156	8,548	*0.00*
INF23_qcdlat_0	800,000	804,874	100.61	-4,874	-0.61	156	341,918	*235.40*
INF23_qftatcol_0	1,000	0	0.00	1,000	100.00	156	427	*0.00*
INF23_quantum_0	160,000	76,503	47.81	83,497	52.19	156	68,384	*111.87*
INF23_sft_0	130,000	131,793	101.38	-1,793	-1.38	156	55,562	*237.20*
INF23_sim_0	650,000	585,489	90.08	64,511	9.92	156	277,808	*210.75*
INF23_teongrav_0	200,000	99,947	49.97	100,053	50.03	156	85,479	*116.93*
INF23_test_0	819,000	715,102	87.31	103,898	12.69	156	350,038	*204.29*
INF23_virgo_0	1,000	3,319	331.90	-2,319	-231.90	156	427	*776.56*
TOTALE	***14,920,000***	***14,045,477***	***94.14***	***874,523***	***5.86***	156	***6,376,767***	***220.26***

NOTE:

Marconi100 dismessa a fine luglio 2023

Risorse di calcolo al CINECA 2023 (consumi al 03/09/2023) —> LEONARDO_B

LEONARDO (booster)								
da	*1-Aug-2023*	*a*	*3-Sep-2023*	*#giorni*	*33*			
account	budget (corehours)	consumo (corehours)	consumo/budget (%)	residuo (corehours)	residuo%	#giorni	consumo linearizzato (su 5 mesi)	consumo/(consumo linearizzato) %
INF23_biophys_2	1,333,333	176,595	13.24	1,156,738	86.76	33	293,333	*60.20*
INF23_enesma_2	1,333,333	1	0.00	1,333,332	100.00	33	293,333	*0.00*
INF23_euclid_2	13,333	8,980	67.35	4,353	32.65	33	2,933	*306.14*
INF23_fldturb_2	1,333,333	0	0.00	1,333,333	100.00	33	293,333	*0.00*
INF23_gagra_2	13,333	1	0.01	13,332	99.99	33	2,933	*0.03*
INF23_indark_2	1,000,000	0	0.00	1,000,000	100.00	33	220,000	*0.00*
INF23_lhc_2	3,466,667	14,909	0.43	3,451,758	99.57	33	762,667	*1.95*
INF23_lqcd123_2	8,000,000	437,038	5.46	7,562,962	94.54	33	1,760,000	*24.83*
INF23_lspe_2	13,333	0	0.00	13,333	100.00	33	2,933	*0.00*
INF23_monstre_2	40,000	0	0.00	40,000	100.00	33	8,800	*0.00*
INF23_nemesys_2	133,333	0	0.00	133,333	100.00	33	29,333	*0.00*
INF23_neumatt_3	13,333	0	0.00	13,333	100.00	33	2,933	*0.00*
INF23_npqcd_2	8,000,000	469	0.01	7,999,531	99.99	33	1,760,000	*0.03*
INF23_nucsys_2	1,333,333	0	0.00	1,333,333	100.00	33	293,333	*0.00*
INF23_qcdlat_2	5,333,333	0	0.00	5,333,333	100.00	33	1,173,333	*0.00*
INF23_qftatcol_2	666,667	0	0.00	666,667	100.00	33	146,667	*0.00*
INF23_quantum_2	133,333	0	0.00	133,333	100.00	33	29,333	*0.00*
INF23_sft_2	333,333	0	0.00	333,333	100.00	33	73,333	*0.00*
INF23_sim_2	1,000,000	0	0.00	1,000,000	100.00	33	220,000	*0.00*
INF23_teongrav_2	1,333,333	990	0.07	1,332,343	99.93	33	293,333	*0.34*
INF23_test_2	5,160,000	0	0.00	5,160,000	100.00	33	1,135,200	*0.00*
INF23_virgo_2	13,333	0	0.00	13,333	100.00	33	2,933	*0.00*
TOTALE	***39,999,996***	***638,983***	***1.60***	***39,361,013***	***98.40***	33	***3,616,438***	***17.67***

da 01/08/2023

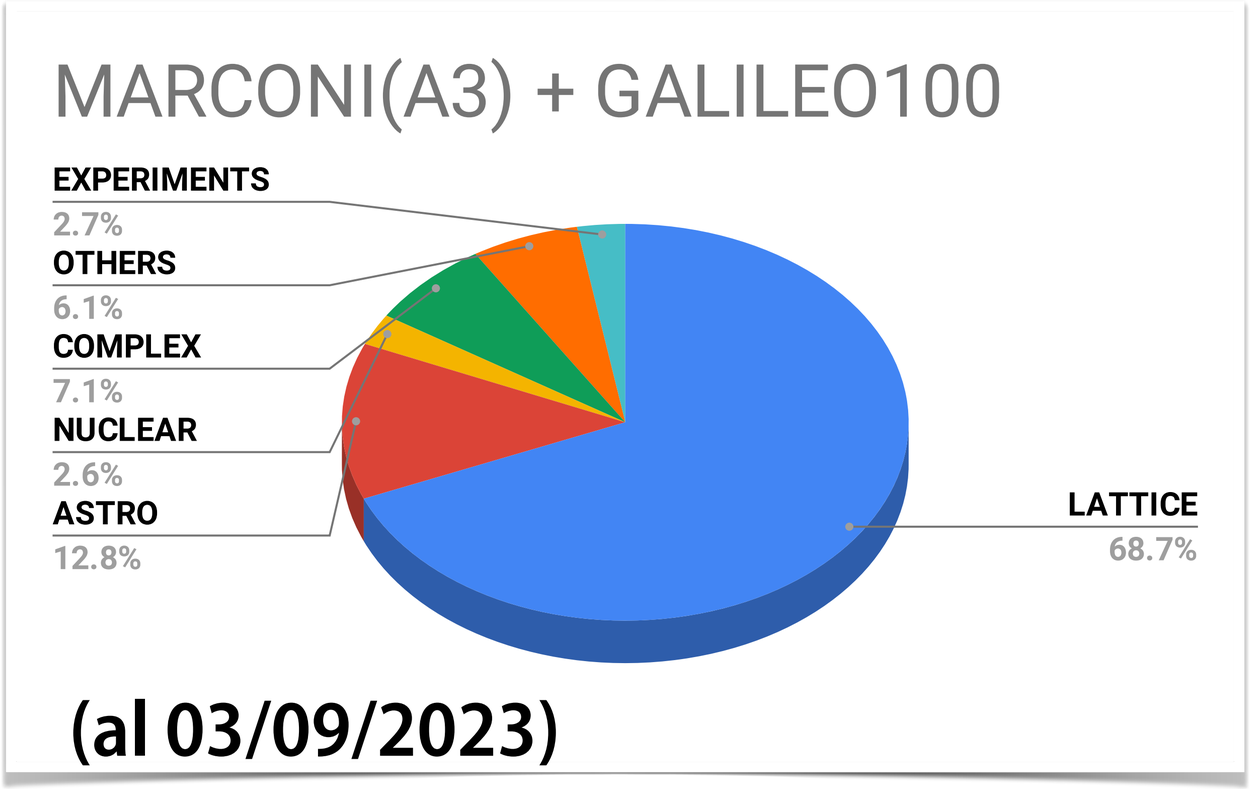
Budget annuo:
3 Mnodehours=(3 x 32) Mcorehours

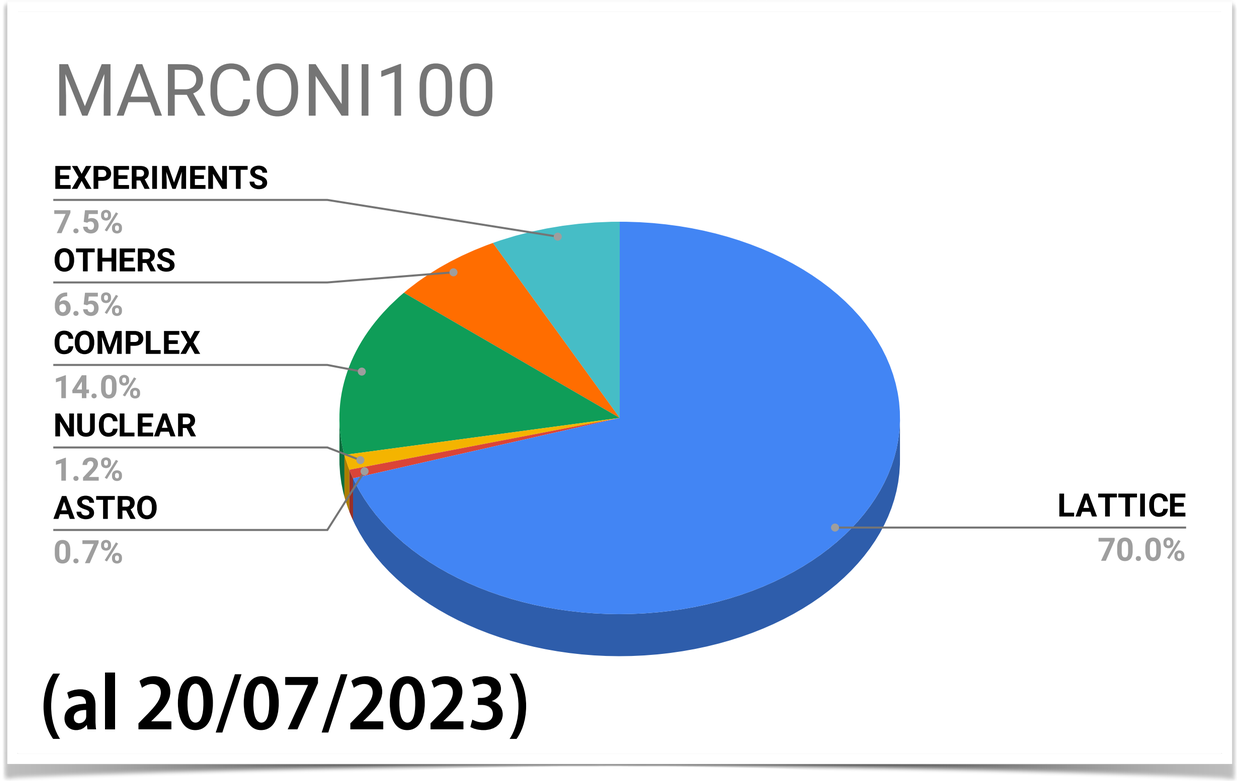
Assegnazione 2023:
5/12 x 96 Mcorehours = 40 Mcorehours

