Report CRESCO 2022

Beatrice Calosso

22 Febbraio 2024

Contents

Riduci zoom

ENEA
Italian National Agency for New Technologies,
Energy and Sustainable Economic Development

1. Cresco report 2022 overview

Number of papers:	33 (2021) - **30 (2022)**
Total number of authors:	156 (2021) - **117 (2022)**

High Performance Computing on CRESCO infrastructure: research activity and results 2022

December 2023

On-line web edition available at:
www.pubblicazioni.enea.it/le-pubblicazioni-enea/edizioni-enea/anno-2023

Contributions provided by a selection of users of the CRESCO infrastructure

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ENEA, TERIN-ICT-HPC

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ENEA, TERIN-ICT

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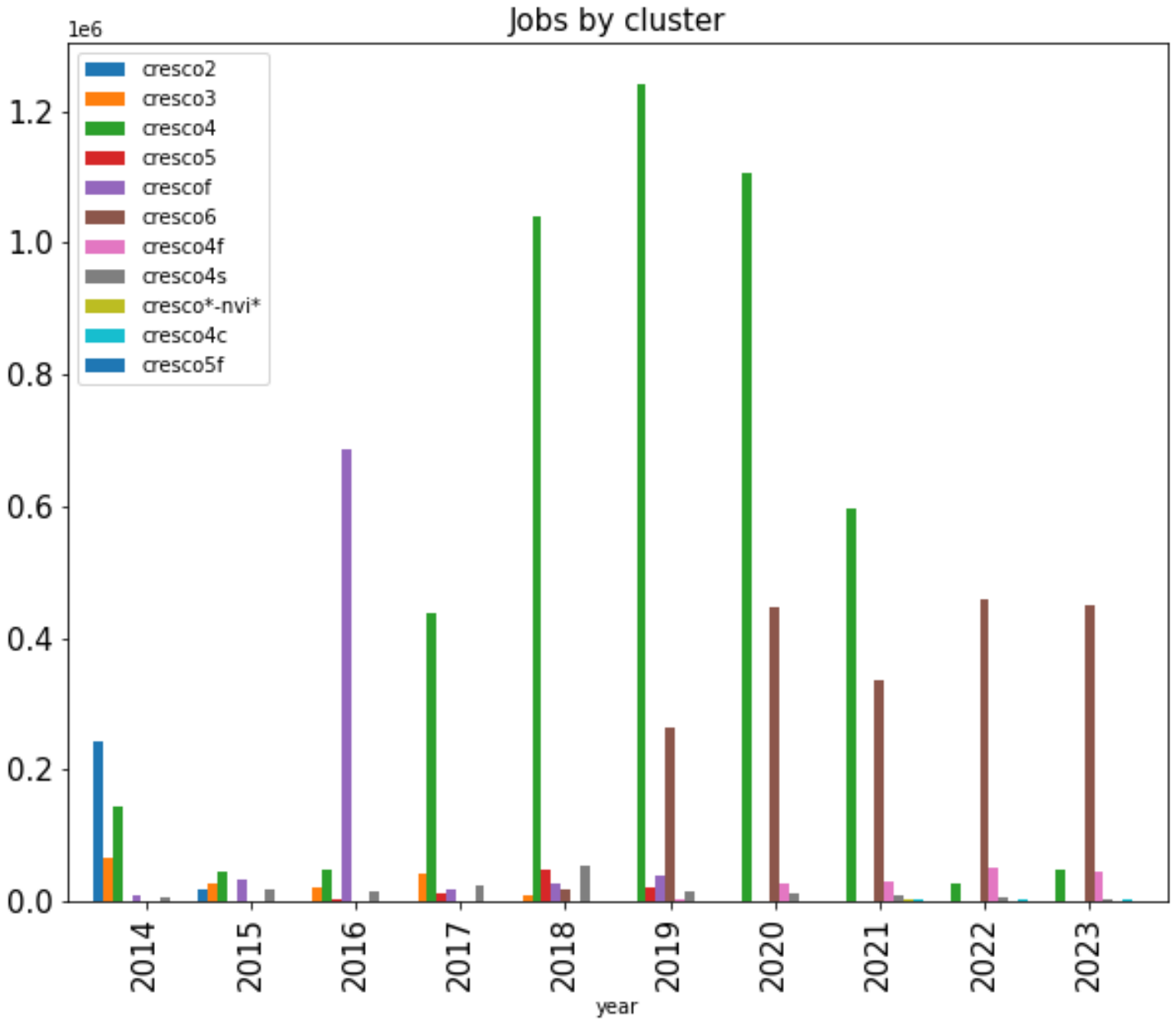
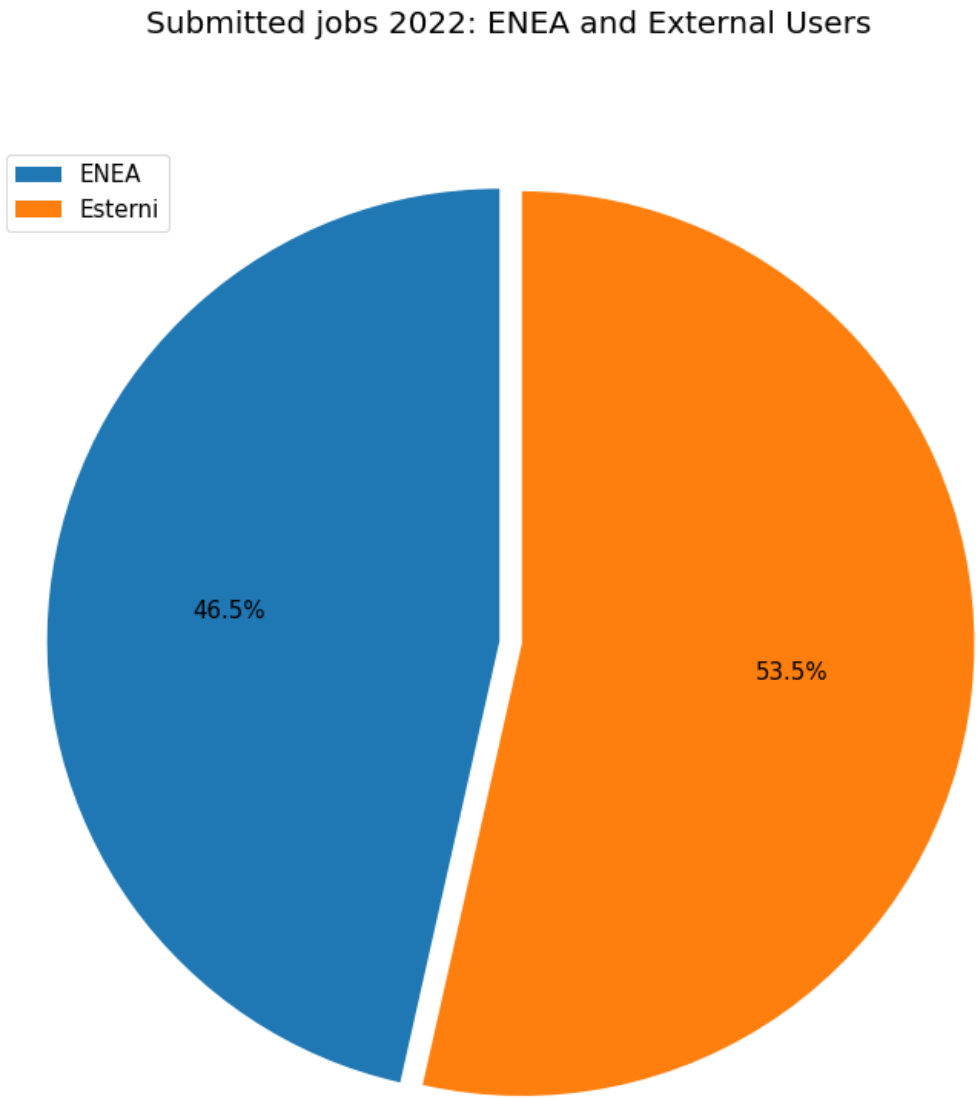
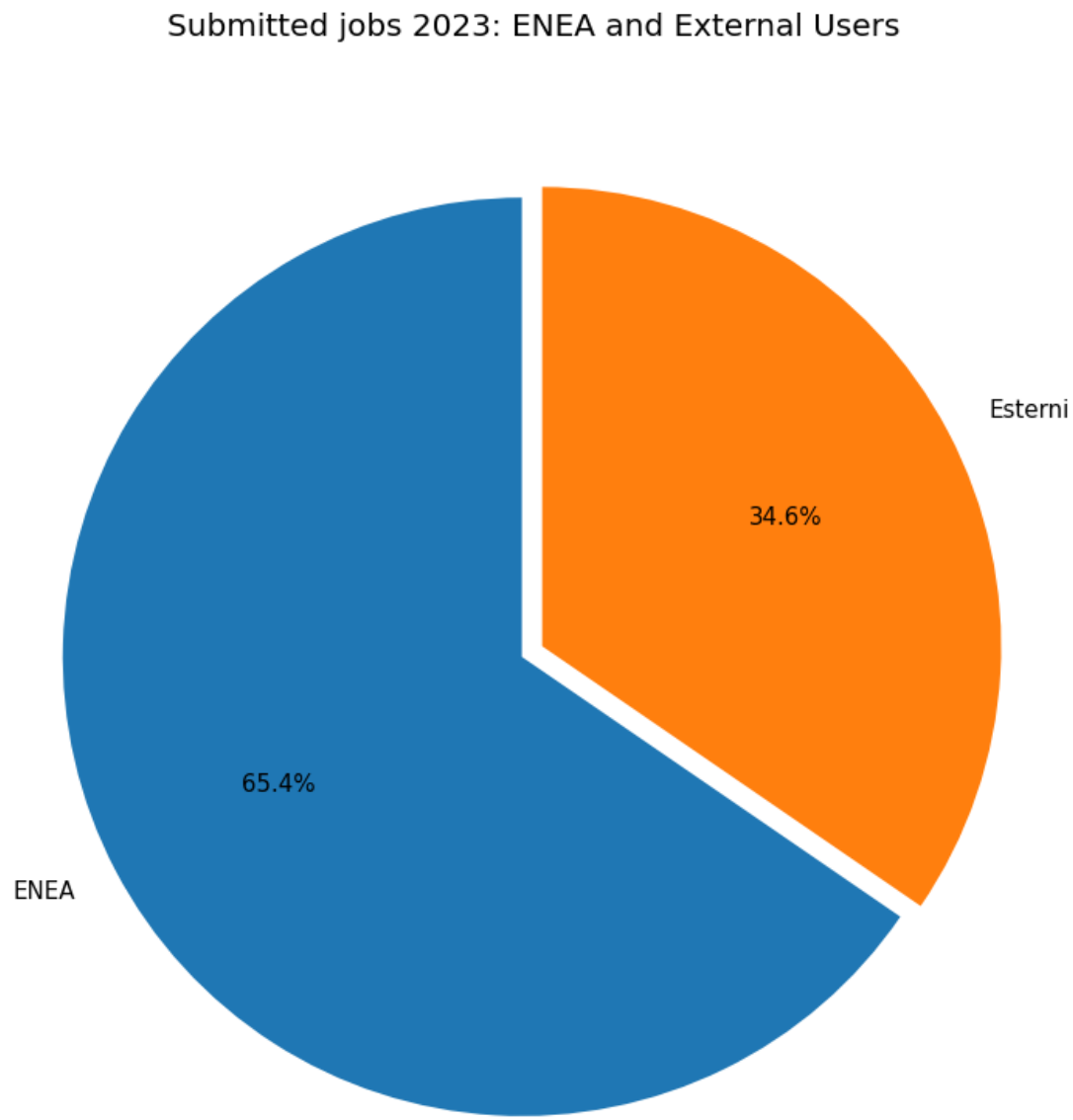
2. CRESCO jobs in details



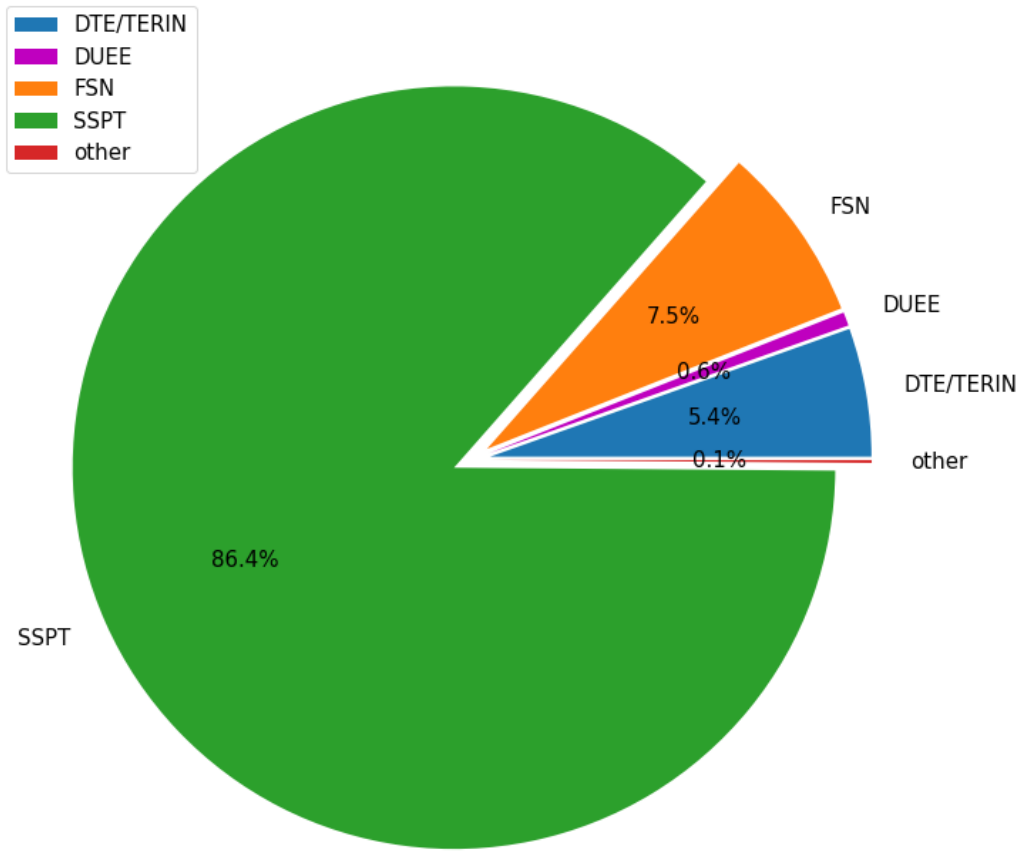
CRESCO6

CRESCO4

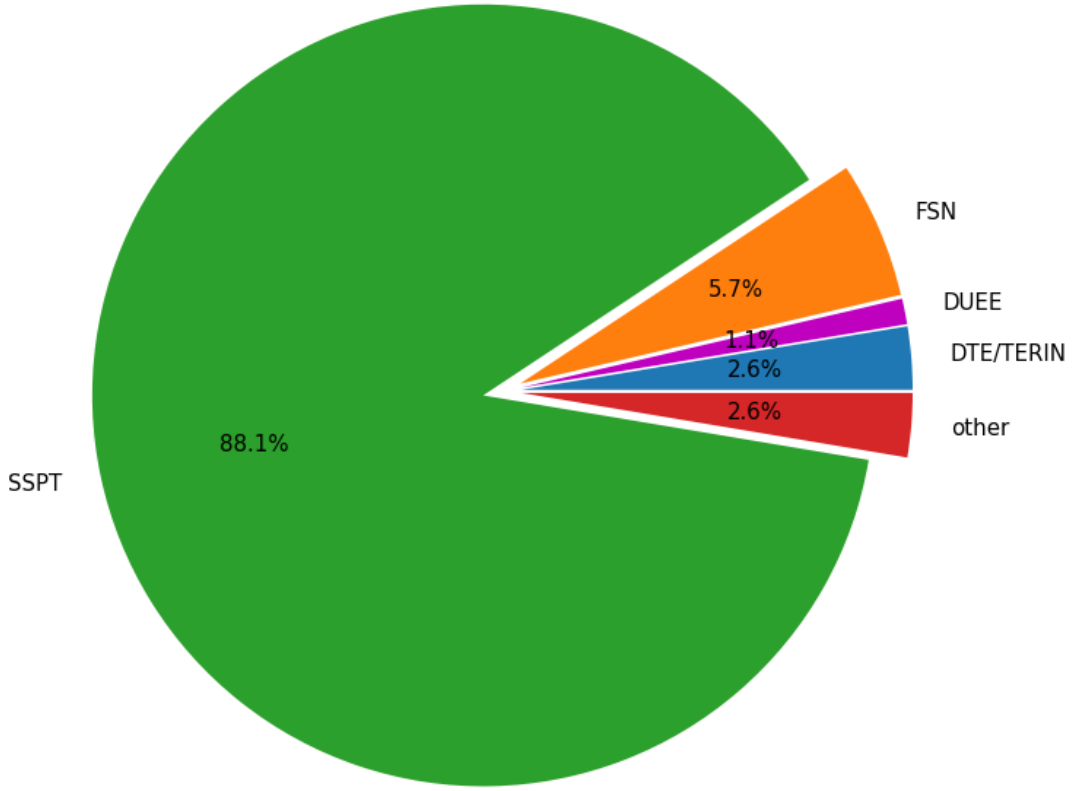

Submitted jobs 2022: ENEA and External Users
ENEA
Esterni
46.5%
53.5%

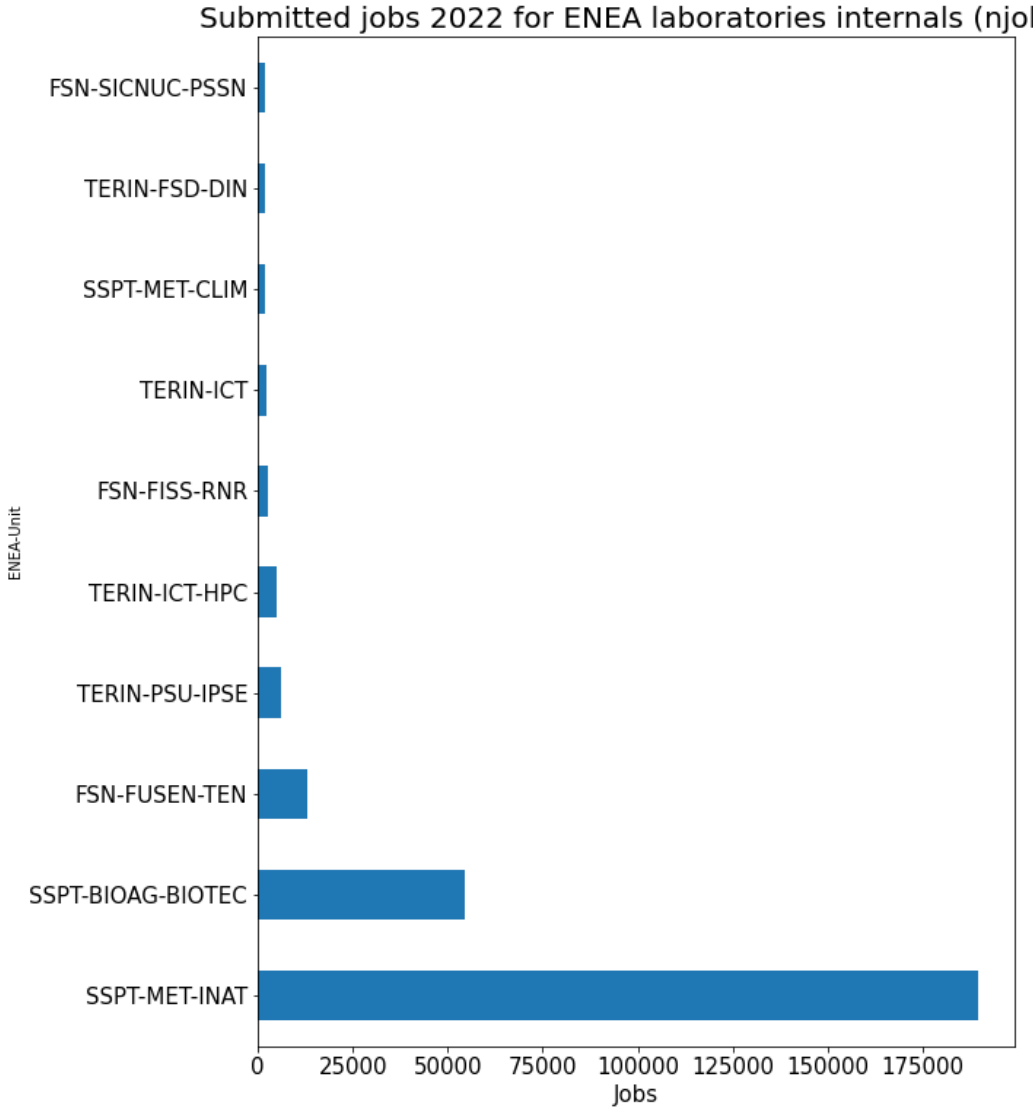

Submitted jobs 2023: ENEA and External Users
Esterni
34.6%
65.4%
ENEA

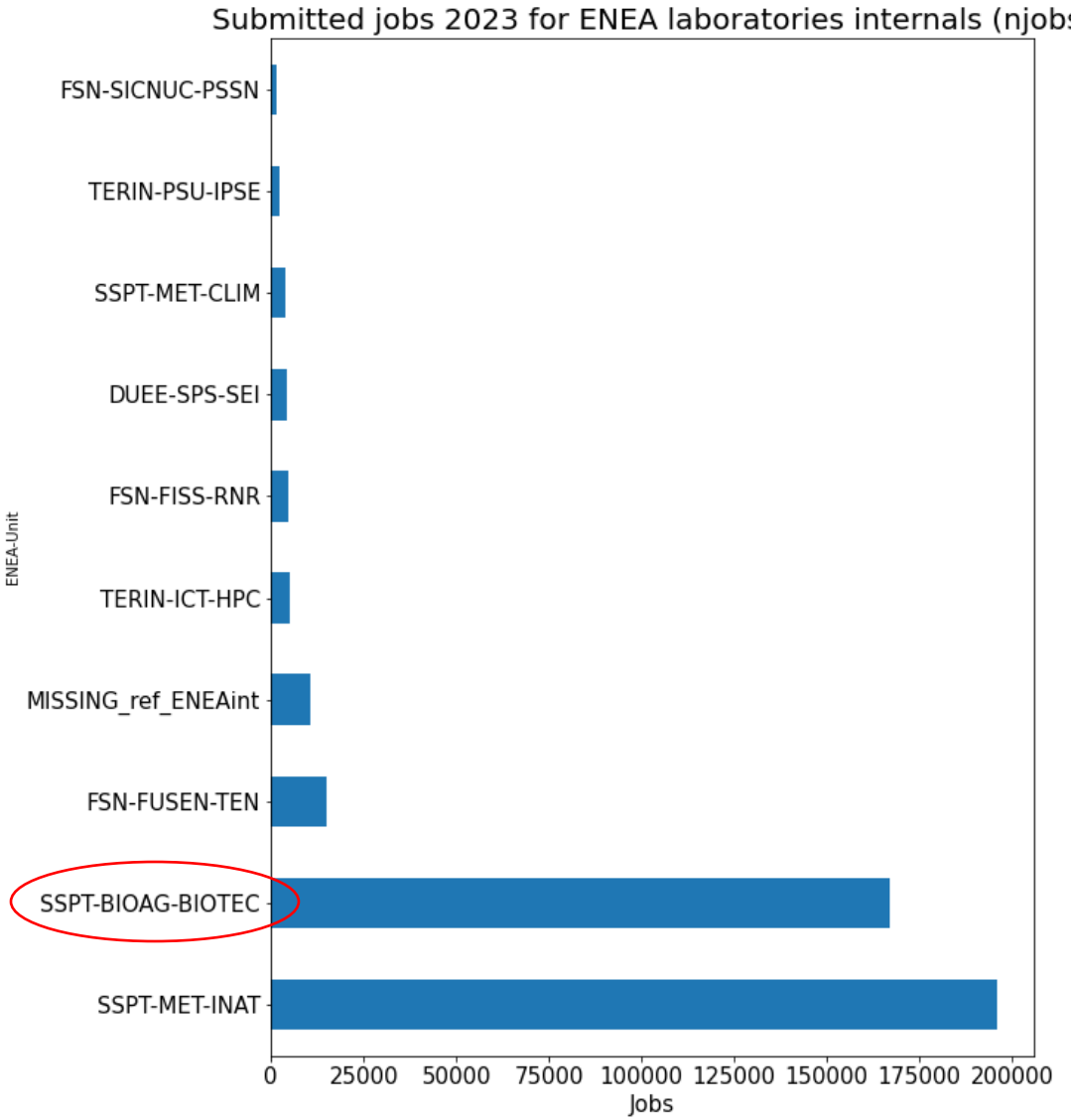
Jobs 2022 for ENEA department internals (njobs)



Jobs 2023 for ENEA department internals (njobs)




Submitted jobs 2022 for ENEA laboratories internals (njobs)
ENEA-Unit
FSN-SICNUC-PSSN
TERIN-FSD-DIN
SSPT-MET-CLIM
TERIN-ICT
FSN-FISS-RNR
TERIN-ICT-HPC
TERIN-PSU-IPSE
FSN-FUSEN-TEN
SSPT-BIOAG-BIOTEC
SSPT-MET-INAT
0
25000
50000
75000
100000
125000
150000
175000
Jobs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ENEA-Unit
FSN-SICNUC-PSSN
TERIN-PSU-IPSE
SSPT-MET-CLIM
DUEE-SPS-SEI
FSN-FISS-RNR
TERIN-ICT-HPC
MISSING_ref_ENEAint
FSN-FUSEN-TEN
SSPT-BIOAG-BIOTEC
SSPT-MET-INAT
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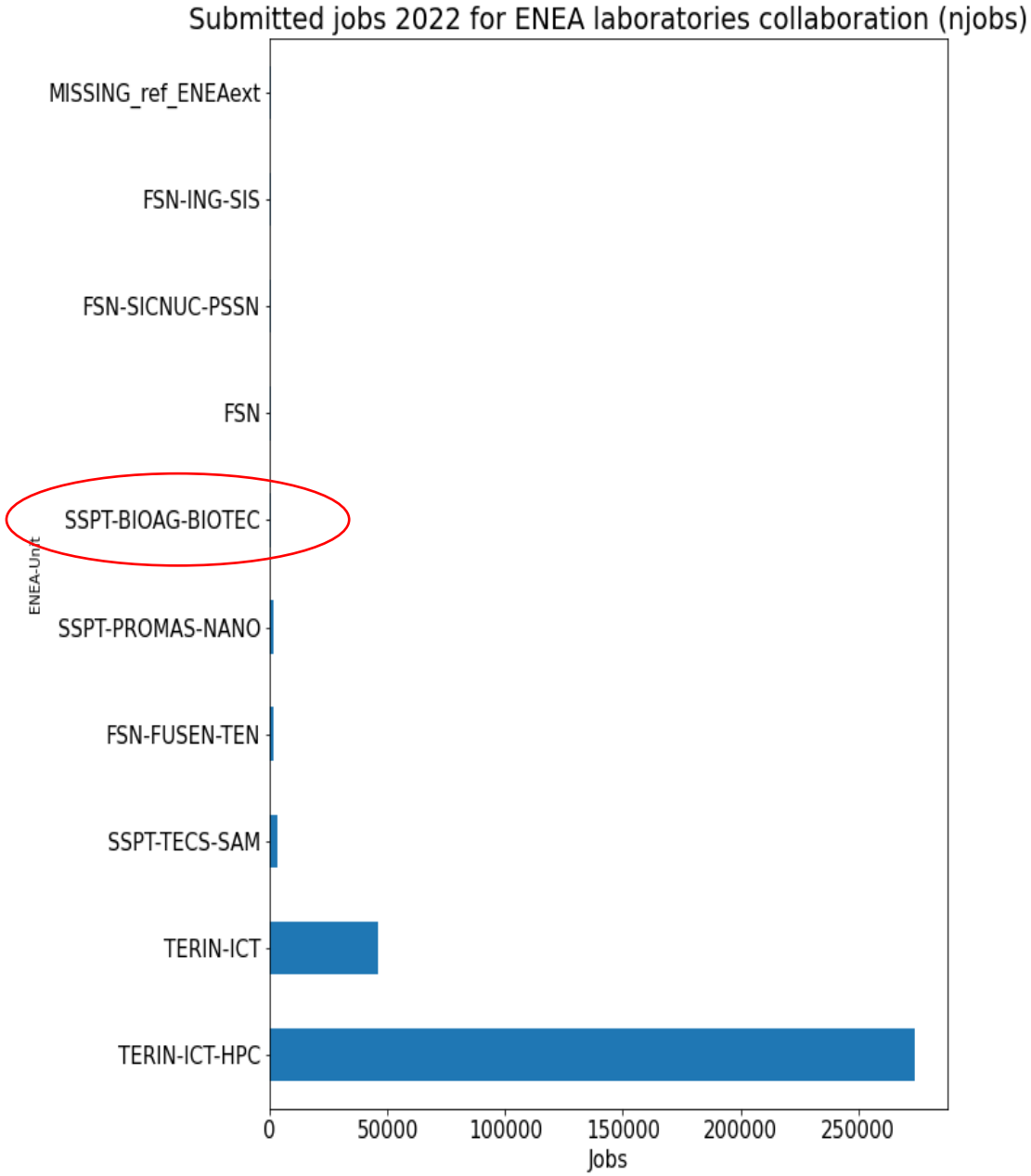
25000
50000
75000
100000
125000
150000
175000
200000
Jobs


Submitted jobs 2022 for ENEA laboratories collaboration (njobs)
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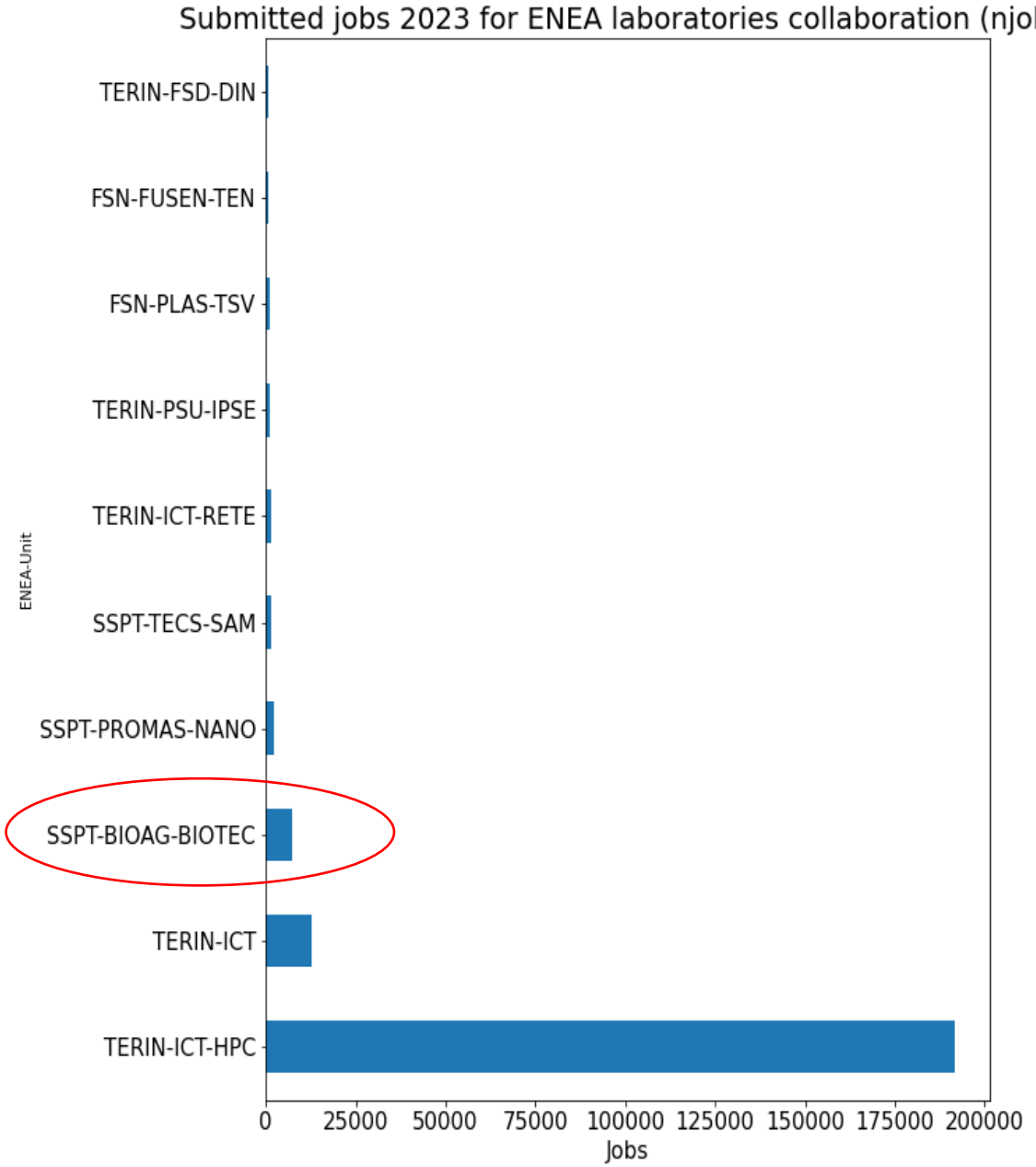
FSN-ING-SIS
FSN-SICNUC-PSSN
FSN
SSPT-BIOAG-BIOTEC
SSPT-PROMAS-NANO
FSN-FUSEN-TEN
SSPT-TECS-SAM
TERIN-ICT
TERIN-ICT-HPC
ENEA-Unit
0
50000
100000
150000
200000
250000
Jobs