Risorse di calcolo al CINECA 2023 (consumi al 03/09/2023) —> GALILEO100

GALILEO100								
da	*14-Feb-2023*	*a*	*3-Sep-2023*	*#giorni*	*201*			
account	budget (corehours)	consumo (corehours)	consumo/budget (%)	residuo (corehours)	residuo%	#giorni	consumo linearizzato (su 12 mesi)	consumo/(consumo linearizzato) %
INF23_biophys_1	45,000	20,380	45.29	24,620	54.71	201	24,781	*82.24*
INF23_enesma_1	2,799	0	0.00	2,799	100.00	201	1,541	*0.00*
INF23_euclid_1	500,001	548,306	109.66	-48,305	-9.66	201	275,343	*199.14*
INF23_fldturb_1	330,000	397	0.12	329,603	99.88	201	181,726	*0.22*
INF23_gagra_1	14,001	0	0.00	14,001	100.00	201	7,710	*0.00*
INF23_indark_1	84,999	0	0.00	84,999	100.00	201	46,808	*0.00*
INF23_lhc_1	999	0	0.00	999	100.00	201	550	*0.00*
INF23_lqcd123_1	9,999	36	0.36	9,963	99.64	201	5,506	*0.65*
INF23_lspe_1	500,001	37,582	7.52	462,419	92.48	201	275,343	*13.65*
INF23_monstre_1	84,999	67,135	78.98	17,864	21.02	201	46,808	*143.43*
INF23_nemesys_1	22,500	21,888	97.28	612	2.72	201	12,390	*176.65*
INF23_neumatt_1	249,999	0	0.00	249,999	100.00	201	137,671	*0.00*
INF23_npqcd_1	650,001	670,203	103.11	-20,202	-3.11	201	357,946	*187.24*
INF23_nucsys_1	71,001	61,717	86.92	9,284	13.08	201	39,099	*157.85*
INF23_qcdlat_1	1,400,001	1,384,166	98.87	15,835	1.13	201	770,959	*179.54*
INF23_qftatcol_1	99,999	0	0.00	99,999	100.00	201	55,068	*0.00*
INF23_quantum_1	17,001	5	0.03	16,996	99.97	201	9,362	*0.05*
INF23_sft_1	150,000	6,699	4.47	143,301	95.53	201	82,603	*8.11*
INF23_sim_1	54,999	136	0.25	54,863	99.75	201	30,287	*0.45*
INF23_teongrav_1	540,000	451,934	83.69	88,066	16.31	201	297,370	*151.98*
INF23_test_1	1,170,699	1,207,581	103.15	-36,882	-3.15	201	644,686	*187.31*
INF23_virgo_1	999	0	0.00	999	100.00	201	550	*0.00*
TOTALE	***5,999,997***	***4,478,165***	***74.64***	***1,521,832***	***25.36***	201	***3,304,108***	***135.53***

Risorse di calcolo al CINECA 2023 (percentuale consumi)



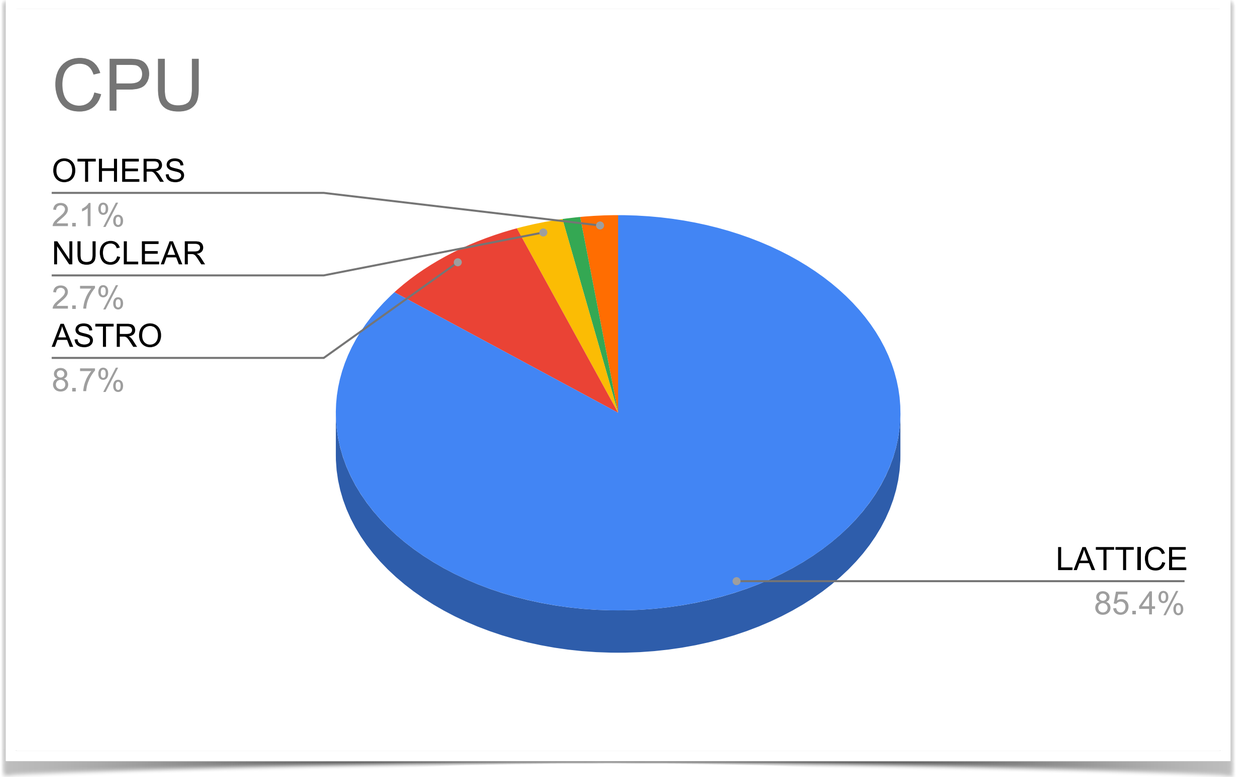


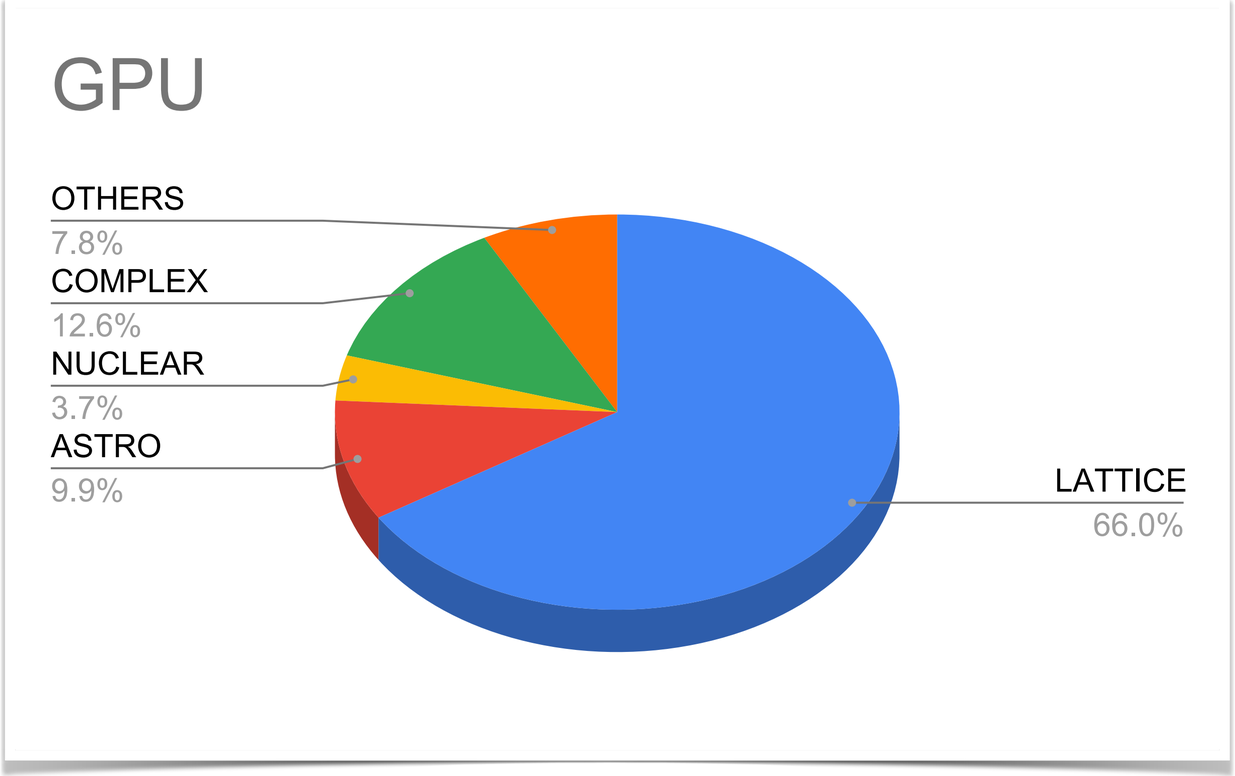
Risorse di calcolo 2024 (proposte)

	sigla	numero max processi MPI per job	connessione	CPU (corehours) RICHIESTE	CPU (corehours) PROPOSTE	possibile utilizzo di sistemi Tier1 e/o Tier2?	Tier1/Tier2 (corehours)	Cineca (corehours)	GPU (nodehours) RICHIESTE	GPU (nodehours) PROPOSTE	possibile utilizzo di sistemi Tier1 e/o Tier2?	Tier1/Tier2 (nodehours)	Cineca (nodehours)
1	**BIOPHYS**	1,000	Infiniband	*1,000,000*	***600,000***	NO	***0***	***600,000***	*100,000*	***100,000***	NO	***0***	***100,000***
2	**ENESMA**	100	Infiniband	*0*	***10,000***	NO	***0***	***10,000***	*300,000*	***150,000***	NO	***0***	***150,000***
3	**FLDTURB**	1,000	Infiniband	*1,000,000*	***1,000,000***	SI	***100,000***	***900,000***	*100,000*	***100,000***	SI	***10,000***	***90,000***
4	**GAGRA**	1,000	Infiniband	*400,000*	***300,000***	NO	***0***	***300,000***	*15,000*	***15,000***	SI	***0***	***15,000***
5	**INDARK**	100	Farm	*2,000,000*	***1,200,000***	NO	***500,000***	***700,000***	*200,000*	***175,000***	NO	***0***	***175,000***
6	***LINCOLN***	1,000	Farm	*750,000*	***400,000***	NO	***200,000***	***200,000***	*7,500*	***7,500***	NO	***0***	***7,500***
7	**LQCD123**	>5000	Infiniband	*25,000,000*	***20,000,000***	NO	***0***	***20,000,000***	*700,000*	***600,000***	NO	***0***	***600,000***
8	**MONSTRE**	1,000	Infiniband	*2,600,000*	***2,000,000***	NO	***0***	***2,000,000***	*3,000*	***3,000***	NO	***0***	***3,000***
9	**NEMESYS**	1,000	Infiniband	*3,500,000*	***500,000***	SI	***100,000***	***400,000***	*250,000*	***100,000***	SI	***10,000***	***90,000***
10	**NEUMATT**	5,000	Infiniband	*5,000,000*	***2,500,000***	NO	***0***	***2,500,000***	*1,024*	***1,000***	NO	***0***	***1,000***
11	**NPQCD**	>5000	Infiniband	*45,000,000*	***40,000,000***	SI	***2,500,000***	***37,500,000***	*700,000*	***600,000***	SI	***30,000***	***570,000***
12	**NUCSYS**	1,000	Infiniband	*2,200,000*	***2,000,000***	NO	***0***	***2,000,000***	*200,000*	***100,000***	NO	***0***	***100,000***
13	**QCDLAT**	>5000	Infiniband	*67,500,000*	***63,500,000***	SI	***10,000,000***	***53,500,000***	*500,000*	***470,000***	SI	***23,500***	***446,500***
14	**QFTATCOL**	5,000	Farm	*3,600,000*	***2,000,000***	SI	***1,000,000***	***1,000,000***	*250,000*	***200,000***	NO	***0***	***200,000***
15	**QUANTUM**	1,000	Infiniband	*500,000*	***500,000***	NO	***100,000***	***400,000***	*10,000*	***10,000***	NO	***0***	***10,000***
16	**SFT**	5,000	Farm	*2,000,000*	***1,500,000***	SI	***500,000***	***1,000,000***	*30,000*	***30,000***	SI	***0***	***30,000***
17	**SIM**	1,000	Infiniband	*2,000,000*	***2,000,000***	NO	***0***	***2,000,000***	*200,000*	***125,000***	NO	***0***	***125,000***
18	**TEONGRAV**	1,000	Infiniband	*13,000,000*	***10,000,000***	NO	***0***	***10,000,000***	*130,000*	***100,000***	SI	***0***	***100,000***
	TOTALE			***177,050,000***	***150,010,000***		***15,000,000***	***135,010,000***	***3,696,524***	***2,886,500***		***73,500***	***2,813,000***

Le proposte risultano dalla valutazione dei referee sulle richieste pervenute

Risorse di calcolo 2024 (proposte)

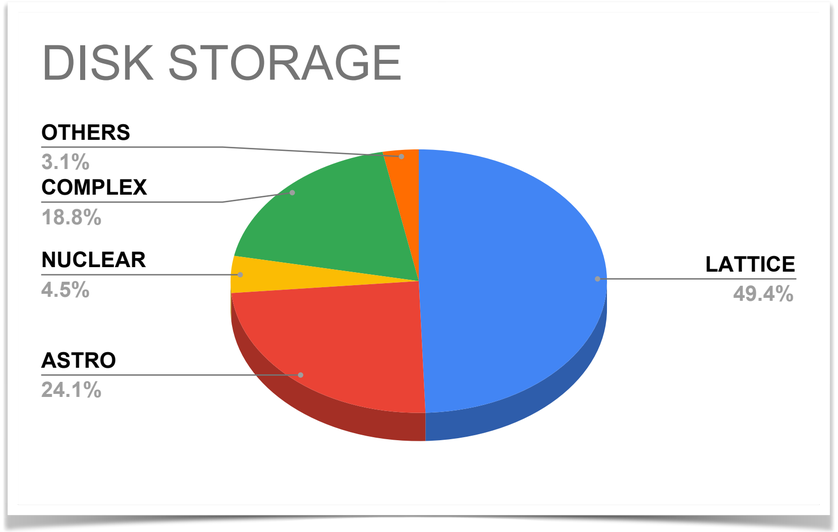


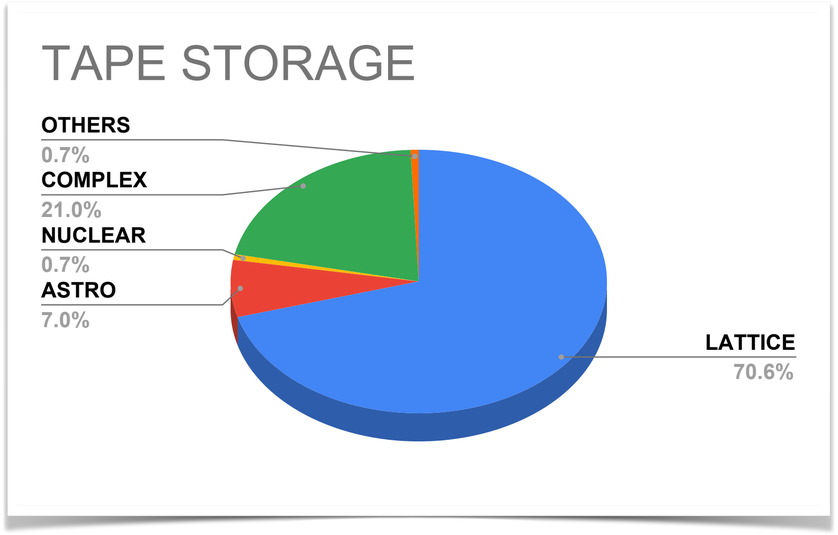


Nota:
i job di LQCD scalano meglio su pre-exascale

Risorse di calcolo 2024 (storage su disco e su nastro)

sigla	DISCO (TB)	NASTRO (TB)
BIOPHYS	100	0
ENESMA	50	0
FLDTURB	100	300
GAGRA	2	10
INDARK	200	100
LINCOLN	1	0
LQCD123	350	0
MONSTRE	50	10
NEMESYS	10	10
NEUMATT	20	0
NPQCD	100	300
NUCSYS	10	0
QCDLAT	0	500
QFTATCOL	25	0
QUANTUM	5	0
SFT	4	0
SIM	200	200
TEONGRAV	100	0
Totale	1327	1430





BACKUP SLIDES:

Attività 2024 delle sigle

LQCD123

Computation time requests for year 2024

A) Fifth lattice spacing of simulations of 2+1+1 QCD with physical pion mass: O(300) trajectories with very fine lattice spacing (ensemble “cE112” L = T/2 = 5.46 fm, a=0.049 fm), using the framework discussed in *PoS* LATTICE2022 (2023) 340, arXiv:2212.06635.

Motivation: improve the continuum limit extrapolation, especially for the heavy-light observables and the hadronic vacuum polarization contribution to the muon g-2.

Estimated cost: 300k node-hours on Leonardo (GPU cluster)

B) QED and isospin breaking contribution to the g-2 of the muon and to the electron-positron hadronic cross section $R(E)$.

Motivation: remove the largest systematic uncertainties on the determination of muon g-2 and R(E). See *Phys.Rev.D* 107 (2023) 7, 074506 and *Phys.Rev.Lett.* 130 (2023) 24, 241901

Estimated cost: 6M core-hours on Marconi A3/Leonardo (CPU cluster)

C) determination of the form factors for heavy-light to heavy-light semileptonic transitions, of the form $B_s \to D_s^* \ell\nu$ decay, along the line of Phys.Rev.D 99, 099902 (2019).