Submitted jobs 2023 for ENEA laboratories collaboration (njobs)
TERIN-FSD-DIN
FSN-FUSEN-TEN
FSN-PLAS-TSV
TERIN-PSU-IPSE
TERIN-ICT-RETE
SSPT-TECS-SAM
SSPT-PROMAS-NANO
SSPT-BIOAG-BIOTEC
TERIN-ICT
TERIN-ICT-HPC
ENEA-Unit
0
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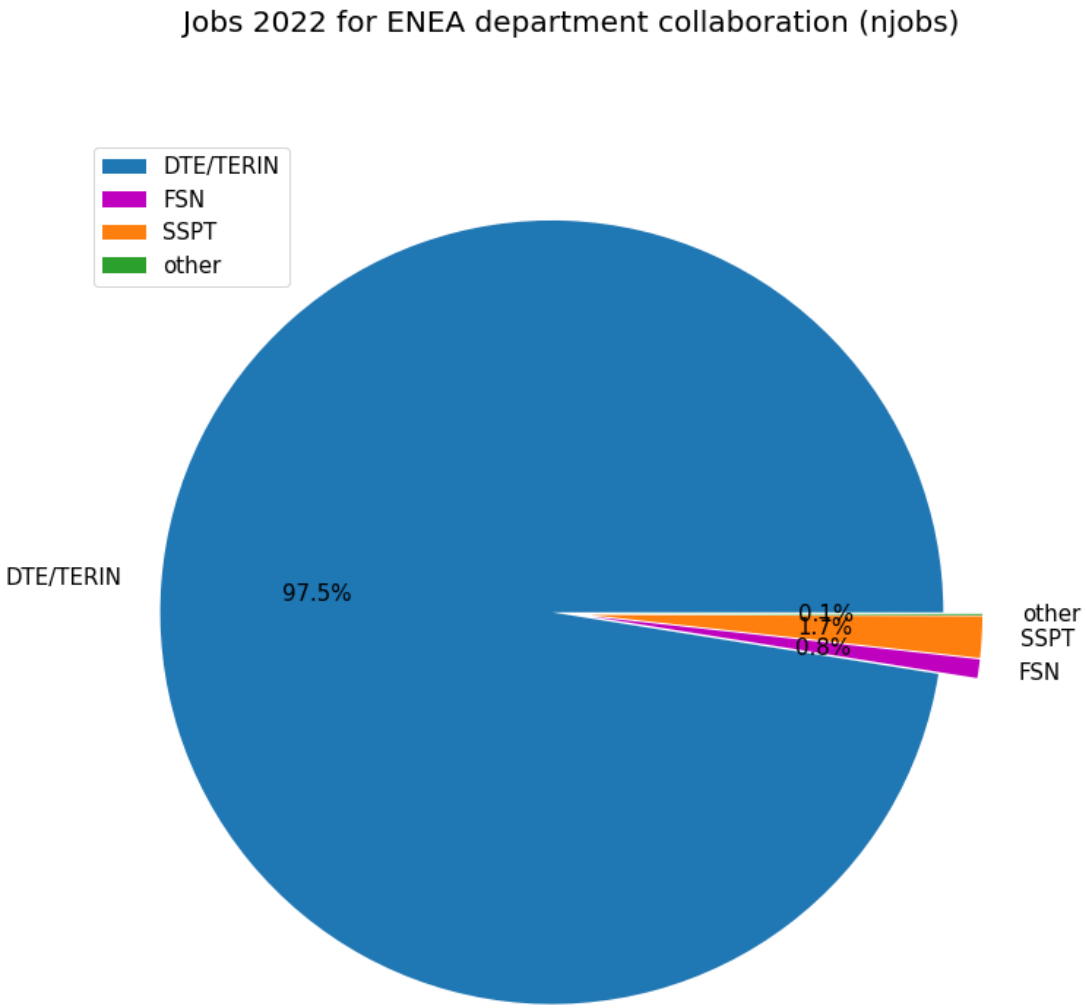
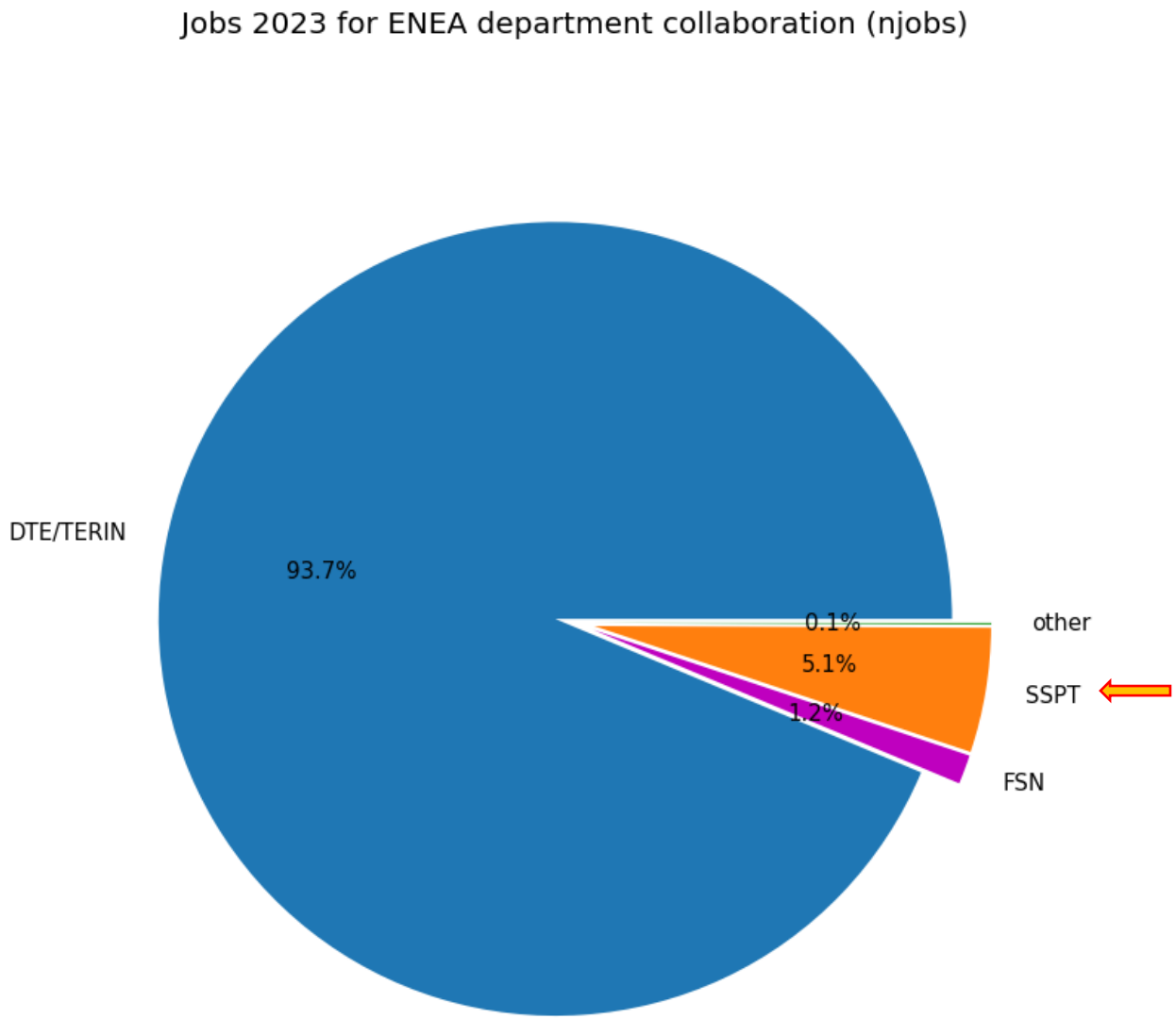
50000
75000
100000
125000
150000
175000
200000
Jobs


Jobs 2022 for ENEA department collaboration (njobs)
DTE/TERIN
FSN
SSPT
other
DTE/TERIN
97.5%
0.1%
1.7%
0.8%
other
SSPT
FSN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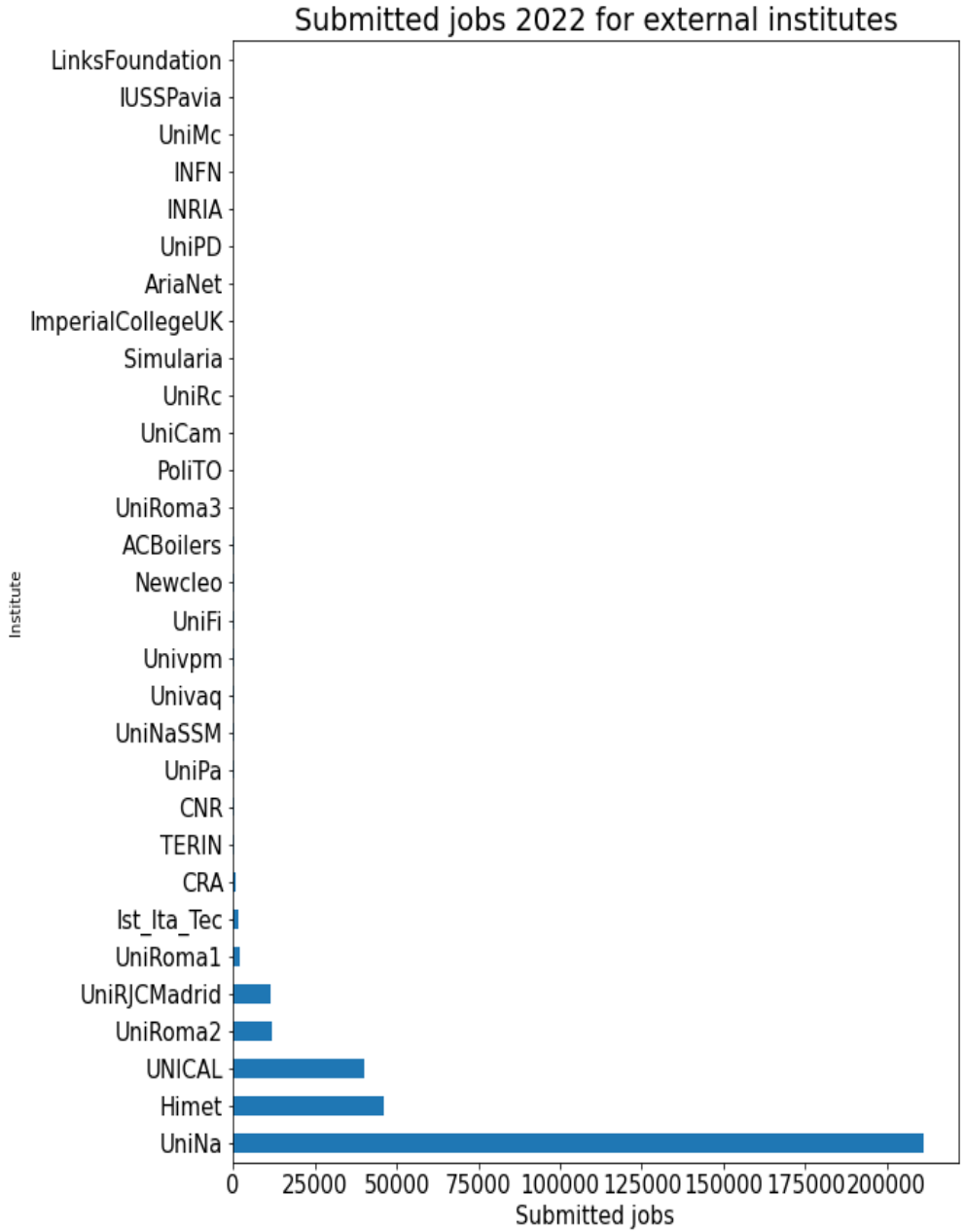
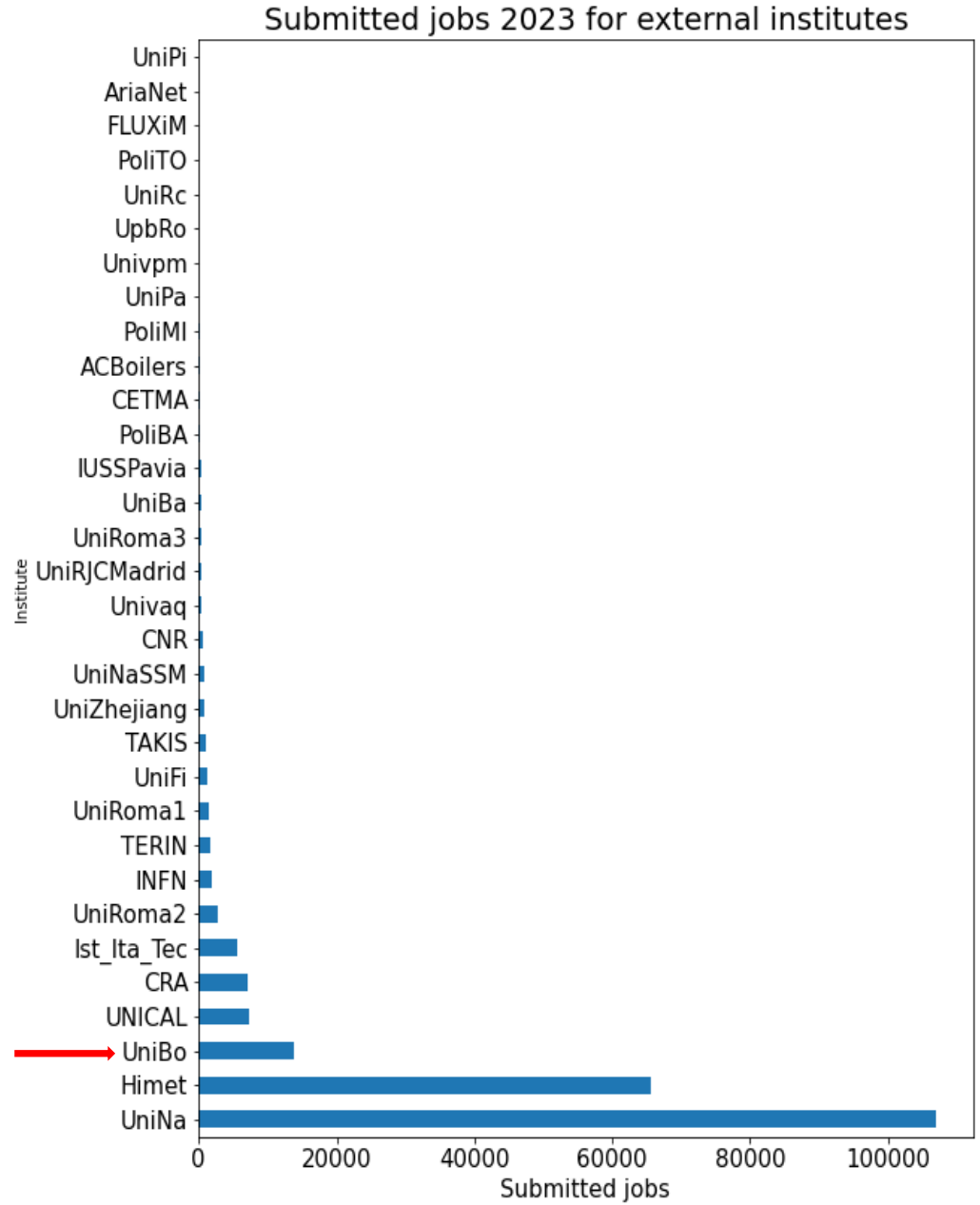
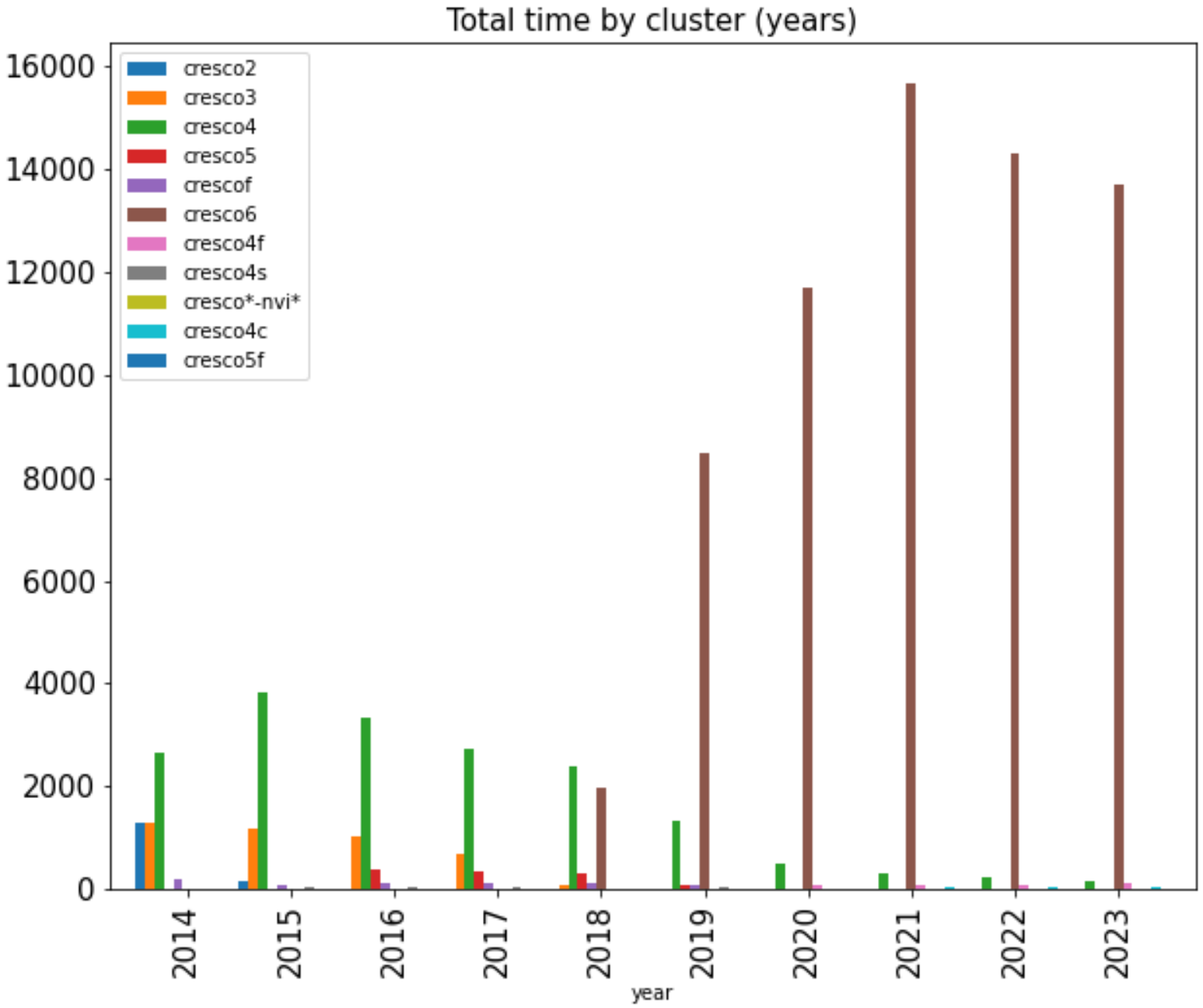
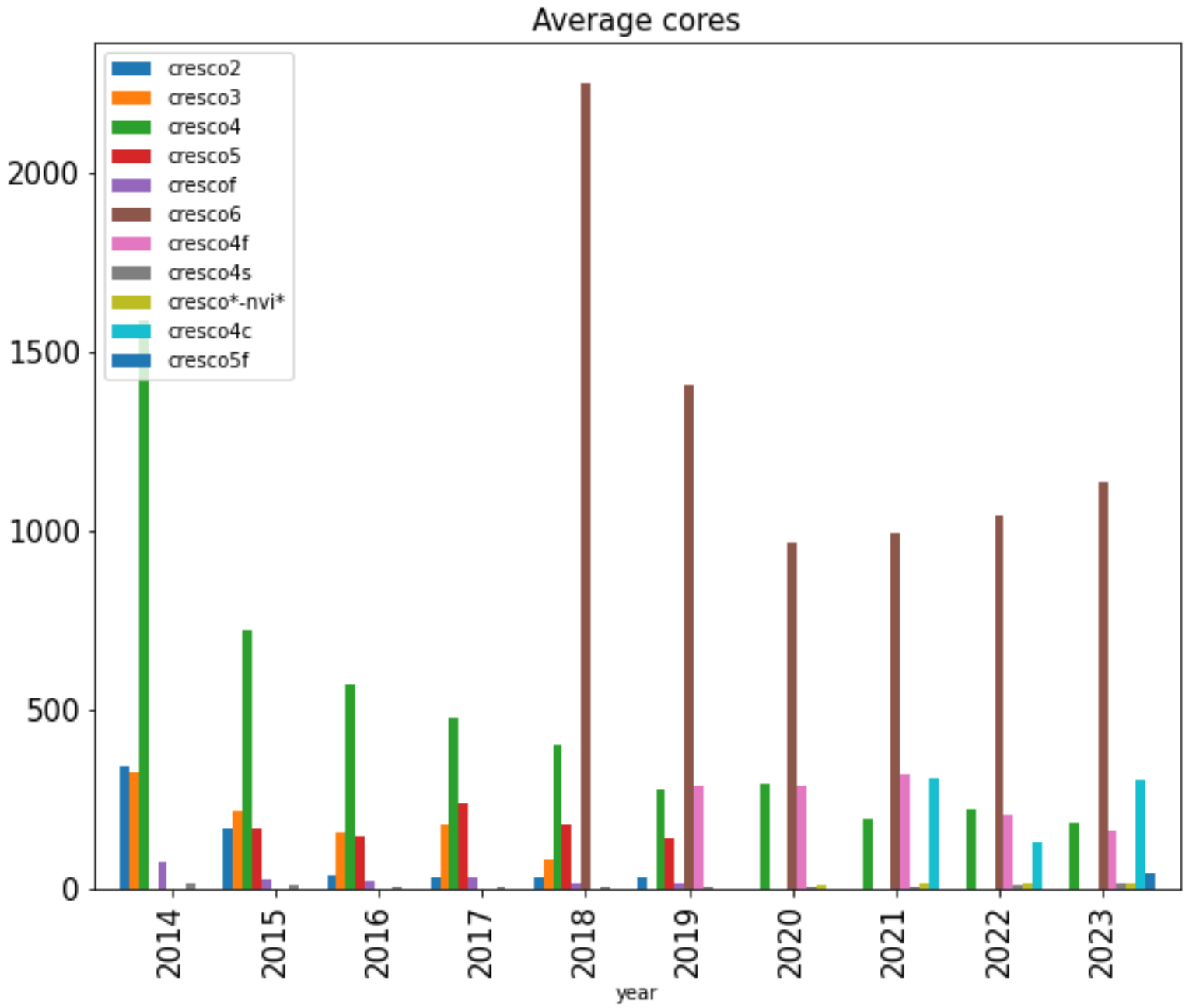
DTE/TERIN
93.7%
0.1%
5.1%
1.2%
other
SSPT
FSN


Submitted jobs 2022 for external institutes
LinksFoundation
IUSSPavia
UniMc
INFN
INRIA
UniPD
AriaNet
ImperialCollegeUK
Simularia
UniRc
UniCam
PoliTO
UniRoma3
ACBoilers
Newcleo
UniFi
Univpm
Univaq
UniNaSSM
UniPa
CNR
TERIN
CRA
Ist_Ita_Tec
UniRoma1
UniRJCMadrid
UniRoma2
UNICAL
Himet
UniNa
Institute
0
25000
50000
75000
100000
125000
150000
175000
200000
Submitted jobs


Submitted jobs 2023 for external institutes
UniPi
AriaNet
FLUXiM
PoliTO
UniRc
UpbRo
Univpm
UniPa
PoliMI
ACBoilers
CETMA
PoliBA
IUSSPavia
UniBa
UniRoma3
UniRJCMadrid
Univaq
CNR
UniNaSSM
UniZhejiang
TAKIS
UniFi
UniRoma1
TERIN
INFN
UniRoma2
Ist_Ita_Tec
CRA
UNICAL
UniBo
Himet
UniNa
Institute
0
20000
40000
60000
80000
100000
Submitted jobs

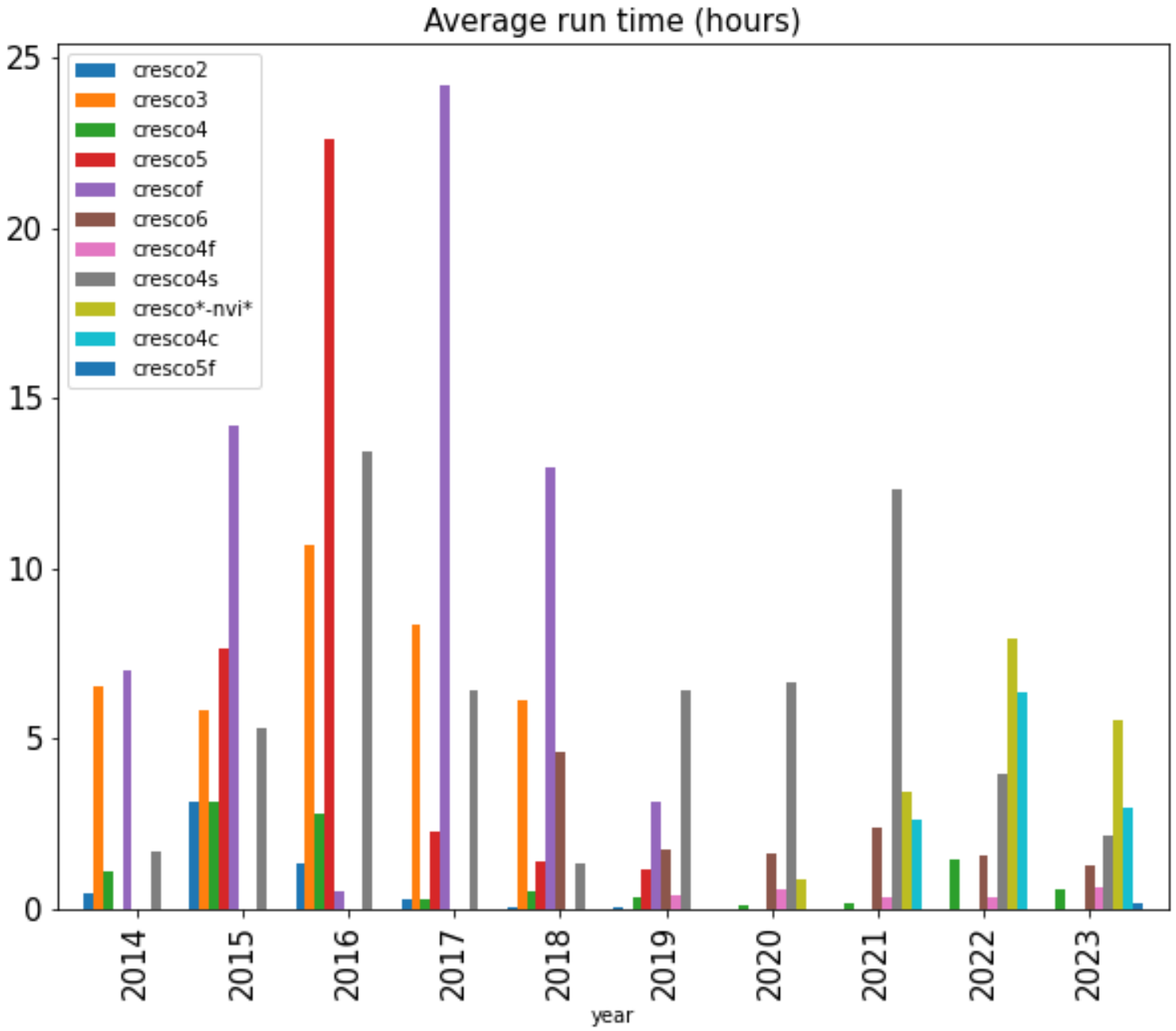
3. CRESCO usage: trends in recent years

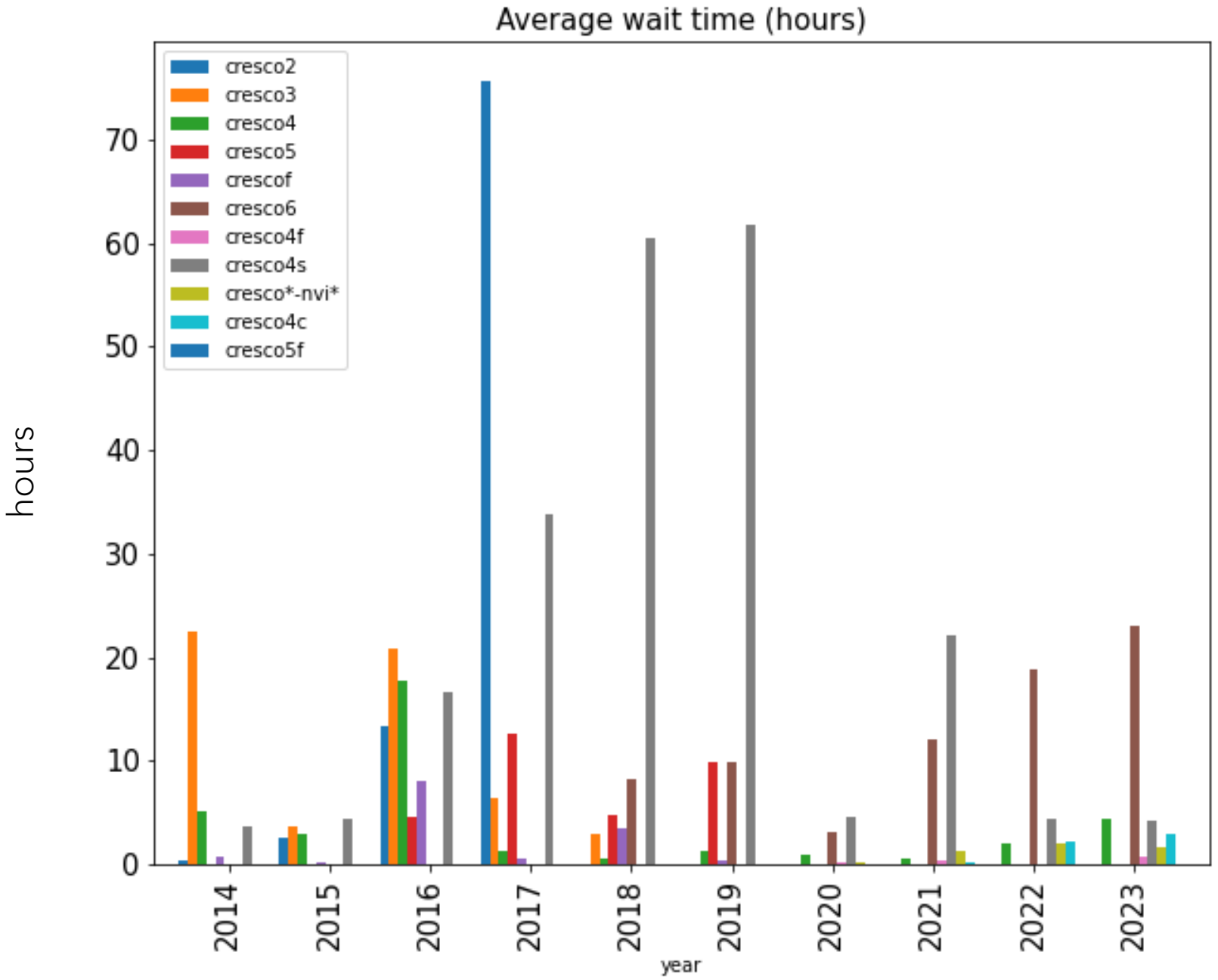

Total time by cluster (years)
cresco2
cresco3
cresco4
cresco5
crescof
cresco6
cresco4f
cresco4s
cresco*-nvi*
cresco4c
cresco5f
16000
14000
12000
10000
8000
6000
4000
2000
0
2014
2015
2016
2017
2018
2019
2020
2021
2022
2023
year

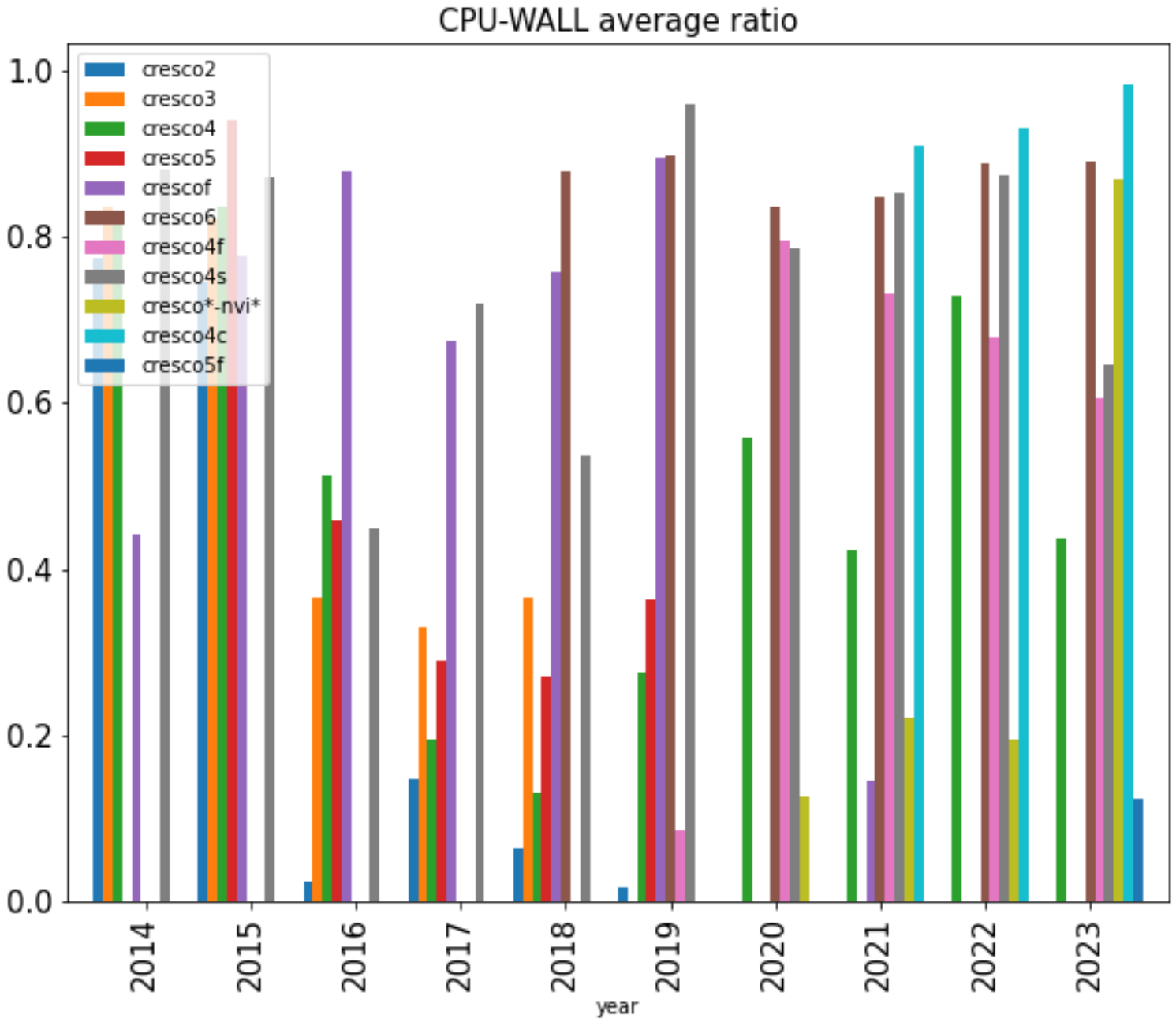


CRESCO6

CRESCO4C

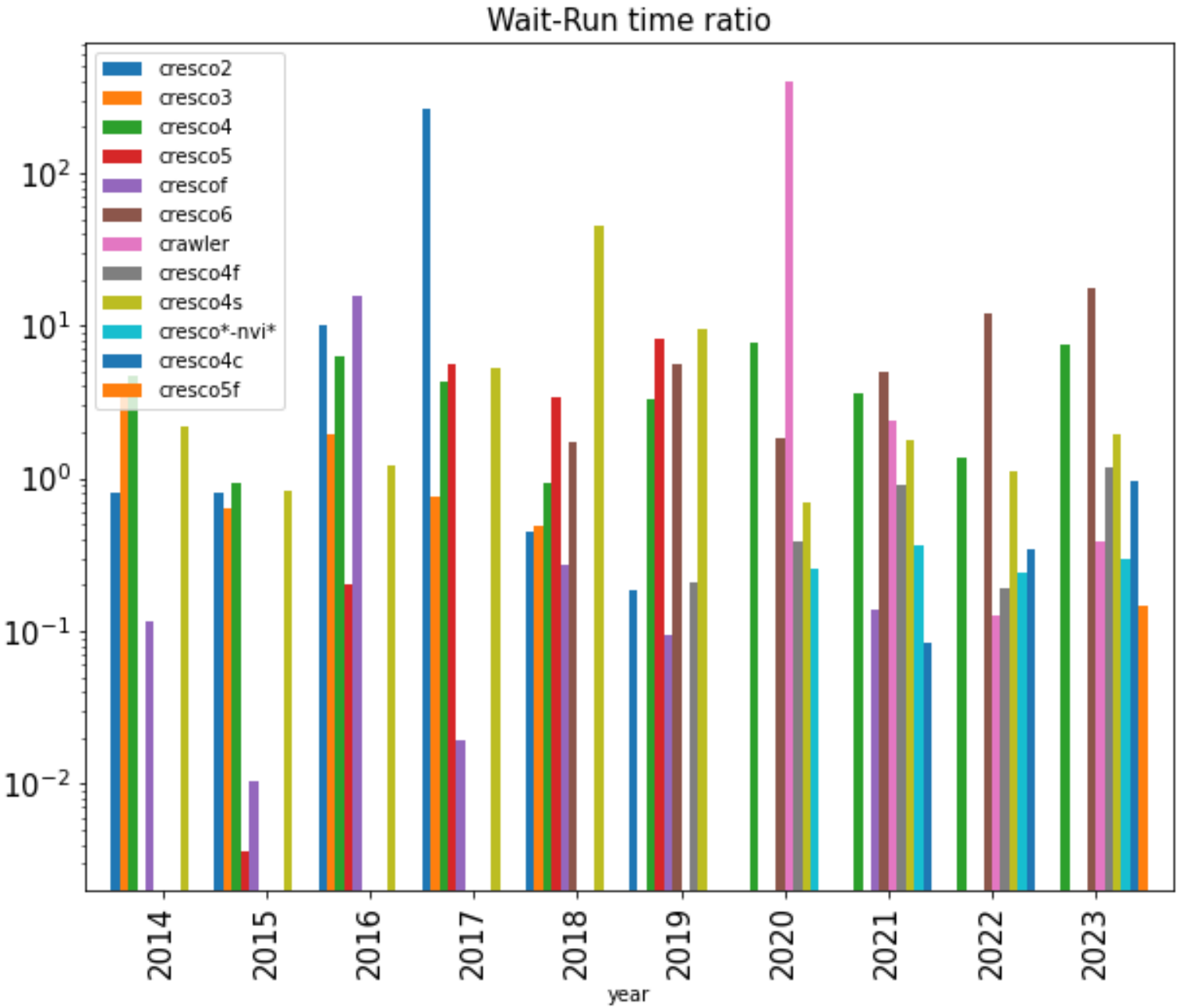

Average run time (hours)
cresco2
cresco3
cresco4
cresco5
crescof
cresco6
cresco4f
cresco4s
cresco*-nvi*
cresco4c
cresco5f
25
20
15
10
5
0
2014
2015
2016
2017
2018
2019
2020
2021
2022
2023
year


Average wait time (hours)
cresco2
cresco3
cresco4
cresco5
crescof
cresco6
cresco4f
cresco4s
cresco*-nvi*
cresco4c
cresco5f
hours
0
10
20
30
40
50
60
70
2014
2015
2016
2017
2018
2019
2020
2021
2022
2023
year



Utilizzo effettivo delle CPU:

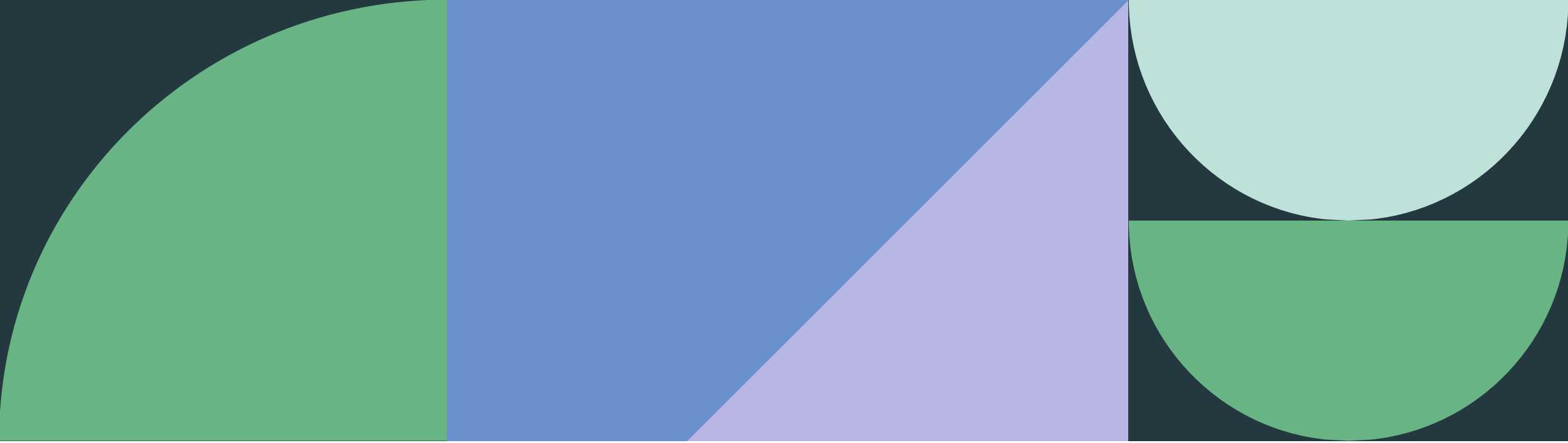
quanto più vicino al valore 1 tanto più i processori sono impegnati al massimo



Rapporto tra tempo di attesa in anni e il tempo di utilizzo dei precessori.