Motivation: A longstanding tension exists between the inclusive and the exclusive determinations of the CKM matrix element $|V_{cb}|$. Lattice simulations are needed to compute the relevant form factors, including those relevant for search of physics beyond the Standard Model, to clarify the tensions.

Estimated cost: 7M core-hours on Marconi A3/Leonardo (CPU cluster)

D) Determination of the radiative decay of mesons, of the form $P \to \ell\nu\gamma$ and $P \to \ell\ell\gamma$ with a novel approach based on spectral density reconstruction, along the line of arXiv:2306.07228, on physical point ensembles, for a range of flavor channel of interest and in particular for the Kaon channel.

Motivation: the novel approach allows for the first time to determine electroweak amplitude directly on euclidean lattice simulations, bypassing a longstanding limitation of lattice methodology related to the Maiani-Testa no-go theorem. This allows several phenomenologically important comparisons, and to verify precisely the flavor sector of the SM in a substantially unexplored field.

Estimated cost: 7M core-hours on Marconi A3/Leonardo (CPU cluster)

E) Computation of the inclusive hadronic decay rate of $\tau \to X_s$, applying the methodology proposed in *PoS* LATTICE2022 (2023) 296, arXiv:2301.00796 to the case of the up-strange channel, to determine $|V_{us}|$

Motivation: clarify the tension between the value of $|V_{us}|$ coming from inclusive τ decays and the other determinations.

Estimated cost: 300k node-hours on Leonardo (GPU cluster)

NPQCD

HPC Research Program for year 2024, I.S. NPQCD

Our research program concerns frontier open problems in the non-perturbative aspects of strong interactions and other QCD-like theories. We have a long-standing tradition in the use of HPC resources, also through competitive calls such as PRACE or ISCRA. Our numerical simulations are mostly based on codes developed by researchers of our team or collaborators, running on GPUs [1, 2] or standard [3] clusters, but also on other publicly available codes [4].

The main research topics to be pursued in 2024 are the following:

B) QCD TOPOLOGY AND AXION PHENOMENOLOGY
We will pursue our efforts for a reliable determination of the topological properties of QCD with physical quark masses at finite temperature, in particular reaching T $\sim$ 1 GeV and above (with lattice spacings down to 0.02 fm), which is the range relevant for axion phenomenology. That will be possible thanks to the extension to full QCD of the algorithm to defeat topological freezing developed for Yang-Mills theories in Ref. [5], which implements parallel tempering on boundary conditions. We plan to run this part of the project on GPUs with a double level of parallelization (parallel tempering with multiple multiGPUs runs). Gauge configurations produced in this context will be used to determine other quantities relevant for axion phenomenology, in particular the so-called sphaleron rate, for which we have already developed a well definite computational strategy in pure Yang-Mills theories [6].

Restricting to the pure gauge case, we plan to extend the study of the theta dependence of the deconfinement temperature to SU(N) gauge theories with $N > 3$ and to study the θ-dependence of the spectrum of the theory (string tension, glueball masses and, for the finite temperature case, screening masses. This part of the project will run mostly on CPUs.

Finally, we plan to investigate the relation between chiral properties and topology by an investigation of the chiral condensate and of the mass dependence of the topological susceptibility through the staggered spectral projectors. This part of the project will run both on GPUs (production of gauge configurations) and on CPUs (analysis).

B) QCD flux tubes and color confinement/deconfinement
We plan to extend our analysis about the properties of the confining flux tube [7, 8] to (2+1)-flavor QCD with physical quark masses, where only preliminary results are available so far, and to the finite temperature case (both in pure SU(3) and in full QCD) across the deconfinement transition. We also plan to assess the impact of perturbing the zero-temperature vacuum with external fields on the shape of the flux tube and, in general, on the distribution of all color fields and currents around the static sources. This part of the project will run mostly on GPUs, with part of the analysis on CPUs.

A precision determination of the flux tube properties and a comparison with effective string theory predictions for the static quark-antiquark potential will be performed in pure gauge theories, extending results of Refs. [9, 10] with and without the insertion of a θ-term, with and without the addition of a trace deformation in the case of compactified theories. This part of the project will run mostly on CPUs.

C) Phase Diagram of QCD and QCD-like theories
We will pursue our efforts in the study of the phase diagram of QCD in the presence of external background fields, in particular by determining the latent heat of the first order transition which is found at strong magnetic fields [11], by studying the dependence of the Roberge-Weiss transition on magnetic background fields, and by extending the investigation to the case of chromomagnetic fields. This part of the project will run extensively on GPUs.

In this context, we also plan to determine the transport properties of QCD in extreme conditions, with a particular emphasis on the electric conductivity. That will mostly involve the analysis of already existing gauge configurations and will run mostly on CPUs.

Part of the computational efforts will be dedicated to the study of three dimensional strongly coupled gauge models coupled to fermionic fields, in order to investigate the confining properties of these theories and the possible existence of continuous phase transitions which can be relevant for finite temperature transitions of 4d gauge theories. We will also investigate the phase diagram of dual models representing a possible solution to the sign problem. This part of the project will run mostly on CPUs

Our computational program involves the production of many gauge configurations which should be stored for further analysis. This is at the basis of our requests for storage, both on disk and on tape.

References

[1] C. Bonati, E. Calore, S. Coscetti, M. D'Elia, M. Mesiti, F. Negro, S. F. Schifano, G. Silvi and R. Tripiccione, Int. J. Mod. Phys. C **28**, no.05, 1750063 (2017) doi:10.1142/S0129183117500632 [arXiv:1701.00426 [hep-lat]].

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QCDLAT

QCDLAT
INFN Research Project of the Theory Group (CSN4)

Title: Non-perturbative QCD on the lattice: advancing the frontiers of extreme conditions and of precision physics

National Coordinator from 2024: Michele Pepe (Michele.Pepe@mib.infn.it)

INFN sections of people involved: Milano Bicocca, Parma, Roma Sapienza, Roma Tor Vergata

Number of Participants: 16

Description of the research activity

The purpose of this proposal is to expand the frontiers of QCD research: we push its boundaries into unexplored regimes characterized by extreme conditions and its theoretical predictions to high accuracy for searching potential signals of physics beyond the Standard Model (SM).

The lattice regularization will allow us to perform non-perturbative investigation from first principles by Monte Carlo simulations. The development of new theoretical methodologies and of innovative algorithmic techniques will be essential in pursuing our project and for attaining final numerical precisions at the percent level or less.

The research activity of this proposal involves many important and interesting phenomena, covering a broad range of energy scales. Indeed, the behavior of QCD in extreme conditions – namely at high temperature and/or at finite chemical potential – plays a central role for nuclear physics as well as for cosmology and astrophysics, and sheds light on early stages of the Universe. Precise comparisons between theory and experiments for a selected number of ElectroWeak and Strong processes may detect hints of new particles or interactions beyond our current understanding of particle physics.

The research activity of the people involved in this project crucially depends on the allocation of computer resources that INFN provides and which are also essential for being competitive when participating to national and European calls for computer time.

The project is organized in four groups of objectives and the tasks that are planned to be pursued during the year 2024 using the INFN computational resources are the following:

- **Flavour physics in the SM and beyond**: precise calculation of the hadronic contribution to the muon anomalous magnetic moment searching for BSM physics; precise determination of fundamental SM parameters; kaon-mixing matrix elements to constraint extensions of the SM; computation of isospin breaking corrections.
- **QCD in extreme conditions**: computation of the Equation of State at μ=0 up to T≈100 GeV as well as of other quantities like baryonic screening masses, transport coefficients, …; search for the QCD critical point via singularity structures in the T-μ phase diagram; Lefschetz thimble approach to study systems with a sign problem.
- **Theoretical developments:** non-perturbative renormalization of the QCD energy-momentum tensor and of other composite operators; Renormalization Group evolution of fundamental SM parameters; strings in non-Abelian gauge theories and QCD; computation of improvement coefficients of lattice operators; computation of scattering amplitudes and of time-like observables.
- **Algorithmic advances:** factorization of the fermionic determinant and multi-level algorithms; shifted boundary conditions for QCD at finite T; simulations with light quarks and large volumes (master field simulations); numerical stochastic perturbation theory.

The people participating to the QCDLAT project are internationally renowned experts in the Monte Carlo simulations of QCD on the lattice exploiting HPC systems; international collaborators are involved in the research activity discussed above.

Request of computational resources at Cineca:

- **CPU**-based partition: **50 Mch**
- **GPU**-based partition: **400 Knh**

Request of computer-time allocation on HPC systems for R&D

The people participating to the project QCDLAT have performed since very long time a very intense research activity on the non-perturbative dynamics of QCD. This sort of studies can be accomplished from first principles only by numerical simulations on the lattice: they are extremely demanding from the computational viewpoint and they can be pursued only on HPC systems available at supercomputing centres.

The steady increase of the computational power of HPC systems allows on the one side to increase the accuracy of the calculations and on the other side to extend the target of the numerical investigations, however the most relevant improvements in the efficiency of the numerical computations often come from the development of new algorithms and new computational strategies.

For this reason, a very important part of the activity of QCDLAT has always been dedicated to the search of innovative numerical techniques to boost the Monte Carlo simulations of QCD on the lattice and, indeed, many methods proposed and studied by our group are now well-established computational strategies.

The study and the development of innovative numerical methods can be efficiently carried out only on small size HPC systems, with resources that can be easily accessible and with a fast stop-restart working approach that is essential when studying and testing new algorithms.

In order to continue this very important research of QCDLAT, we would like to ask to have access to 8 nodes with 192 cores each connected by a 200 Gbit/s switch InfiniBand. We are also interested in the possibility of using 8 nodes with GPUs.