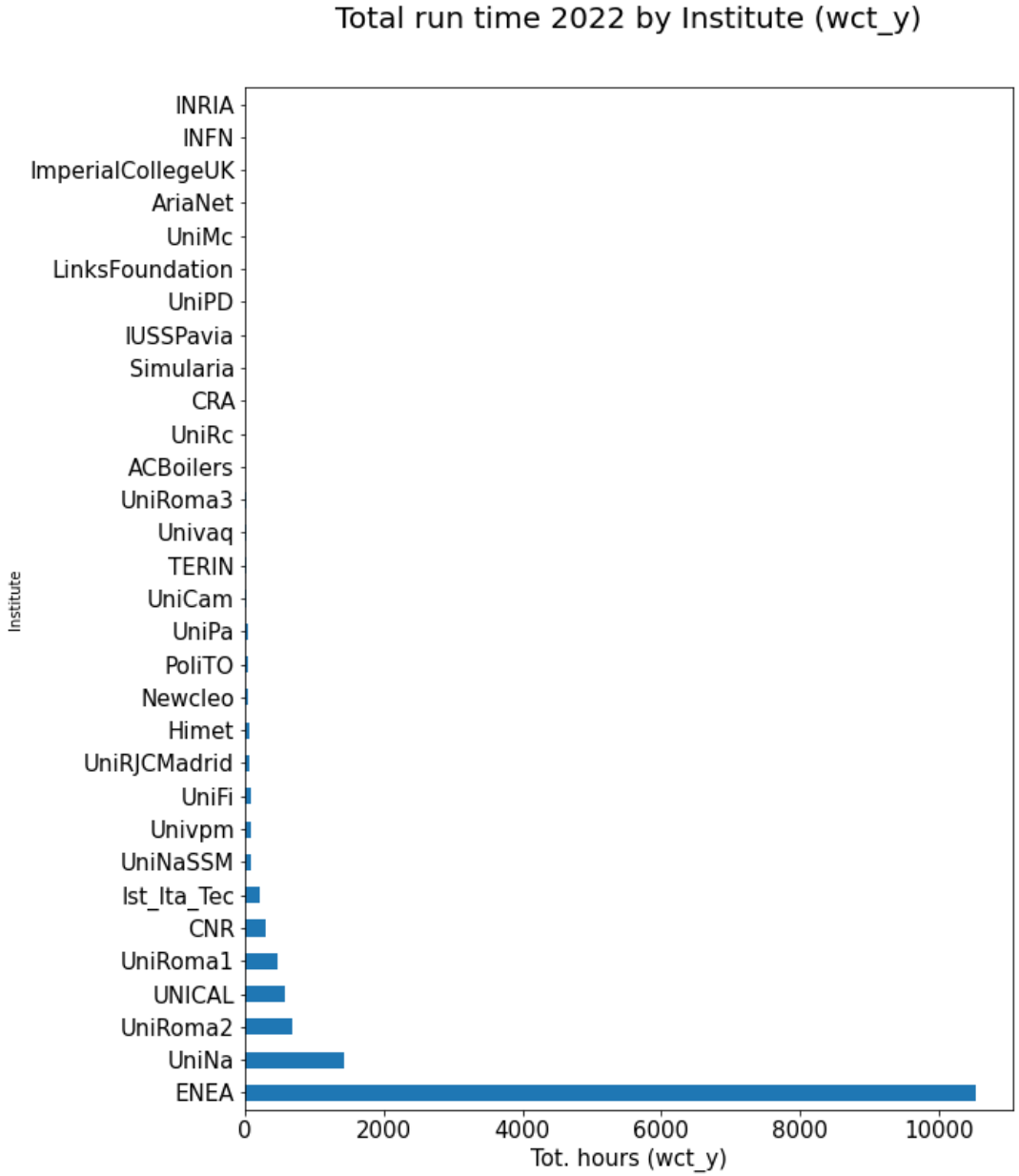
Tempo di attesa ottimale: 10^0 che equivale al tempo di esecuzione di un job.

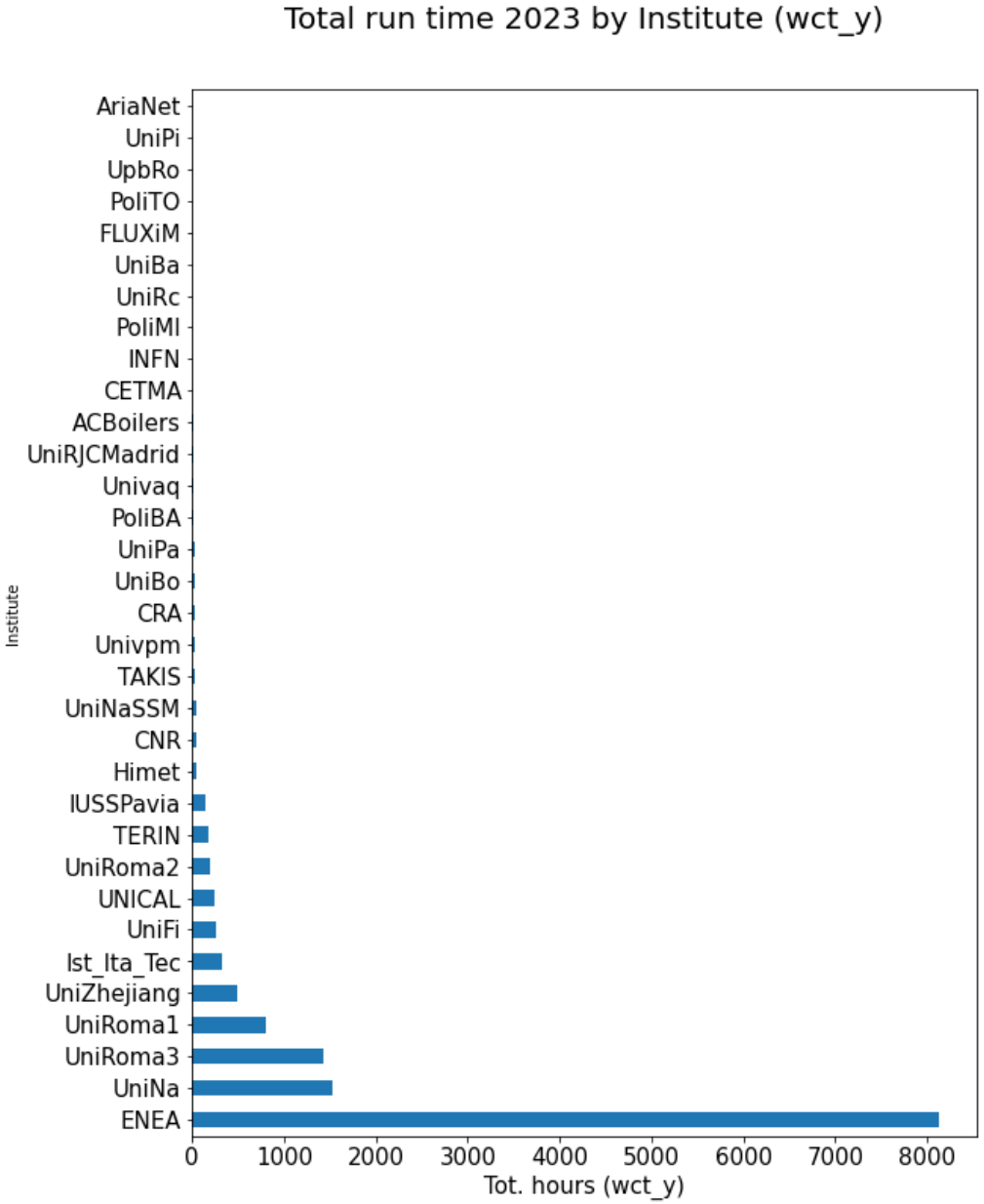
Cresco 5f

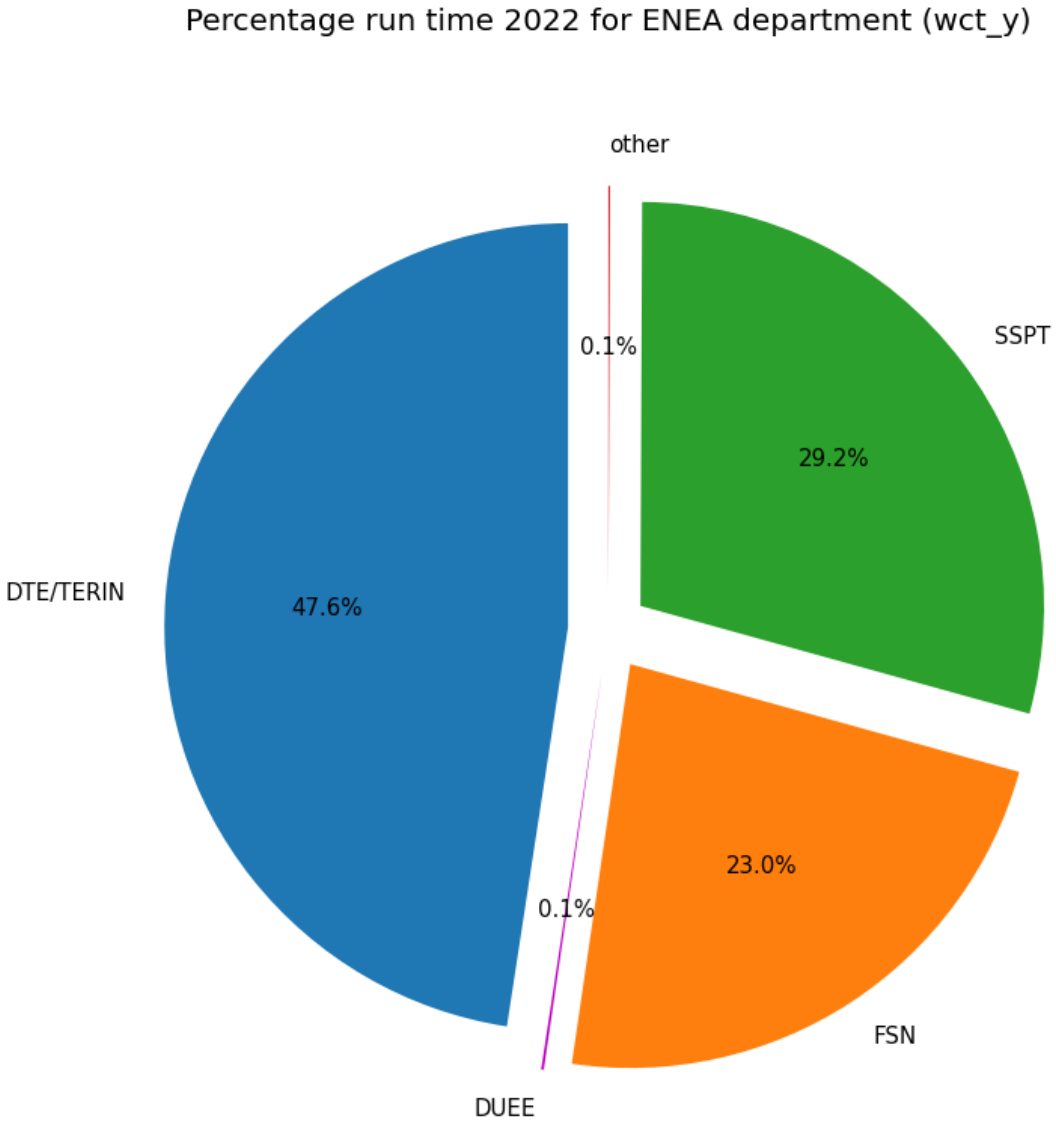


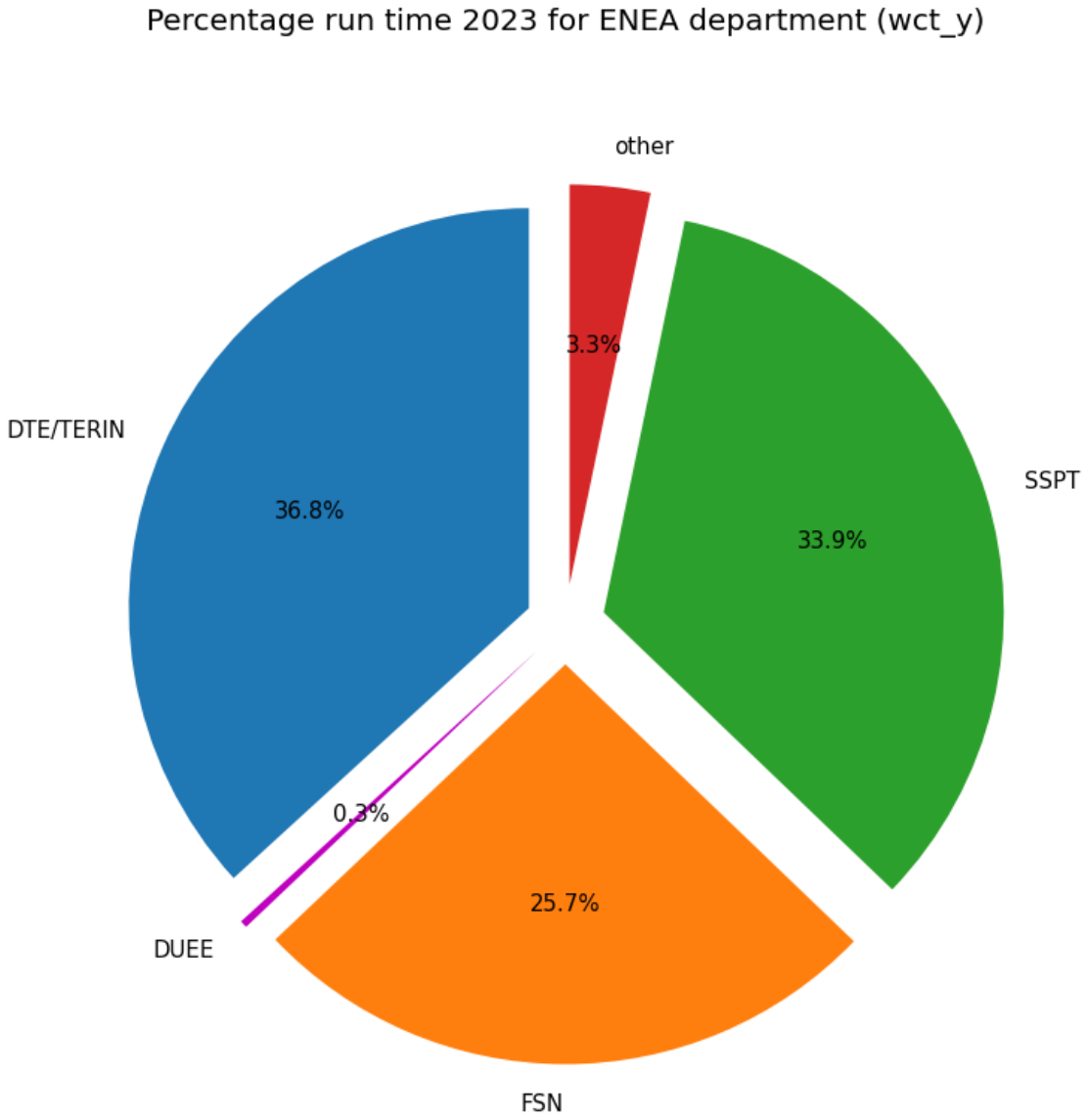
4. Some users and wall clock time_years

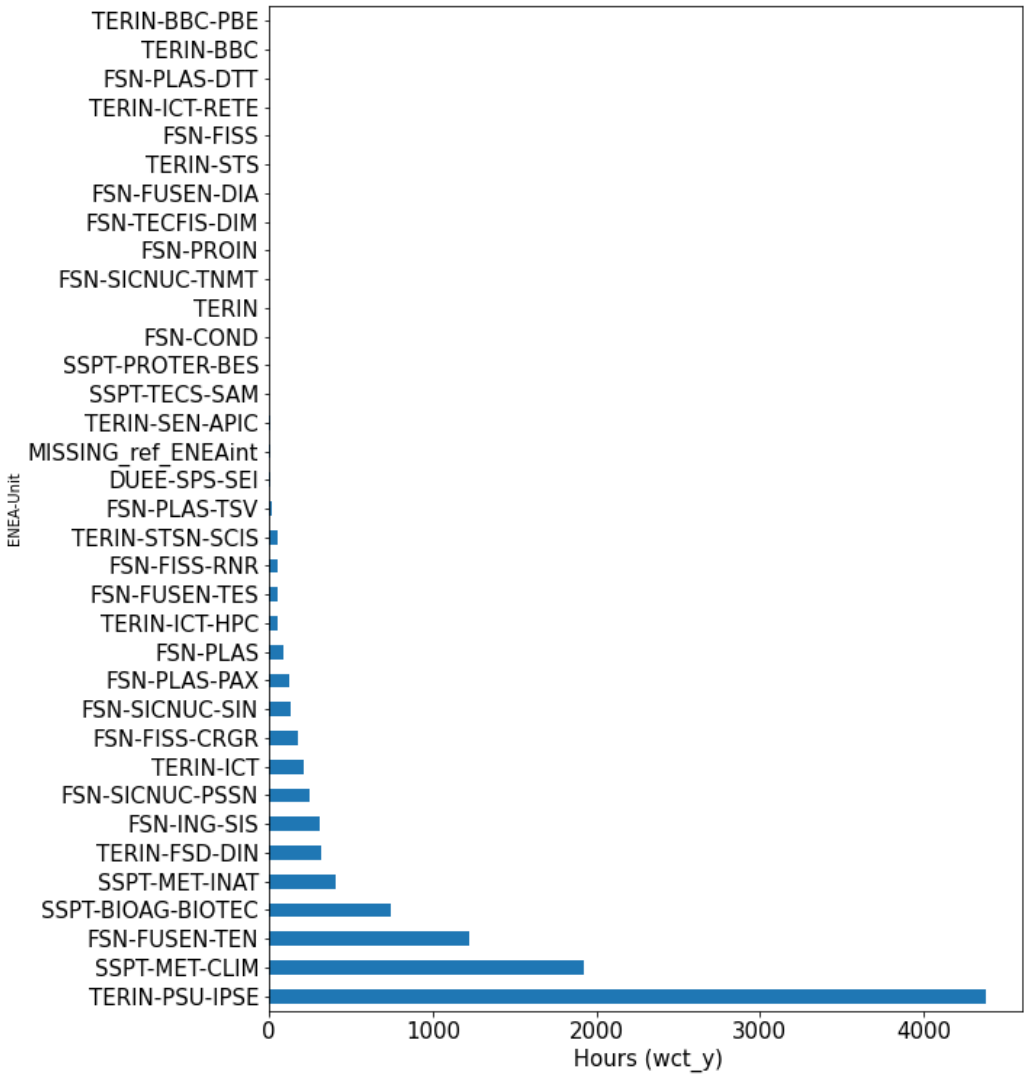
in details

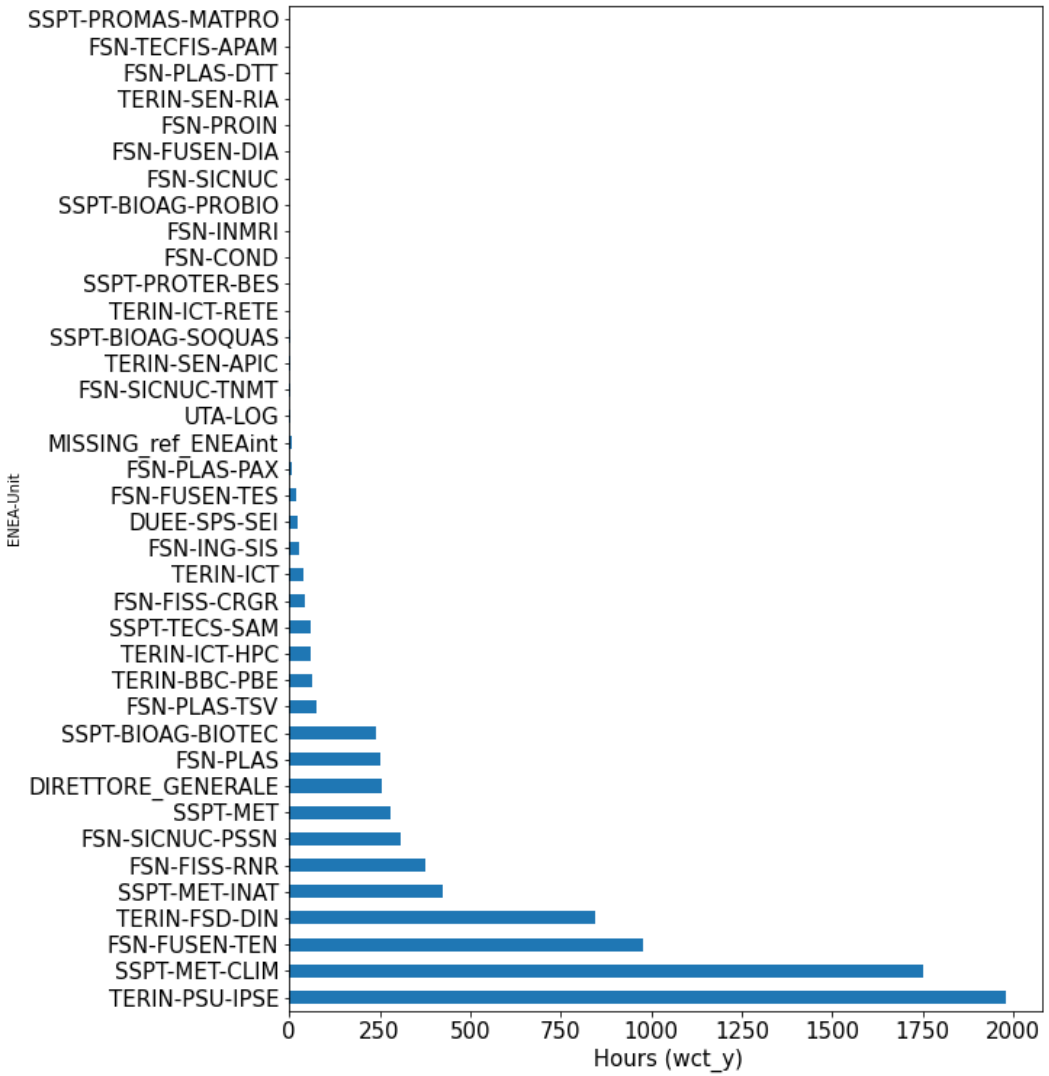

Total run time 2022 by Institute (wct_y)
INRIA
INFN
ImperialCollegeUK
AriaNet
UniMc
LinksFoundation
UniPD
IUSSPavia
Simularia
CRA
UniRc
ACBoilers
UniRoma3
Univaq
TERIN
UniCam
UniPa
PoliTO
Newcleo
Himet
UniRJCMadrid
UniFi
Univpm
UniNaSSM
Ist_Ita_Tec
CNR
UniRoma1
UNICAL
UniRoma2
UniNa
ENEA
Institute
0
2000
4000
6000
8000
10000
Tot. hours (wct_y)


Total run time 2023 by Institute (wct_y)
AriaNet
UniPi
UpbRo
PoliTO
FLUXiM
UniBa
UniRc
PoliMI
INFN
CETMA
ACBoilers
UniRJCMadrid
Univaq
PoliBA
UniPa
UniBo
CRA
Univpm
TAKIS
UniNaSSM
CNR
Himet
IUSSPavia
TERIN
UniRoma2
UNICAL
UniFi
Ist_Ita_Tec
UniZhejiang
UniRoma1
UniRoma3
UniNa
ENEA
Institute
0
1000
2000
3000
4000
5000
6000
7000
8000
Tot. hours (wct_y)


Percentage run time 2022 for ENEA department (wct_y)
other
0.1%
SSPT
29.2%
DTE/TERIN
47.6%
23.0%
0.1%
FSN
DUEE


Percentage run time 2023 for ENEA department (wct_y)
other
3.3%
DTE/TERIN
36.8%
SSPT
33.9%
0.3%
25.7%
DUEE
FSN


Total run time 2022 for ENEA laboratories (wct_y)
TERIN-BBC-PBE
TERIN-BBC
FSN-PLAS-DTT
TERIN-ICT-RETE
FSN-FISS
TERIN-STS
FSN-FUSEN-DIA
FSN-TECFIS-DIM
FSN-PROIN
FSN-SICNUC-TNMT
TERIN
FSN-COND
SSPT-PROTER-BES
SSPT-TECS-SAM
TERIN-SEN-APIC
MISSING_ref_ENEAint
DUEE-SPS-SEI
FSN-PLAS-TSV
TERIN-STSN-SCIS
FSN-FISS-RNR
FSN-FUSEN-TES
TERIN-ICT-HPC
FSN-PLAS
FSN-PLAS-PAX
FSN-SICNUC-SIN
FSN-FISS-CRGR
TERIN-ICT
FSN-SICNUC-PSSN
FSN-ING-SIS
TERIN-FSD-DIN
SSPT-MET-INAT
SSPT-BIOAG-BIOTEC
FSN-FUSEN-TEN
SSPT-MET-CLIM
TERIN-PSU-IPSE
ENEA-Unit
0
1000
2000
3000
4000
Hours (wct_y)


Total run time 2023 for ENEA laboratories (wct_y)
SSPT-PROMAS-MATPRO
FSN-TECFIS-APAM
FSN-PLAS-DTT
TERIN-SEN-RIA
FSN-PROIN
FSN-FUSEN-DIA
FSN-SICNUC
SSPT-BIOAG-PROBIO
FSN-INMRI
FSN-COND
SSPT-PROTER-BES
TERIN-ICT-RETE
SSPT-BIOAG-SOQUAS
TERIN-SEN-APIC
FSN-SICNUC-TNMT
UTA-LOG
MISSING_ref_ENEAint
FSN-PLAS-PAX
FSN-FUSEN-TES
DUEE-SPS-SEI
FSN-ING-SIS
TERIN-ICT
FSN-FISS-CRGR
SSPT-TECS-SAM
TERIN-ICT-HPC
TERIN-BBC-PBE
FSN-PLAS-TSV
SSPT-BIOAG-BIOTEC
FSN-PLAS
DIRETTORE_GENERALE
SSPT-MET
FSN-SICNUC-PSSN
FSN-FISS-RNR
SSPT-MET-INAT
TERIN-FSD-DIN
FSN-FUSEN-TEN
SSPT-MET-CLIM
TERIN-PSU-IPSE
ENEA-Unit
0
250
500
750
1000
1250
1500
1750
2000
Hours (wct_y)

Limesurvay statistics

LimeSurvey

Users selected and invited to partecipate at the survay: 115 (2021) – **105 (2022)**

Selection criterium is:

wct_y > 1.0 || (av_totcore* > 5000)

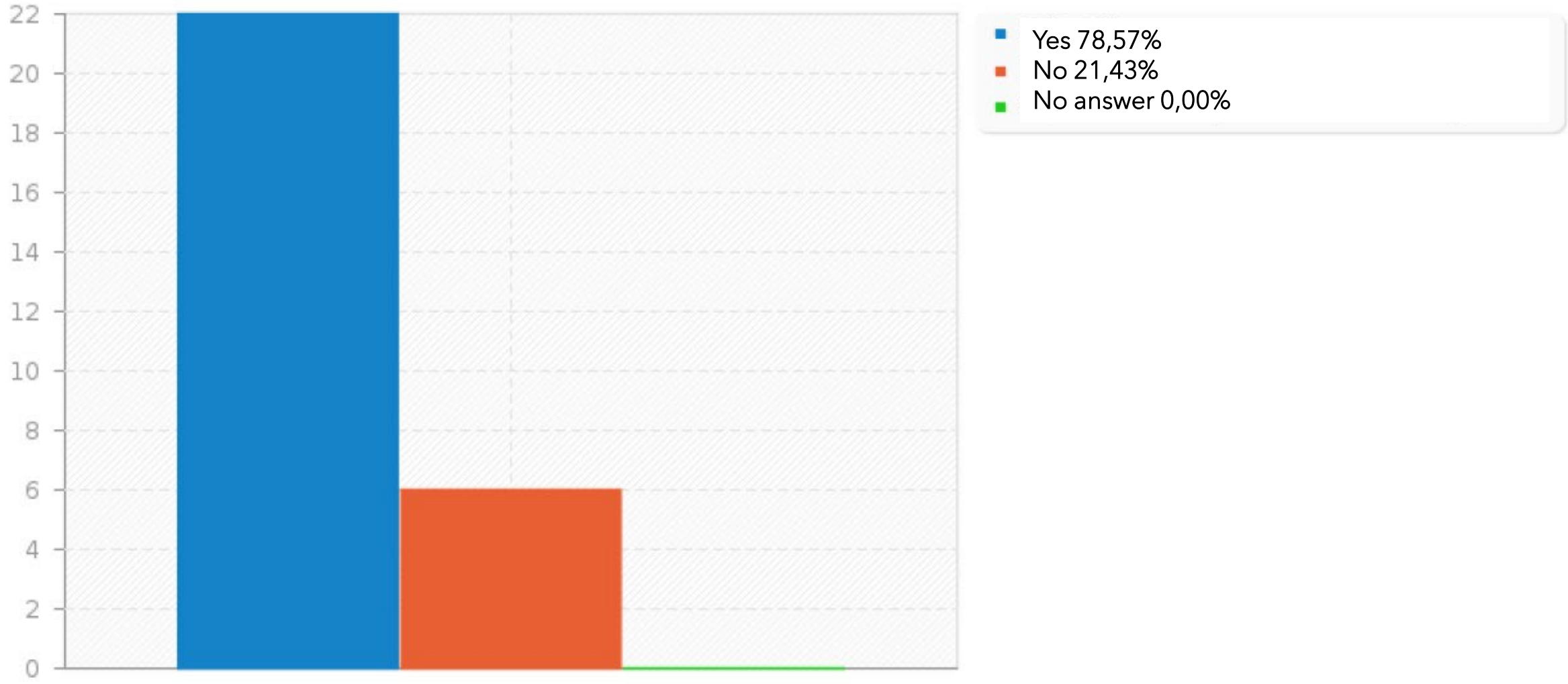
wct_y: total wall clock time (years)
njobs: number of submitted jobs
av_nc: average number of used cores
av_totcore: njobs*av_nc

Start: 03.05.2023

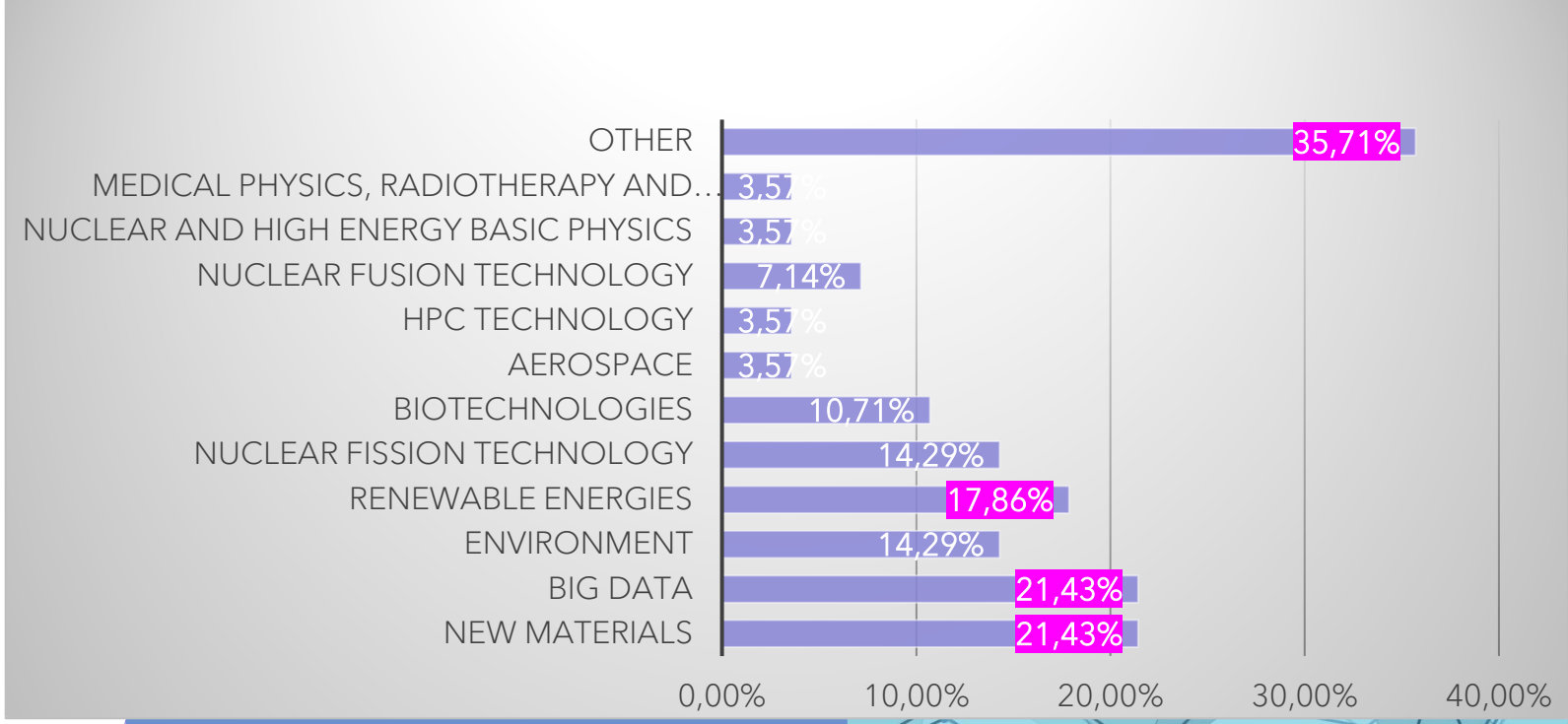
Deadline: 01.10.2023

N. completed questionnaires: 28
Incomplete: 4
Total: 32

Have you already contributed in a previous Cresco Annual Report?