Request of computational resources on Tier1/Tier2 clusters:

- **CPU**-based partition: **13.5 Mch**
- **GPU**-based partition: **70 Knh**

Request of storage space on tape

People participating to the project QCDLAT have been awarded relevant computer resources (European Calls PRACE) at supercomputing centres. In pursuing those projects, many gauge field configurations have been generated: those data are very important since the measurement of physical quantities is, in general, performed in a successive step with respect to the production of the configurations.

Thus, it is important to store those configurations in a long-term way so that one can access at any time that Database to measure new quantities that have turned out interesting to compute. Considering that also many other configurations will be produced, **we would like to confirm the request of 500 Tb of storage on tape.**

GAGRA

1. GAGRA research project

The lattice regularisation of gauge theories offers the unique possibility of computing the functional integral numerically without any approximation through Monte Carlo techniques. One can thus obtain theoretical informations about the low-energy, non-perturbative regime of Yang-Mills theories and QCD with any number of colours N.

The main interest of our research project is the numerical computation of the low-energy spectrum of gauge theories. We are thus planning to compute the lowest glueballs and mesons masses in the large-N limit in order to compare them against the predictions of the models developed to solve analytically such theories (see e.g. Ref. [1,2]).

In the last year we have written a code for the simulation of SU(N) pure gauge theories and the computation of the two-point correlation functions of Wilson loops of several lengths, classified according to the transformation properties under the cubic group and discrete symmetries (parity and charge conjugation). From the two-point correlators we have implemented the extraction of the low-lying glueball spectrum through the solution of the Generalized Eigenvalue Problem.

This computation faces the long standing problem of the exponential deterioration of the signal-to-noise ratio of the two-point correlation functions at large Euclidean time. This problem has been partially solved in the glueball case [3] allowing for the state of the art computation in [4]. After this study a new one [5] has been recently presented which goes up to $N = 12$ (the largest value of N ever simulated so far) and perform an extrapolation to $N = \infty$.

The study in [5] does not implements the algorithmic improvement developed in [3] and presents errors which seems exceedingly small, giving rise to tensions in the values of the mass of some states with respect to previous published results (e.g. in [4]). In the last months we have implemented in our code the algorithmic improvement proposed in [3] together with the smearing of gauge links used to build the Wilson loops which creates or annihilates the glueball states and we are presently testing such improvements. We thus plan to be able to start very soon new extensive simulations to compute the low-lying glueball spectrum at large values of N and small lattice spacings, in order to be able to perform systematically the continuum limit at each N and then a safe extrapolation to the $N = \infty$ limit.

In the case of the meson spectrum, the problem of the exponential deterioration of the signal-to-noise ratio does not affects the pseudoscalar channel while in the other channels is less dramatic than in the glueball case. Despite this, even in the most recent/state of the art study of meson masses at large-N [6], no continuum limit has been taken. We are thus planning to perform a study in which the continuum limit is taken for each N, possibly increasing the number of N on which the large-N limit is taken.

2. References

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SFT

SFT Scientific Initiative – Planned Research Activities for 2024

The SFT scientific initiative of the Italian Nuclear Physics Institute (INFN) is focused on theoretical research in statistical field theory. The main scientific activities involving high-performance computing (HPC) are in the area of lattice field theory. The HPC research carried out by SFT distinguishes itself from the other scientific initiatives working in lattice field theory for:

- its particular focus on fundamental theoretical problems, which are often best studied in simple models, including the purely gluonic sector of QCD, low-dimensional spin and gauge theories, etc.;
- the broad variety of physical topics that are studied, which range from conventional lattice QCD studies (with direct phenomenological applications) to models for new physics beyond the Standard Model (including studies of composite-Higgs models and particle dark matter), to the entanglement entropy in quantum system, to the critical behavior of spin models.

This unique combination of features makes the research activities carried out by SFT in the area of high-performance scientific computing particularly attractive towards national and international collaborators, boosting the publication output and research impact of SFT. Indeed, it is worth pointing out that while the requested computing resources for SFT are a small fraction of those that are appropriate for other INFN Scientific Initiatives, the number of publications in high-impact journals like JHEP, PRD, PRL, etc. and other bibliometric parameters from numerical studies carried out by SFT are nevertheless significant. This feature is also particularly attractive for a growing number of junior users (including graduate and undergraduate students), who are also granted access to the resources and trained in massively parallel HPC, in the development and use of code running on GPU's, and in machine-learning applications, with evident benefits for their scientific education and future career prospects.

The main research lines for 2024 are:

1. **Reconstruction of spectral functions from the lattice** In a series of works with collaborators from Rome and from other groups, we are applying the spectral-reconstruction techniques pioneered by M. Hansen *et al.* in Phys. Rev. D 99 (2019) 094508 to investigate the spectrum of glueballs, the properties of states in non-Abelian gauge theories with matter fields in multiple representations, and the study of semileptonic decays of heavy mesons (the latter is part of a large-scale, long-term computational effort with the Extended Twisted-Mass Collaboration).

2. **Composite dark matter in the early universe** We will continue an ongoing study with collaborators from Milan and from Swansea, analyzing the equation of state of a model based on the Sp(4) gauge group, which could provide a viable framework for a secluded type of particle dark matter.

3. **Entanglement entropy from lattice calculations** Having completed a first study in the Ising model, we will study the entanglement entropy and entropic c-function in statistical models based on O(N) symmetry in three dimensions, in collaboration with members of SFT studying this topic with analytical techniques, and with collaborators from Madrid.

4. **Universal ratios and form factors in the tricritical, three-state dilute Potts model** Novel high-precision numerical simulations of the tricritical, three-state dilute Potts model will be carried out, to test a class of approximate analytical predictions for form factors and universal ratios.

5. **Quantum simulation of $\mathbf{CP}^{N-1}$ models** Inspired by constructions from non-commutative geometry, we will perform quantum simulations of CP^{N-1} models with a suitable truncation of the Hilbert space, which preserves more symmetries than those that are preserved in conventional approaches.

SIM

We would like to use the resources for

QCD Plasma studies for experiments and cosmology

The participants are: Maria Paola Lombardo, Andrey Kotov (Juelich FZK), Anton Trunin (Samara) and we greatly benefit from help of the ETMC colleagues, in particular in this phase QCD Bartosz Kostrzewa.

Our project has two long term interrelated main objectives: firstly, it aims at a characterisation of the strongly coupled Quark Gluon Plasma region, addressing some of the main open issues; second, we wish to make further progress and impact on axion physics. We have a running exploratory application (ISCA Class C) and we plan to apply for B as soon as possible. This INFN allocation will be most helpful in complementing the little C budget, and help finalising more demanding proposals.

We will use the tmLQCD software suite which has recently been extended with a full interface to the QUDA lattice QCD GPU library, enabling its Hybrid Monte Carlo implementation to make use of the optimized Dirac operators and solvers in QUDA, in particular the highly efficient multigrid-preconditioned GCR solver, which speeds up inversions at the physical point by two orders of magnitude compared to mixed-precision CG. This enables large scale studies to be performed directly at the physical pion mass at a reasonable computational cost.

From a computational viewpoint, our codes are ready, making use of the highly efficient QUDA lattice QCD library through the tmLQCD software suite.Our observables will be the order parameter for the chiral transition, and two point functions in the relevant channels. We will further study the scaling window of the chiral transition, the nature of an anomalous threshold observed at around T= 300 MeV, and improve limits on the QCD axion mass from topological susceptibility.

INDARK

InDark - Description of the research program for 2024

M. Lattanzi for the InDark affiliates

In 2024, computational resources will continue to be used to support the InDark activities on the development of robust tools for the analysis and scientific exploitation of observations from next-generation cosmological experiments. This includes CMB observations from the ground (Simons Observatory, CMB-S4) and from space (LiteBIRD), as well as galaxy surveys (Euclid), as well as their cross-correlation. We detail the activities in more detail in the following.

CMB B-mode polarization has been recognized as a unique probe of cosmic inflation and it will be the target of a large number of international experiments planned for the coming years. Their success, however, deeply relies on the exquisite control of systematic effects and astrophysical foreground contamination in the data. The same holds for other scientific targets, like neutrino masses and the effective number of relativistic degrees of freedom. As experiments from the ground and from space will feature a wide frequency coverage and an unprecedented number of detectors (up to 10^5), we will expand and optimise available tools for the simulation of systematic effects and foregrounds, and we will analyse their impact on the estimate of the cosmological parameters. Innovative algorithms and efficient HPC software solutions will be explored, including those based on GPUs.

We will develop and run different estimators for the Cosmic Birefringence (CB) effect, the in-vacuo rotation of the linear polarization plane of photons during propagation caused by parity violating EM (e.g. photon-axion coupling). The estimators can be based on CMB maps or CMB spectra. The estimators produce estimates of the isotropic rotation angle (if we consider an isotropic effect) or of the CB spectra/maps (if we consider an anisotropic effect).

We plan to continue our simulation-based study of galaxy clustering on non-linear scales, aimed at measuring both cosmological and primordial non-Gaussian parameters in different inflationary scenarios. Our current pipeline includes a joint power spectrum and bispectrum analysis and has been so far tested in real space. In the coming year, we intend to: extend the analysis to redshift space; add extra-summary statistics, which can be sensitive to higher order correlation functions (e.g. wavelets); apply the procedure to the actual analysis of BOSS data.

We are currently developing a new N-body simulation code for extended cosmologies based on the Gadget-4 code which was publicly released in 2021. This code will allow to run cosmological simulations for any model defined through the Effective Field Theory of Dark Energy formalism, also including large-scale relativistic effects by exploiting the synergy with the relativistic code Gevolution. We expect to have the first production version of this new code by the end of the year. Therefore, in 2023 we expect to be able to proceed with the first cosmological simulations of EFToDE models with this new code.