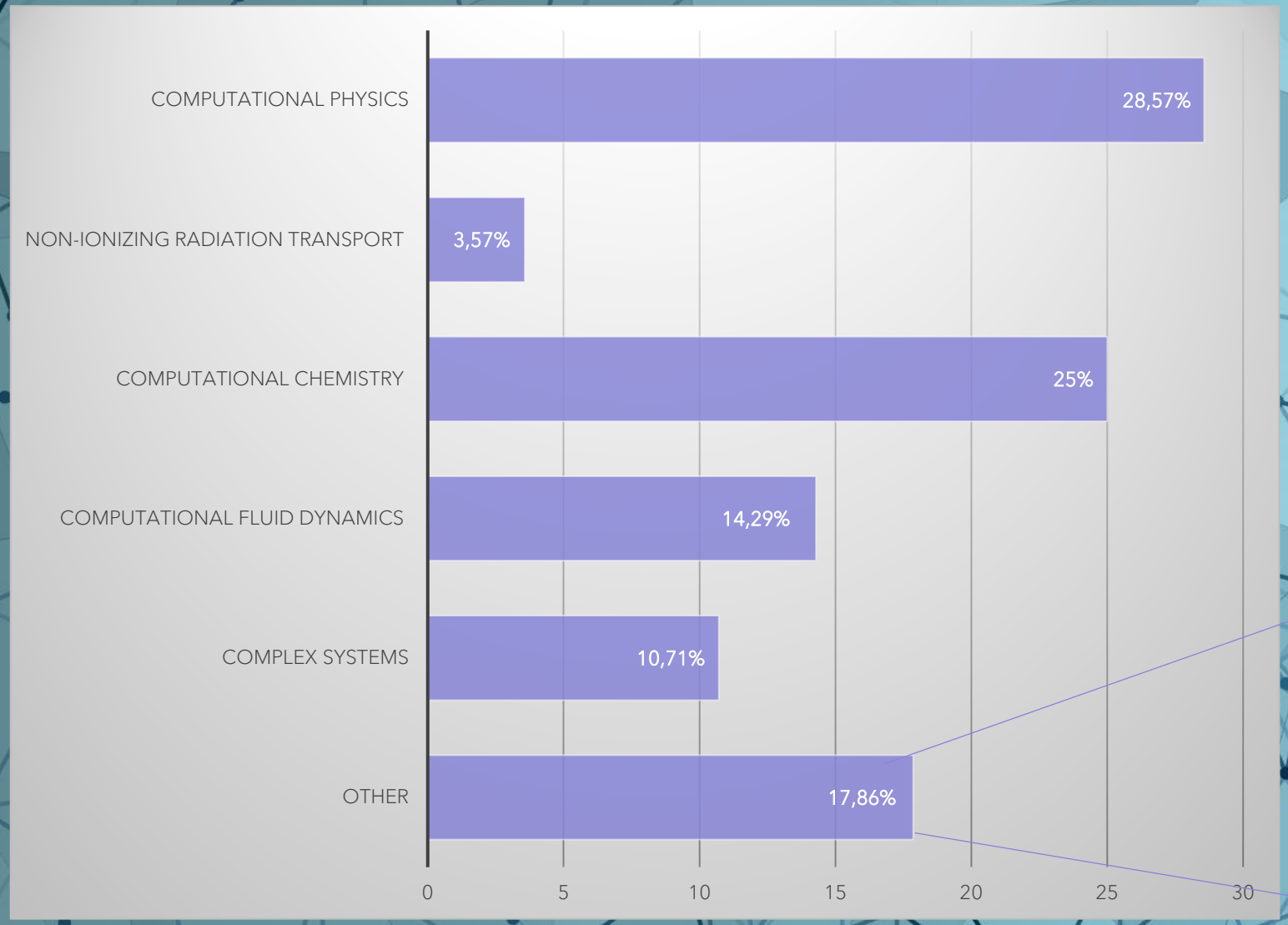
Research & Development Domain	
New Materials	21,43%
Big Data	21,43%
Environment	14,29%
Renewable Energies	17.86%
Nuclear Fission Technology	14.29%
Biotechnologies	10.71%
Aerospace	3.57%
HPC Technology	3.57%
Nuclear Fusion Technology	7.14%
Nuclear and High Energy Basic Physics	3.57%
Medical Physics, Radiotherapy and Dosimetry	3.57%
Other	35.71%



- Soft Matter
- Computational Nanoscience
- Storage
- Statistical Physics
- Structural Biology
- Artificial Intelligence
- Drug Discovery and Structural Bioinformatics
- Infectious Diseases
- Radiological Characterization
- Agriculture

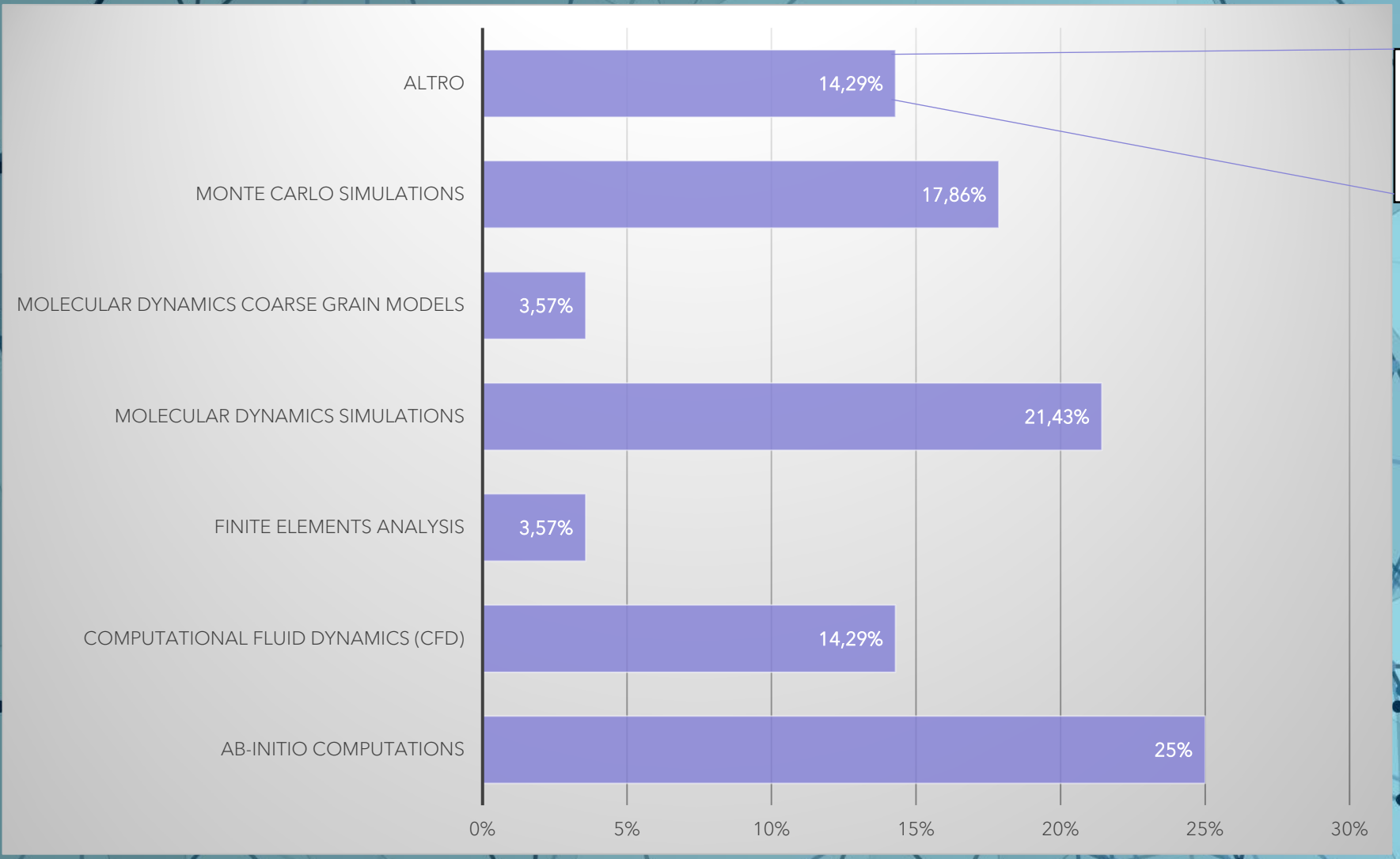
Modeling & Simulation Background

What is the scientific context on which the modeling and simulations are based?



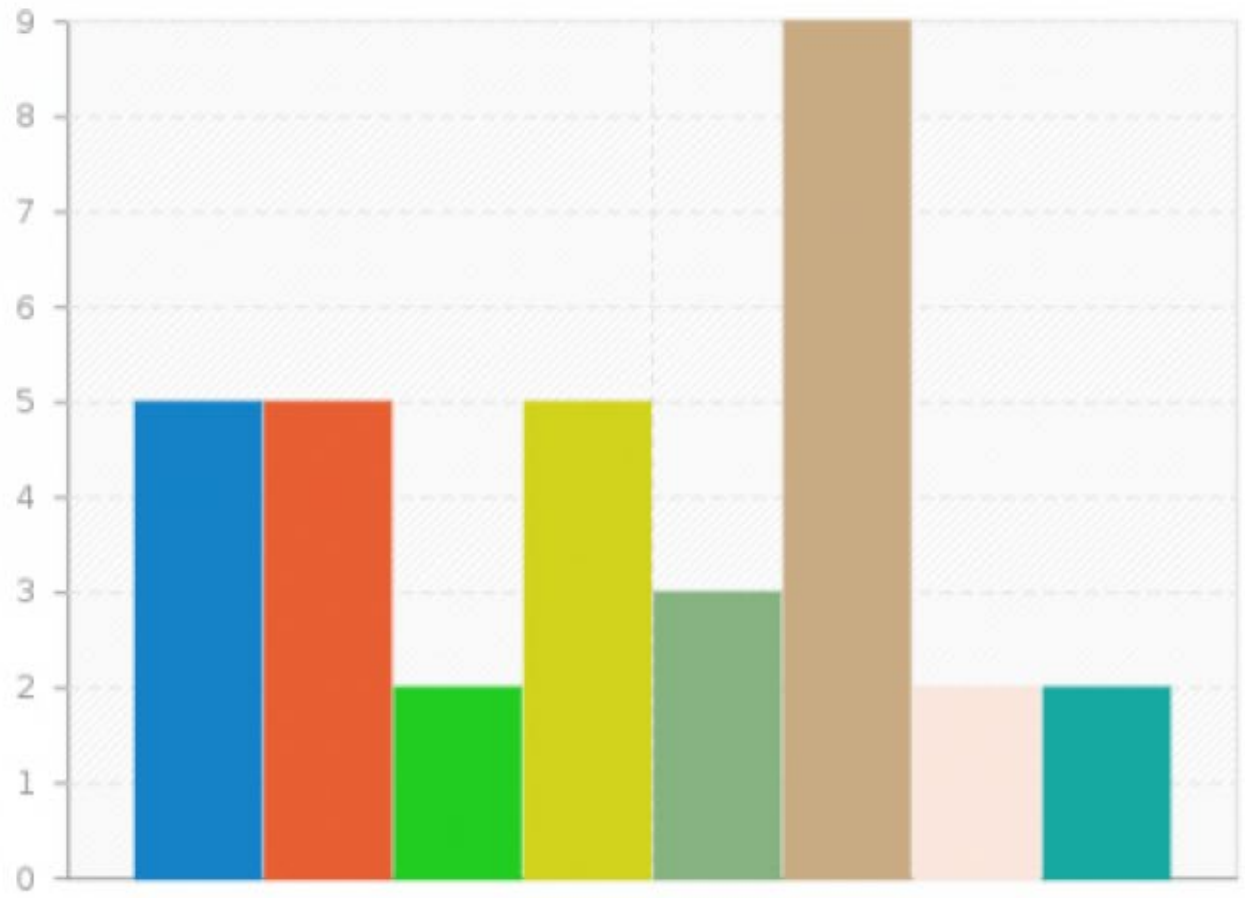
- MC Transport of Nuclear Particles
- Radiation Damage Analysis
- Radiation Transport
- Digital Platform
- Machine Learning

Computational Methodology



- Density Functional Theory
- Neural Networks
- Digital Platform

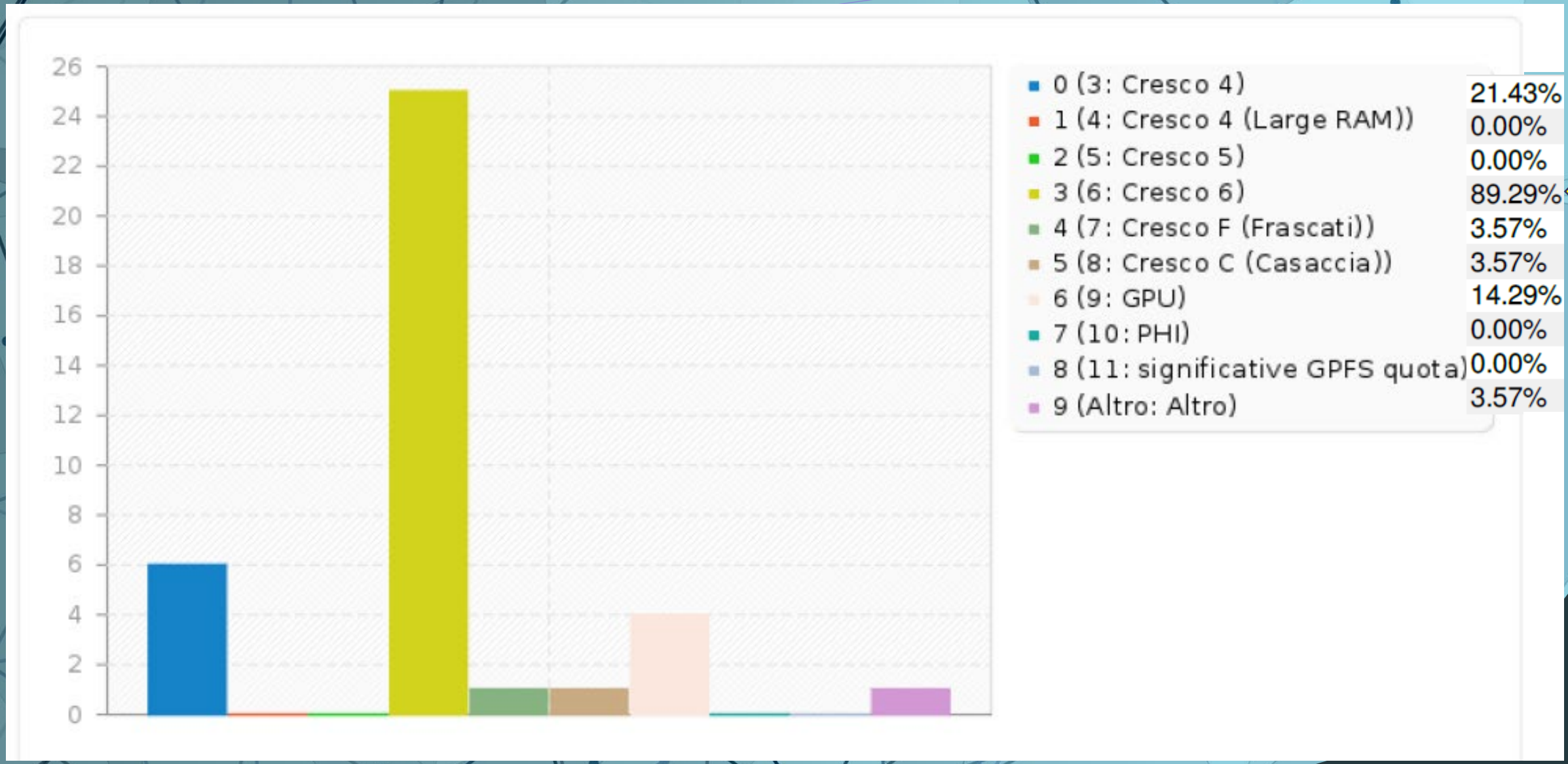
Context of the activity



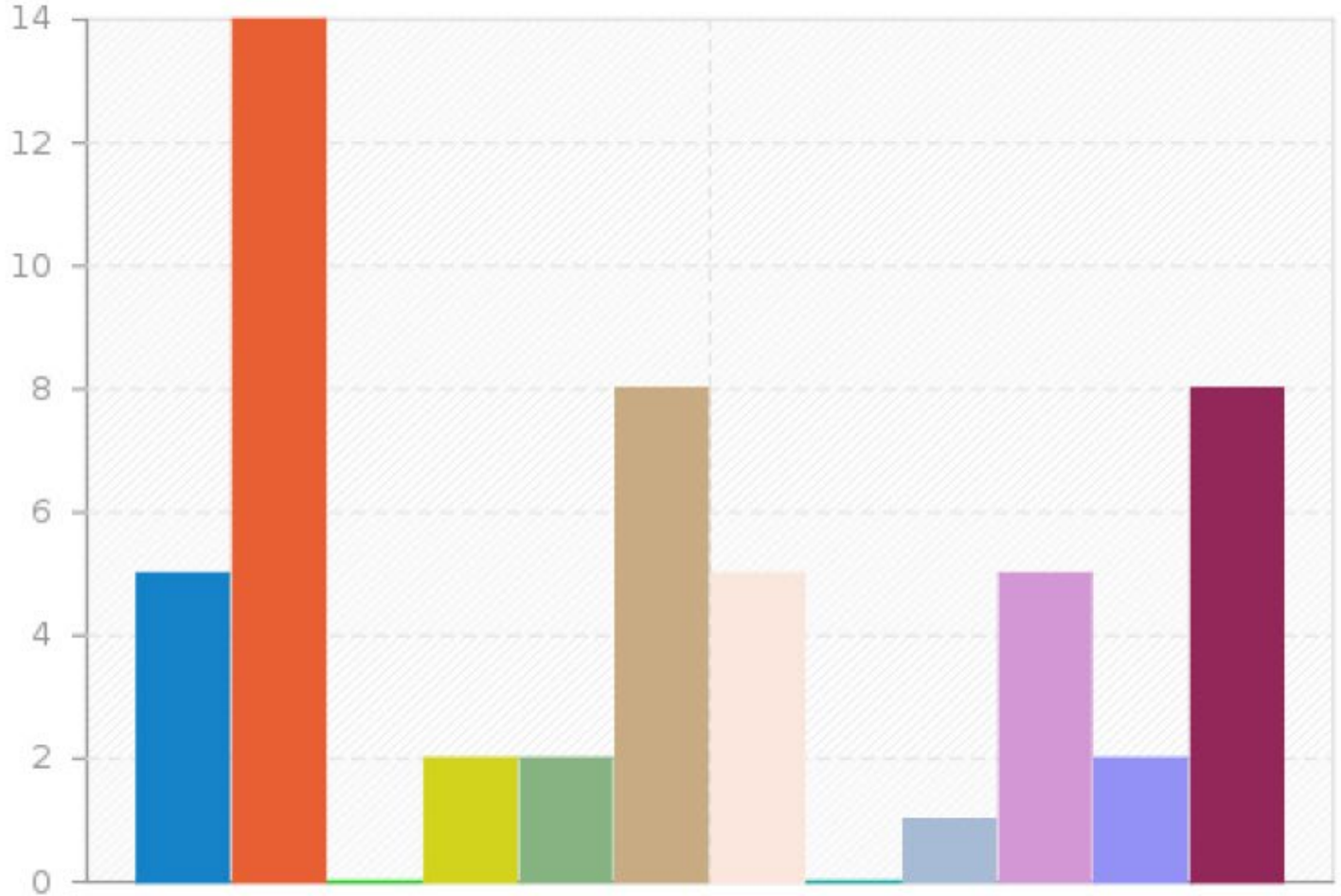
- European Project 17.86%
- Italian National Project 17.86%
- Programme agreement 7.14%
- ENEA Institutional Activities 17.86%
- University projects 10.71%
- Base research 32.14%
- Contracts with external entities 7.14%
- Other 7.14%

Hardware

Choose the Cresco hardware used for the report; In "other" you can specify one or more entries that are not yet in the list.



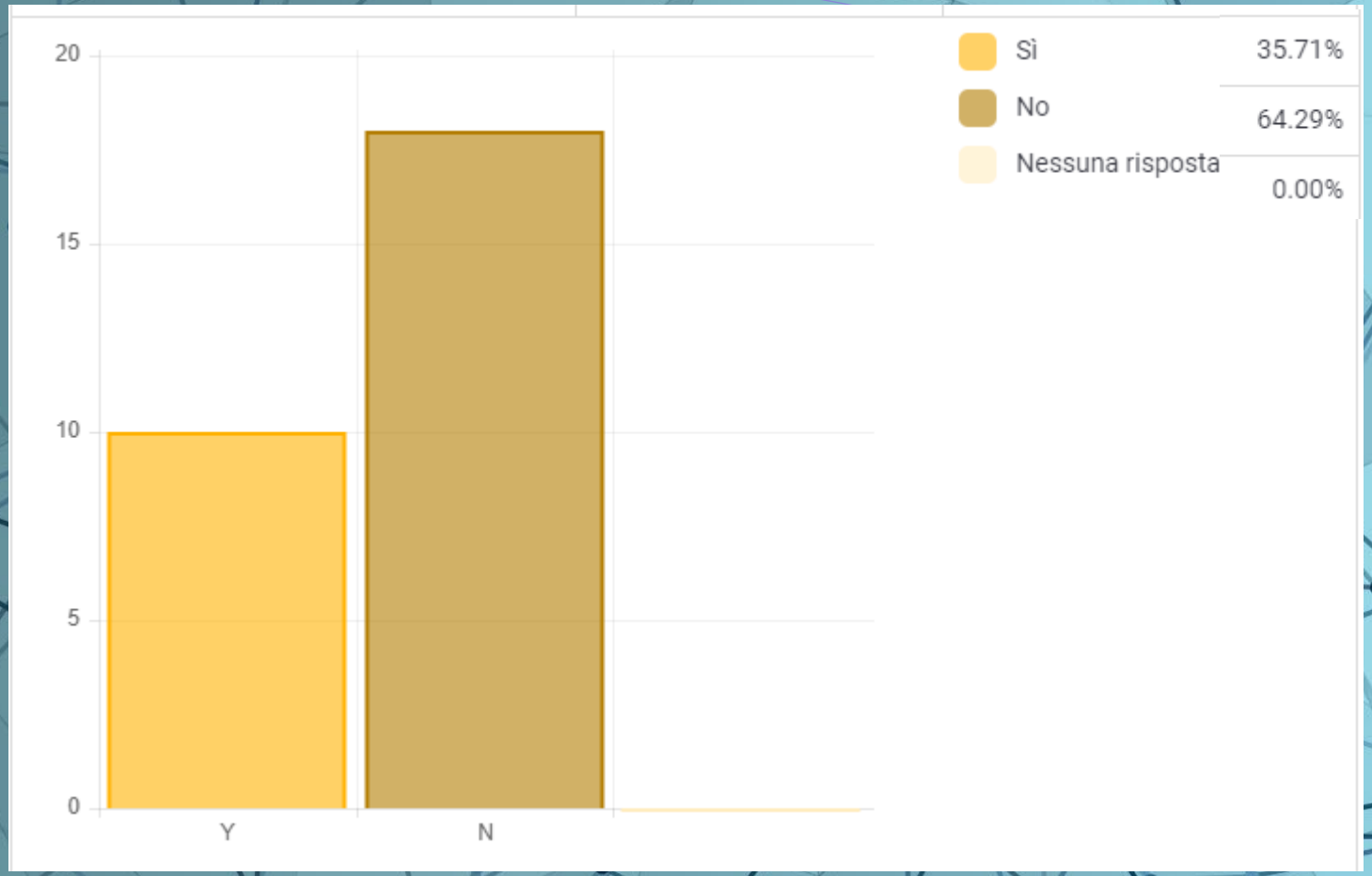
Data Visualization
Tools used to view simulation results



0 (1: Gnuplot)	17.86%
1 (2: Python)	50.00%
2 (3: Matlab)	0.00%
3 (4: Paraview)	7.14%
4 (5: R)	7.14%
5 (6: Visual Molecular Dynamics (VMD)	28.57%
6 (7: Grace)	17.86%
7 (8: IDL)	0.00%
8 (9: Ansys)	3.57%
9 (10: Excel)	17.86%
10 (11: MCNP[X])	7.14%
11 (Altro: Altro)	28.57%

Octave, Microcal Origin
None (VESTA on local machines)
Octave
Material Studio Visualizer
Origin
pyvista
Tecplot
xCrysDen

Scalability: Have you done scalability tests of the code?



Software #1

GNU Octave
Python
pYTHON
VASP
ORAC6.1
FLUKA
GROMACS
Siesta
VASP 5.4.4
fhi-aims
MCNP
LAMMPS
Gromacs
MCNP
NAMD
OpenFOAM
OpenFOAM based solvers for SARS-Cov-2 Thermo-Fluid Dynamics
MCNPX
Quantum Espresso
AiiDA

Software #2

R
cp2k
PHITS
LAMMPS
Quantum Espresso
DMOL3
Phyton
HOOMD
VMD
GROMACS
Pytorch
Quantum Espresso
R

Software #3

OCCAM MD
PyMOL
VMD
EXCEL

SW	N. of Users
Quantum Espresso	5
GROMACS	4
Python	3
LAMMPS	3
OpenFOAM	3
VASP	2
MCNP	2
Pytorch	2
R	2

AiiDA
cp2k
PHITS
DMOL3
HOOMD
VMD
OCCAM MD
PyMOL
VMD
EXCEL
ORAC6.1
FLUKA
Siesta
fhi-aims
NAMD
MCNPX
GNU Octave
ANSYS CFX

Software #1

GNU Octave
Python
pYTHON
VASP
ORAC6.1
FLUKA
GROMACS
Siesta
VASP 5.4.4
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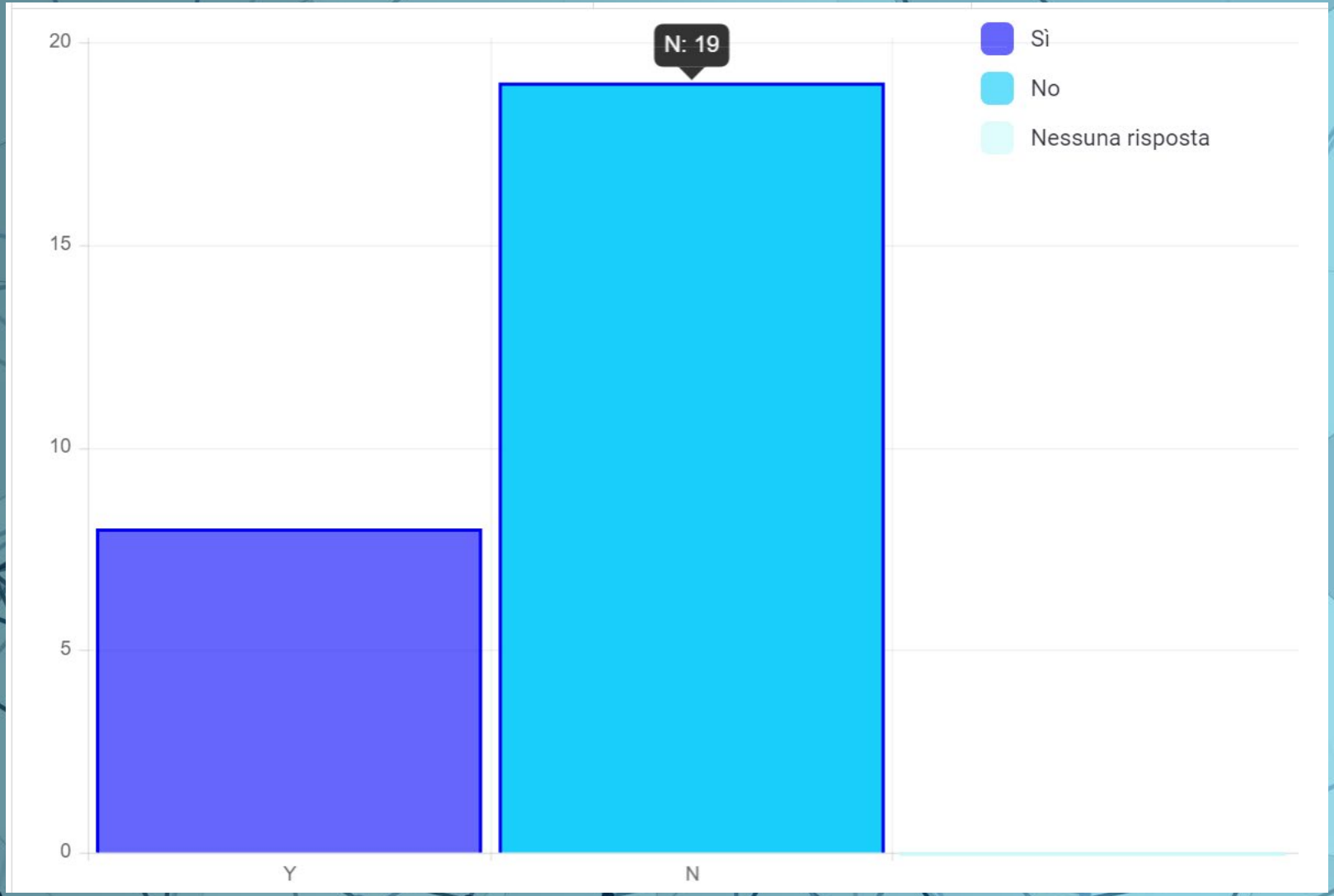
MCNP
LAMMPS
ANSYS CFX
Gromacs
MCNP
NAMD
OpenFOAM
OpenFOAM based solvers for SARS-Cov-2 Thermo-Fluid Dynamics
MCNPX
Quantum Espresso
AiiDA

License type

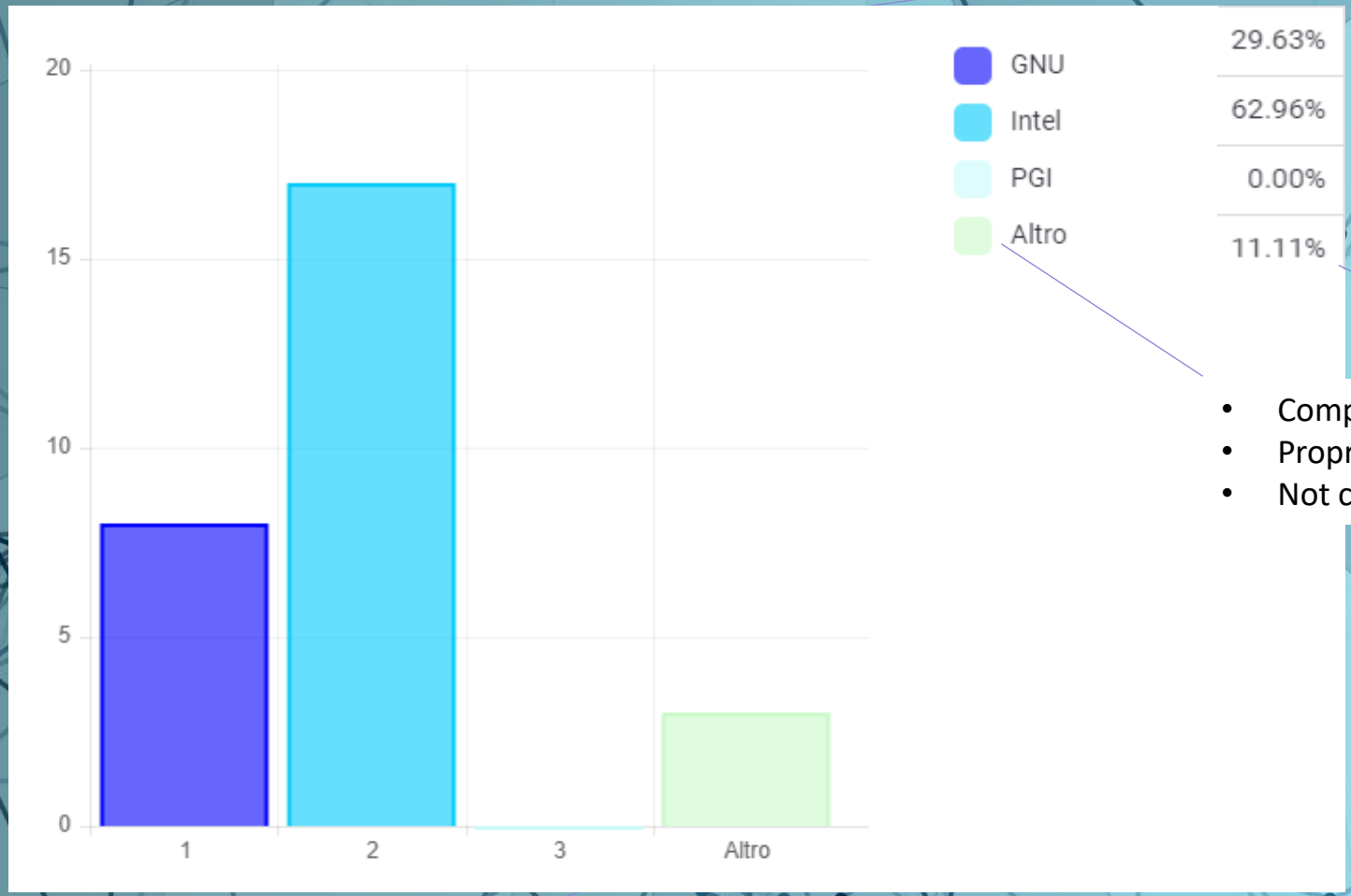
Have you developed the code or part of it?



Programming language(s) used in the software

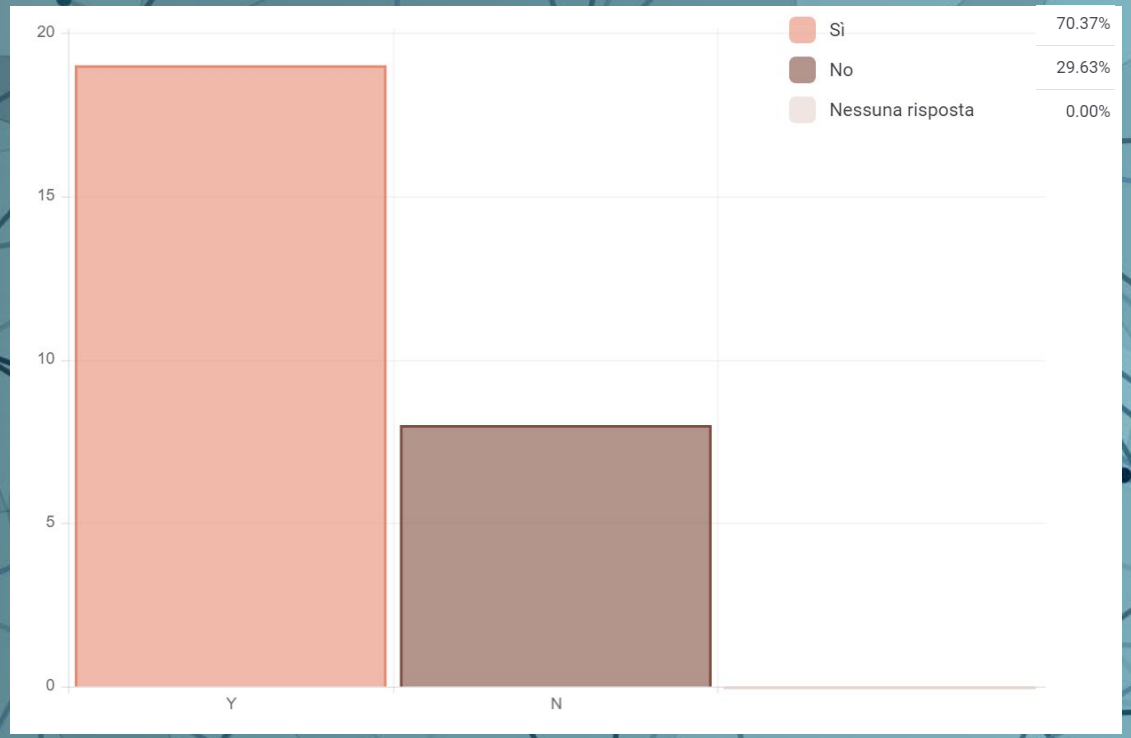
Octave
Python
JavaScript
CFX Command Language (CCL) and PERL
python
Python
pYTHON

Compilers used for the compilation

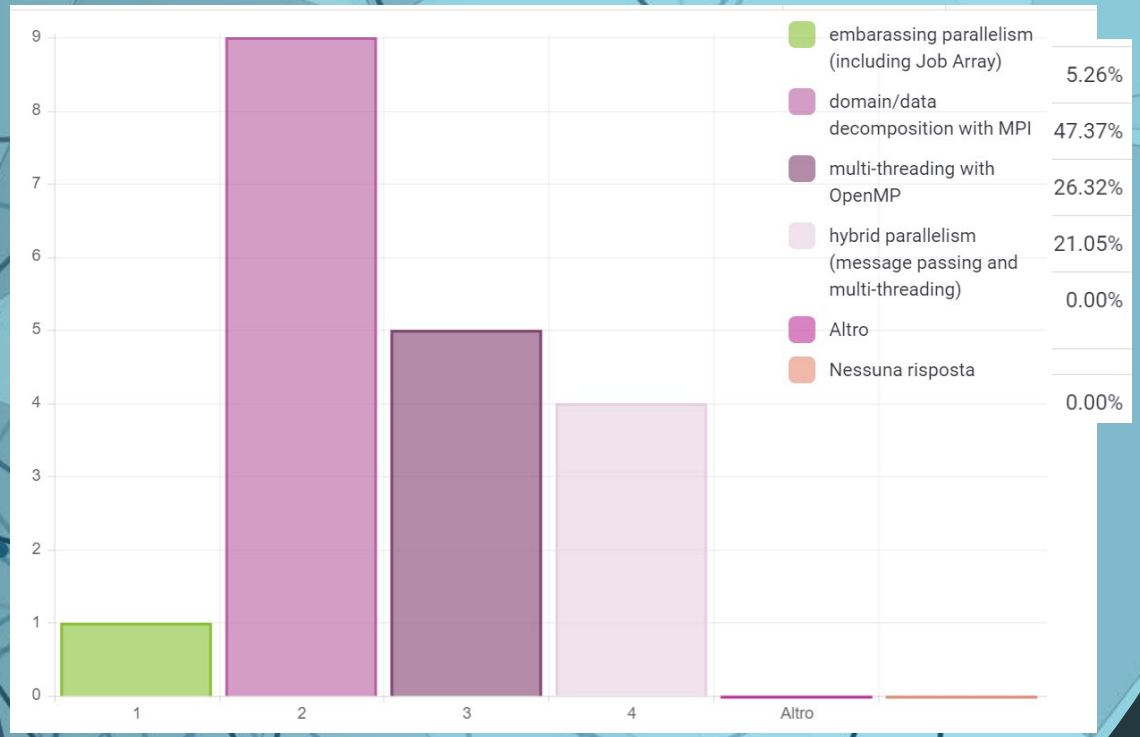


- Compiled version
- Proprietary compiler
- Not compiled

Parallelism implemented



Parallelism type



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