We will develop and test statistical methods for next generation CMB and LSS experiments, such as Simons Observatory, CMB-S4, LiteBIRD, Euclid, including validation phase on synthetic datasets through Monte Carlo analysis.

We will investigate models beyond LCDM with available CMB and LSS data and assess the sensitivity of future experiments. Some examples of the models of interest are: early Universe physics (inflation, non-adiabatic initial conditions, primordial magnetic fields); modified gravity; reionization; CB and generalized Faraday rotation through power spectrum analyses; decaying dark matter; neutrinos and other light relics (axions, sterile neutrinos, majorons). This activity is based on Einstein-Boltzmann codes and associated Markov Chains MonteCarlo samplers, all massively parallelized and CPU-based.

We foresee that these activities will continue to use mainly CPU-based machines, as opposed to GPUs. However, we plan to exploit computational time on GPU-based machines to explore the possibility of migrating a fraction of our codes to GPUs.

In general, as we come closer to the actual data taking stage (SO will see first light in late 2023, the first Euclid data will arrive in 2024) an increase in computing needs is expected for the coming year. Thus, our activity will likely intensify, which might lead to higher computational needs, both in terms of machine-hours and storage space (to store simulations etc). Moreover, the personnel affiliated to InDark is continuously increasing. Some of the members who have joined recently were heavily relying, in the past, on HPC resources other than CINECA. These resources will not be available to them anymore in 2024. For all these reason, it would be good to increase the currently allocated time by 25-50%.

NEUMATT

Scientific project for the year 2024
Iniziativa Specifica **NEUMATT**

NEUMATT (composed by the Ferrara, LNGS, Catania, and Pisa Units) aims to study strongly interacting matter's properties through neutron stars' complex and rich phenomenology. The main focus of the computational request is to study the effect of the EOS for nuclear matter on the gravitational signal generated by Neutron Star Mergers. The study of this effect is particular timing for the year 2024 since the LVK interferometers will be running for the whole year, and it expects that at least one event like GW170817 with a multi-messager-observation of a binary neutron star merger that will need to be interpreted to infer the properties of the EOS.

The computational resources requested are motivated to simulate the mergers of compact stars in numerical relativity and the subsequent kilonovae light curves: we aim to investigate how different models for the EoS and different astrophysical scenarios (one or two families of compact stars) affect those kind of signals. In particular, the amount of mass ejected, its entropy, and its chemical composition are key for determining the properties of the kilonovae. These simulations will include magnetic fields and (code in development) magneto-resistive effects. These simulations will be performed using the EinsteinToolkit code plus customs extensions. The code is known to scale well up to more than 16000 cores.

The typical cost of a 3D merger simulation (with magnetic fields) at the resolution 225 m (the minimum resolution required) for an evolution lasting 50 ms requires 237 GByte of allocated memory and are performed using 512/1024 cores and **200k core hours,** while the activation of magneto resistive double the CPU time needed. Higher resolution simulations require 2048 cores. We estimated the need to simulate at least 20 configurations at different resolutions. That would lead to an estimate of **4 Mcore hours** for the simulation at the best resolution. To that should be added the additional request cost of the lower resolution simulation and the development and optimization of the code. The simulation will include

- Simulations using different astrophysical scenarios for the EoS describing neutron stars including one or two families of compact stars. They aim to determine the amount of mass ejected, its entropy, and its chemical composition since they are key for determining the properties of the kilonovae.
- Study of the effect of magneto-resistive on the post-merger dynamics.

The request also aims to fulfill the need to develop the code further and do the preparatory simulation needed for performing PRACE allocation for large-scale simulations.

The request is for **6 Mcore hours** on CPU clusters (Marconi A3/Galielo100/Leonardo CPU cluster.) All the possible systems are appropriate to run the EinsteinToolkit. A small amount of 1024 node-hours is requested on GPU machines to start code porting.

Recent publications most relevant to the proposal:

1. M.Miravet-Tenés, F. L. Castillo, R. De Pietri, et all., **Phys. Rev. D** 107, 103053 (2023)
2. F. Di Clemente, A. Drago and G. Pagliara, **Astrophys.J**. 929 (2022) 1, 44.
3. K. Franceschetti, ed all.. **Universe. 8**. 172. 10.3390/universe8030172 (2022).
4. R. De Pietri, A. Drago, A. Feo, G. Pagliara, M. Pasquali, S. Traversi, G. Wiktorowicz, **Astrophys.J.** 881 (2019) 2, 122.

TEONGRAV

TEONGRAV needs HPC resources for the following projects:

1. Numerical Relativity Simulations of Compact Binary Mergers: we will use the publicly available Einstein Toolkit code to run simulations of compact binary mergers, neutron stars (NSs) and black holes (BHs), in order to study their gravitational wave (GW) and electromagnetic (EM) emission. The Einstein Toolkit uses a hybrid parallelization approach (OpenMP and MPI). The toolkit has been already used on Marconi A3 and Galileo 100 at CINECA. A new version of the toolkit able to run on GPUs is currently being developed, but it is not yet ready for production runs.

2. Numerical Relativity Simulations of Black Hole Mergers Beyond General Relativity: We will simulate the gravitational collapse of fundamental fields and BH mergers in motivated extensions of General Relativity both within an effective field theory approach and at the fully nonperturbative level. In both cases we shall use codes developed in the Einstein Toolkit and in GRChombo, as well as domestic codes.

3. Bayesian parameter estimation with Markov chain Monte Carlo: We shall perform Bayesian inference of single GW events and population studies, both to study parameter estimation and waveform systematics, and also to assess whether current and future GW detectors can infer the properties of multiple formation channels for BH binaries. We will use the BILBY and pyCBC infrastructures.

4. *N*-body simulation of stellar clusters to investigate the formation channels of compact binary mergers: We will simulate the evolution of massive stellar clusters (1e5-1e6 Msun) to study the formation of compact binary mergers in such dense environments. We will use the state-of-the-art code PETAR, a high-performance code that exploits hybrid parallelization methods (MPI, OpenMP, GPU), coupled with the single and binary population synthesis codes MOBSE and SEVN. In parallel, we will use the MPI hydrodynamic code RAMSES to simulate star-forming regions and generate more realistic conditions for the *N*-body simulations.

5. Hydrodynamical simulation of massive star mergers: We will perform simulations of massive star mergers to investigate the formation of BHs in the so-called BH upper mass gap (52-150 Msun). We will use the hydrodynamic code STARSMASHER exploiting both the MPI and GPU parallelization.

6. Special relativistic MHD simulations of short GRB jets: We will use the PLUTO code to investigate the propagation of jets across realistic NS-NS post-merger environments, with the ultimate goal of connecting our models with short GRB observations. We already tested our simulations on the CINECA clusters Marconi and Galileo100. A GPU version of PLUTO is currently under development, our simulations are for now only CPU-based.

7. Hydrodynamical simulations of Massive Black Hole formation and evolution: We will employ the public code GIZMO to study the formation and evolution of massive BHs in the cosmological context, to study in detail potential GW sources for LISA and ET. We will investigate the conditions under which these objects form and how they evolve and pair in binaries. GIZMO has been used on the Galileo100 and Marconi CINECA clusters, and is fully parallelised with MPI and OpenMP, but no GPU parallelisation is present at the moment.

BIOPHYS

The INF23_biophys project (coordinator Giovanni La Penna) collects the activity of 7 groups involved in high-performance computing in the field of biophysics. Below the list and the actual PIs:

- University of Roma Tor Vergata (UNITOV), Velia Minicozzi;
- Politecnico of Torino (POLITO), Andrea Gamba;
- University of Torino (UNITO), Michele Caselle;
- University of Trento (UNITN), Luca Tubiana;
- University of Napoli (UNINA), Mario Nicodemi;
- Scuola Normale Superiore of Pisa (SNS), Giuseppe Brancato;
- University of Milano (UNIMI), Guido Tiana;

Each group applies original and advanced computational methods, all requiring HPC resources, to different scales relevant to biology: macromolecules described as atoms; coarse grained models; crowded environments; networks. Methods range from quantum mechanics, atomic interactions, polymer physics, network science, machine learning, and extended cutting-edge statistical methods.

Below is a short summary of some of the activities that will be continued in year 2024.

UNITOV - Development and application of computational methods (mainly generalized statistical ensembles) to determine the structure and the dynamics of biologically relevant molecules. We use molecular dynamics at different space and time scales, based on classical and first principles models, all requiring massive HPC resources. We analyse experimental results obtained exploiting large scale facilities such as synchrotrons and free electron lasers (FEL).

POLITO - We use a computational model that we have recently introduced to model region/activity localization in eukaryotic cells, based on the idea that protein sorting naturally emerges from the combination of spontaneous molecular aggregation with vesicle nucleation. We take into account the effects of molecular crowding to understand how the efficiency of sorting may depend on the number of molecular species involved. This task is performed by extensive numerical simulations of the model for varying numbers of molecular species and values of control parameters using parallelized computer code.

UNITO - We apply topic modelling techniques for the identification of cancer subtypes, extending a specific class of topic models to allow a multi-omics approach. We are able to clearly distinguish healthy from tumour samples as well as the different cancer subtypes. The integration of different layers of information is crucial for the observed classification accuracy. Our approach naturally provides the genes and the microRNAs associated to the specific topics that are used for sample organization.

UNINA - We develop polymer models to study the three-dimensional (3D) organization of DNA and its temporal dynamics. In particular, we investigate the physical mechanisms (e.g. phase separation or polymer adsorption) that shape chromosome structure and control genome activity. The research will use massive parallel molecular dynamics simulations, machine learning methods and analyses of public genomic databases.

SNS - Research activities are focused on the development and application of numerical simulation methods for modeling complex macromolecular systems of biological interest through the use of various HPC resources and facilities. In particular, we will investigate the structural and dynamic properties of voltage-gated ion channels and the effects of some pathogenic mutations causing their dysfunction.

ENESMA

Project description

1 Turbulent hemodynamics

The main objective of the project is to carry out a direct numerical simulation of the whole cardiac hemodynamics, solving up to the smallest fluid dynamics spatial scale ($\sim 40\mu$m) and investigate the transitional nature of the impulsive jets originated by the chambers contraction, namely aortic, mitral, tricuspid and pulmonary jets. We will consider the case of a healthy heart with an ejection fraction of about 65% beating at 70 bpm, the experience of the group in the cardiac modelling will ensure a fast start of the project. This is also a preliminary step before investigating pathologic cases.
The hemodynamics within the whole human heart will be solved using a multi–physics computational approach capable of tackling the electrophysiology, the elasto–mechanics and the fluid dynamics of the heart, along with their multi–way coupled interactions. The developed tool embodies accuracy, versatility and computational efficiency, thus allowing cardiovascular simulations in realistic conditions and it has been developed and validated by our group through comparisons with the literature, ad–hoc experiments and clinical data in a sequence of papers, see [1,2,3].

The pulsatile and transitional character of the hemodynamics is obtained by solving directly the incompressible Navier–Stokes equations using a staggered finite differences method. All spatial derivatives are discretized by central second–order accurate finite-difference schemes including the nonlinear terms and the time advancement of the solution is obtained by a low storage 3rd–order Runge-Kutta scheme. The nonlinear terms are treated explicitly, while the viscous terms are computed implicitly (or explicitly with a small time step so that the stability constraints of the viscous terms and the CFL condition for the non-linear terms are both satisfied). The elliptic equation for pressure is solved using a combination of FFTs, implemented using serial FFTW and the serial tridiagonal solver from LAPACK. Finally, all I/O larger than writing short plain text log-files is done using parallel HDF5. The parallelization of the Navier–Stokes solver is based on a domain decomposition where the Cartesian domain is split into slabs. According to this 'one-dimensional slab' parallelisation, each processor needs to store information from the neighbouring processors that is required for computing the derivatives in what is called a 'halo/ghost' layer and since the flow solver employs a second-order finite difference spatial discretisation at most one halo layer is required on each side of a slab. All the simulations will be carried out using our in–house multi–physics solver, which has been GPU accelerated using CUDA Fortran with an extensive use of CUF kernel directories that automatically run single and nested loops on the GPU device without modifying the original CPU code.

The code is complemented with various immersed boundary (IB) techniques to handle complex moving and deforming geometries. The structural mechanics is based on the Fedosov's interaction potential method [1] to account for the mechanical properties of the biological tissues, which are anisotropic and nonlinear. The electrophysiology, responsible for the active potential propagation in the cardiac tissue triggering the active muscular tension, is incorporated by means of a bidomain model [3] that can account for the different cellular models of the various portions of the heart. All these models are three–way coupled with each other, thus capturing the fully synergistic physics of the heart.

Essential bibliography

[1] Viola, F., Meschini, V., & Verzicco, R. (2020). Fluid-Structure-Electrophysiology interaction (FSEI) in the left-heart: a multi-way coupled computational model. European Journal of Mechanics-B/Fluids, 79, 212-232.

[2] Viola, F., Spandan, V., Meschini, V., Romero, J., Fatica, M., de Tullio, M. D., & Verzicco, R. (2022). FSEI-GPU: GPU accelerated simulations of the fluid-structure-electrophysiology interaction in the left heart. Computer physics communications, 273, 108248.

[3] Del Corso, G., Verzicco, R., & Viola, F. (2022). A fast computational model for the electrophysiology of the whole human heart. Journal of Computational Physics, 457, 111084.

FIELDTURB

The FIELDTURB initiative will address different topics with high performance computing.

1. The activity will address the question on how soaring birds exploit thermal plumes in the atmosphere to search for prey or migrate across large distances. The landscape of convective currents is rugged and shifts on timescales of a few minutes as thermals constantly form, disintegrate or are transported away by the wind. The analysis will be based on Large-Eddy Simulations of the turbulent atmospheric boundary layer in the fully convective regime. How soaring birds find and navigate thermals within this complex landscape has been the subject of a recent investigation exploiting the reinforcement learning (RL) technique. Our plan is to perform state-of-the-art LES simulations in synergy with RL techniques to identify optimal strategies to exploit thermals to migrate across large distances while minimizing energy consumption. The RL runs will be done on Leonardo and Leonardo 100 being demanding in terms of computational effort.

2. Phase transition, topological defects in active systems: Here we study the collective behavior of active particles by large scale Molecular Dynamics simulations of Active Brownian particle (ABP). We are interested in studying the role of defects in the topological transitions in ABP, and the effect, at the collective level, of the diffusion properties of clusters of active particles.

3. Modeling of self-propelled droplets and liquid crystals in the presence of external fields and chirality: The interplay between topological defects and flow becomes particularly relevant when complex and active fluids are geometrically confined. We apply multiphase mesoscopic 3D Lattice Boltzmann approaches to study (i) 3D chiral liquid crystal shells where the director field stabilizes helicoidal patterns and high-energy excitations, such as skyrmions. By adding an active stress in models for multicomponent droplets, we also study the emergence of self-propelled directed motion due to the coupling between induced flow and topological defects depending on specific anchoring.

4. The resources will enable the development and testing of novel deep learning models for (i) physics inference, (ii) data assimilation, and (iii) super-resolution of high-resolution 2D and 3D Eulerian configurations of complex flows. We will also investigate the Lagrangian problems of (i) prediction of extreme events (ii) data generation of 3D particle trajectories.

5. 2D and 3D Navier-Stokes turbulence in the presence of microswimmers which force and interact with the flow will be simulated. The goal is to understand how microswimmers can affect the small scale properties of the flow and in particular the intensity and the direction of the energy cascade.

6. We also plan to simulate the 2D Navier Stokes to check the presence of hidden symmetries in the inertial range of a passive scalar advected by the flow, for which we need high-resolution simulations up to 16384^2 grid points.

MONSTRE

MONSTRE:

MOdeling Nuclear STructure and REactions

Our project aims to establish a comprehensive and integrated framework for the study of atomic nuclei, nuclear reactions, and strongly interacting matter. The synergistic efforts of the various units, based on their complementary expertise in advanced many- body and computational methods, will be devoted to the study of complex nuclear phenomena occurring at different scales of energy and size. Modern ab initio techniques will be refined and applied making use of microscopic interactions, derived from nuclear effective field theories. Density functionals will be developed using ab initio and/or phenomenogical constraints and applied to the calculation of bulk, spectroscopic, and decay properties of finite nuclei throughout the whole nuclear chart, Collective modes will be studied making use of many body techniques including beyond mean-field correlations. The consistent merging of structure and reaction theories will offer the opportunity to directly compare theoretical calculations with empirical data for nuclear systems under extreme conditions, also deriving microscopic optical potentials. These investigations will also be performed by developing mathematical methods, quantum computing-based algorithms and machine learning techniques specifically tailored for the study of the nuclear many-body problem. Special attention will be devoted to the current experimental projects related to the production of rare isotopes, dark-matter detection, and the physics of electroweak interactions, including neutrino physics and double-beta decay. Combined astrophysical and terrestrial constraints, together with predictions based on state-of- the-art models, will be employed to achieve an improved, multi-faceted understanding of the nuclear equation of state.

Examples of HPC applications

SHELL model calculations

The KSHELL code, massively employed in shell-model calculations, can easily run on a Linux PC with a many-core CPU and OpenMP library, as well as on a state-of-the-art massive parallel computer with hybrid MPI+OpenMP parallel programming. It exhibits a strong scaling of the parallel computation tested on different HPC systems, included the CINECA Marconi and Galileo100 clusters. In order to store the calculated wavefunctions for all the systems we plan to calculate we need about 1Tb of storage. All the libraries needed are already installed on the CINECA machines.

RPA−based calculations

The nuclear response of atomic nuclei is calculated by using the QRPA approach for deformed systems and the Second RPA for spherical ones. From a computational point of view, the most demanding operations required these calculations are the evaluation of the matrix elements to be diagonalized and the diagonalization of the corresponding eigenvalue problem. The dimensions of the matrices are of the order of $10^7 - 10^9$. PETSC/SLEPC libraries are employed to handle the matrices and for their diagonalization, using the MPI parallel protocol. These libraries are already available on the CINECA infrastracture. The typical storage needed is of the order of 500 Gb.

Quantum Monte Carlo calculations

Nuclear structure calculations are performed using two distinct methods: the Configuration Interaction Monte Carlo code is allows for efficient parallel execution, through MPI, with up to a few hundred cores but we are planning to add also a layer parallelized using OpenMP to allow the code to scale to larger allocations; the Variational Monte Carlo calculations using Network Quantum States are instead based on the NetKet code which is designed to use GPU systems through JAX. At the moment typical simulations involve a single GPU node at a time. For both simulations the typical storage is in the hundreds of Gb.

NUCSYS

Iniziativa Specifica NUCSYS
Nuclear Systems
Attività di ricerca in HPC per il 2024

Lo scopo del progetto NUCSYS è quello di studiare la struttura e la dinamica di sistemi nucleari, in maniera unificata partendo dall'interazione microscopica tra i nucleoni (a due corpi ed a tre corpi). In particolare, si vogliono studiare le reazioni tra pochi nucleoni, l'interazione tra elettroni e neutrini di alta energia con nuclei, la struttura di nuclei medio-pesanti, e decadimenti e transizioni nei nuclei (decadimento gamma, beta e doppio beta, ecc.)

Da notare che dal 2024 il gruppo che si occupa di calcoli di Large Scale Shell-Model (LSSM), fino al 2023 nell'I.S. MONSTRE, si unira' all'I.S. NUCSYS. Poiche' molto del tempo CINECA allocato a MONSTRE veniva usato da questo gruppo, le richieste di NUCSYS per il 2024 sono state maggiorate considerando circa il 70% di quello del 2023 assegnato a MOSNTRE.

In dettaglio, durante l’anno 2024, progetti di studio che faranno uso pesantemente delle risorse HPC del CINECA saranno:

• Sudio di reazioni di fusione di interesse astrofisico e per la produzione di energia, in particolare la deutone-trizio, deutone-3He, e deutone-4He. A tale scopo, si intende sviluppare nuovi codici che utilizzano le GPU per il calcolo degli elementi di matrice necessari.

• Calcolo degli elementi di matrice nucleari di interesse per esperimenti con sonde elettrodeboli (p.e. doppio decadimento beta senza emissione di neutrini) mediante la realizzazione di calcoli di LSSM.

QFTATCOL

The Project (Iniziativa Specifica) QFT@Colliders deals with the application of Quantum Field Theory techniques to the phenomenology of present and future colliders. Important searches and experimental measurements, at modern particle accelerators at energy and intensity frontiers, require the calculation of higher-order corrections to a variety of scattering processes in gauge theories of fundamental interactions. Moreover, such calculations must be available in the form of Monte Carlo event generators, in order to allow for a systematic and meaningful comparison between data and theory. An increasing level of theoretical precision is required to fully exploit the high quality of future data collected at the LHC and high-intensity e^+e^- machines. Many new physics signals are obscured by large Standard Model (SM) backgrounds: improving the accuracy of the modelling of such backgrounds is of crucial importance to explore possible regions of model parameter space, where only an excess over SM expectations and not a clearly standing resonance is expected. In addition, the study of the properties of newly discovered particles requires the availability of precise simulation tools. Precision measurements, in combination with accurate theoretical predictions, may open the way to the detection of fundamental physics phenomena not yet discovered, even if the present lack of clear direct new physics signals will persist at the LHC. Furthermore, the synergy between the research at the energy and intensity frontiers may allow to deeply probe the SM and eventually unravel the existence of new physics beyond it.

This ambitious theoretical program needs computational resources, which are usually CPU intensive, for code development, validation and physics studies. This is even more true because of the increasing accuracy of the Monte Carlo tools, which now aims at reaching QCD/EW NNLO accuracy matched with Parton Showers for a growing number of scattering processes.

The Monte Carlo codes which will exploit the resources are well know tools in the communitiy of high energy phenomenology, such as `GenEva` [1], `POWHEG BOX` [2], `MadGraph5_aMC@NLO` [3], `Mesmer` [4], `BabaYaga@NLO` [5] and possibly more.

References

[1] `stash.desy.de/projects/GENEVA/repos/geneva-public/`

[2] `powhegbox.mib.infn.it/`

[3] `madgraph.phys.ucl.ac.be/index.html`

[4] `github.com/cm-cc/mesmer/`

[5] `wwww.pv.infn.it/~hepcomplex/babayaga.html`

LINCOLN

Research Unit: LINCOLN (group IV, CSN4), Perugia Section.

Associated researchers: 9 people, 7.7FTE
Brodoloni Luca (PhD student, Unicam, 100%), Cantori Simone (PhD student, Unicam, 100%), Costa Emanuele (PhD student, Unicam, 100%), Di Patti Francesca (RTDB, UniPG, 100%), Mancini Stefano (PO, Unicam, 20%), Marini Bettolo Marconi Umberto (Senior associate, 50%), Midei Giovanni (PhD student, Unicam, 100%), Pilati Sebastiano (PhD student, Unicam, 100%, loc. resp.), Scriva Giuseppe (PhD student, Unicam, 100%).

Project title: *Neural Monte Carlo simulations of disordered Rydberg-atom arrays*

Project description: The experiments performed with Rydberg atoms trapped in arrays of optical tweezers represent one of the most promising platforms to perform quantum simulations and, in the long term, to implement scalable quantum computations. Interestingly, the optical tweezers used to trap individual atoms can be displaced essentially at will. This paves the way to exploring disordered lattices, which might host intriguing quantum spin-glass phases.
In recent years, the Camerino Unit has developed self-learning projective quantum Monte Carlo (QMC) algorithms to simulate random spin models [1]. These algorithms are suitable for providing unbiased predictions to guide the explorations of spin-glass physics in Rydberg-atom experiments. Notably, these QMC methods exploit neural networks as guiding variational phase functions. As our preliminary tests demonstrate, this allows them to flexibly address distinct phases of matter, including spin-glass phases. Still, the study of spin-glass models requires averaging over large ensembles of different (random) realizations of the disorder. This significantly increases computational demands.

Our QMC codes exploit shared memory parallelism, implemented via automatic loop parallelization in NUMBA, to propagate the population of random walkers needed in projective QMC algorithms. Furthermore, ensemble averaging can be distributed over different cores and/or nodes, with virtually no data communication. We implemented this job-farming protocol via MPI4PY. Overall, our simulations exploit hybrid OPENMP-MPI parallelism, and efficiently scale on multicore-multinode CPU clusters. Furthermore, we plan to train deep neural networks, implemented in PYTORCH, to perform supervised learning of quantum many-body systems, following a growing research line on which our Unit is continually active [2]. Therefore, we are also requesting a smaller amount of compute time on a GPU cluster.

Requests of HPC resources for 2024:
- CPU cluster [MARCONI-A3, or GALILEO100, or LEONARDO (CPU cluster)]: 750,000 core hours.
- GPU cluster [LEONARDO (GPU cluster)]: 7,000 GPU hours.

Note: in case it is possible to access the HPC resources already in late 2023, this would be quite helpful.

References:

[1] S. Pilati, E. M. Inack, P. Pieri, *Self-learning projective quantum Monte Carlo simulations guided by restricted Boltzmann machines*, Physical Review E **100**, 043301 (2019).
[2] S. Cantori, D. Vitali, S. Pilati, *Supervised learning of random quantum circuits via scalable neural networks*, Quantum Science and Technology **8**, 025022 (2023).

NEMESYS

Time2Quest [CINECA HPC Resources - Research Program]

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As expressed in its project proposal, the specific initiative **Time2Quest** aims at exploring highly demanding computational strategies to unravel excited state properties, collective excitations, transport phenomena and other many-body effects in low dimensional systems of uttermost importance for quantum information processing. The requested CPU hours are needed to progress towards the microscopic understanding of the electronic and optical properties of reliable platforms made of two-dimensional materials, which appears to be suitable for isolating, controlling, and coherently manipulating quantum particles that behave like qubits. Indeed, due to the `naked' nature to the environment of their electronic states and low dielectric screening, emergent quantum phenomena are theoretically predicted and experimentally observed. Moreover, they are promising candidates for novel electronic and opto-electronic devices from quantum technologies to energy saving and production. Specifically, the main focus will be on graphene-like, chalcogen-based, and Kagome-like systems that have shown enhanced many-body effects, expressed in terms of exotic quasi-particles and excitons.

For the ground-state and electronic structure simulations we plan to use density functional theory (DFT) codes like **Abinit** and/or **Quantum-ESPRESSO**. Many-body perturbation theory (MBPT) calculations will be mainly run via the **Yambo** code. All the above-mentioned packages are well configured and parallelized in the Marconi, Galileo 100, and Leonardo clusters of the CINECA consortium. It is also worthwhile noticing that MP from the RM@ unit is a member of the developer/superuser team of YAMBO. We also plan to use specific MBPT and time-dependent density functional theory (TDDFT) codes developed with the CS and RM2 units of the present IS.

DFT will provide geometries and Kohn-Sham (KS) electronic structures using local/semi-local forms for the exchange-correlation functional. Quantitatively correct electronic structures will be computed by performing many body GW calculations and the use of less expensive, hybrid xc-functionals will be tested. Excitonic optical properties will be calculated within linear response theory, by solving the many body Bethe-Salpeter Equation (BSE). This method provides a deep analysis of (intra- and inter-) excitons (energies, spatial localization, weights in terms of single-particle states). Momentum forbidden and spin forbidden excitons which are crucial to understand exciton dynamics after light-excitation, will be also characterized. Exciton radiative lifetimes will be estimated by applying by using a fully ab-initio method developed by MP and collaborators. Non-radiative lifetimes (electron-electron/phonon interactions) can be estimated from the spectral width of the self-energy in the particle and hole sector, by employing recent advances in electron-phonon scattering computations. Due to the modulation of the opto-electronic properties from the number of layers, we will address not only monolayer but also multilayer forms with a particular focus on homo and hetero-bilayers, where twisting angle has been demonstrated recently to be a further degree of freedom to play with.

The DFT step requires moderate computational resources, being essentially a self-consistent one-particle approach. On the other hand, the TDDFT, GW, BSE and, in general, MBPT steps are highly demanding, and can be efficiently run only on HPC resources. The requested CPU time can be barely used to set up one of the applications proposed in the research program of the present IS for 2024.

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