



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

Presentation of the CRESCO annual report: Research activities and results 2021 Accounting 2022

Online, 15/03/2023

Luigi Bucci: TERIN-ICT-HPC



1101 0110 1100
0101 0010 1101
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Italian National Agency for New Technologies,
Energy and Sustainable Economic Development

High Performance Computing on CRESCO infrastructure: research activities and results 2021



December 2022

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Contributions provided by a selection of users of the CRESCO infrastructure

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ENEA, TERIN-ICT-HPC

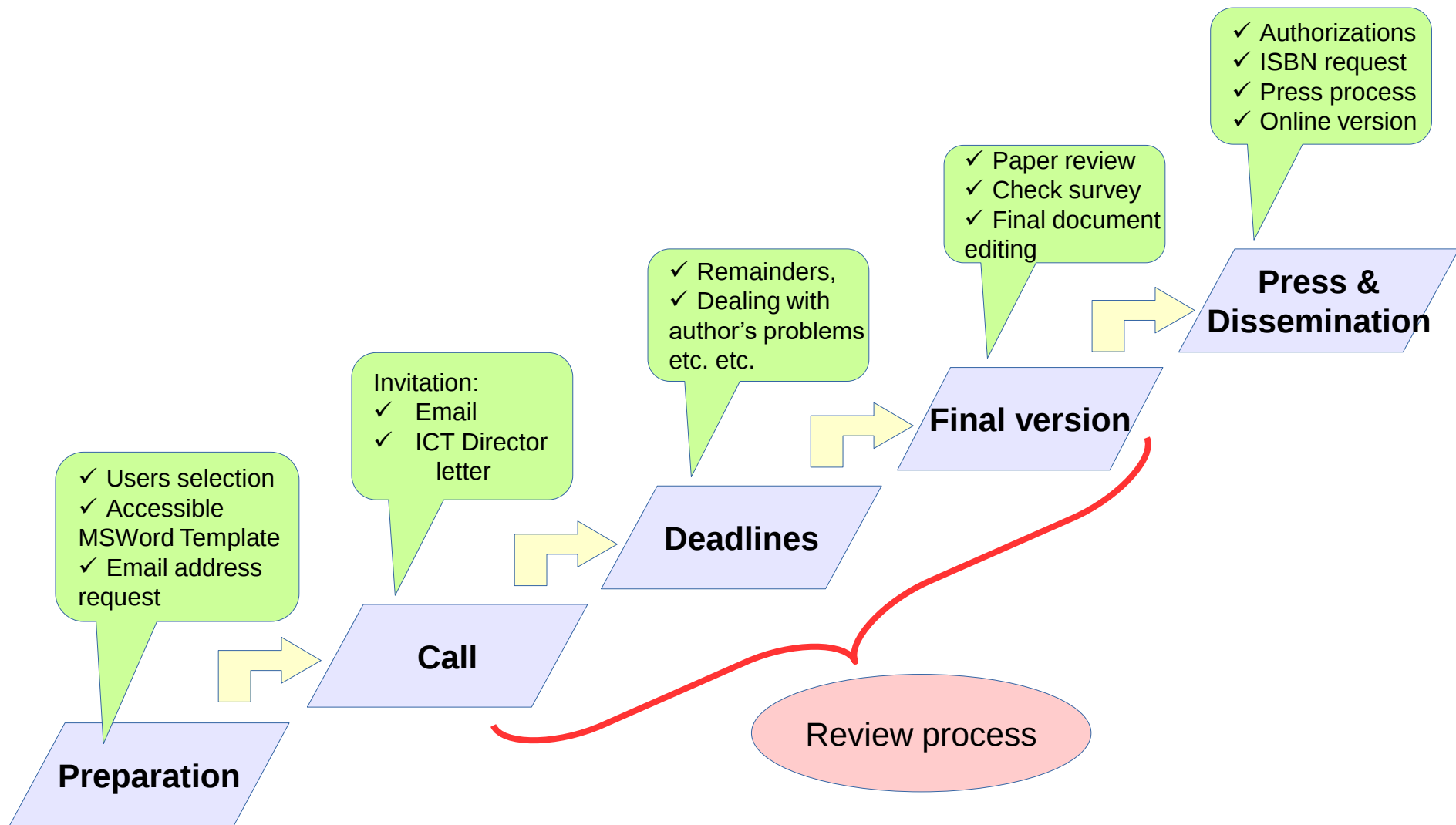
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ENEA, TERIN-ICT

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See also: [/afs/enea.it/project/eneagrid/html/SystemAdministration/CRESCO_Reports](https://afs.enea.it/project/eneagrid/html/SystemAdministration/CRESCO_Reports)
https://www.eneagrid.enea.it/CRESCOreports/Report_CRESCO_2021.pdf



Report Preparation



Report preparation history

- 2022-07:
 - user selection from: Isf accounting (info from kerberos lists and mailing lists);
 - survey tool kit (LimeSurvey: <http://sondaggi.enea.it/index.php/>): user list, mails;
- 2022-08-03: invitation mail (115 invited users);
- 2022-09-30: first deadline;
- 2022-11-30: deadline extensions;
- 2022-12: final check, author index, samples for the cover;
- 2022-12: authorization process for the publication by REL-PROM;
- 2023-01: press & dissemination;
- 2023-03: presentation prepared (this presentation).

◆ PDF version online:

https://www.eneagrid.enea.it/CRESCOreports/Report_CRESCO_2021.pdf

Invited Users

115/193 users invited

Selection criterium is:

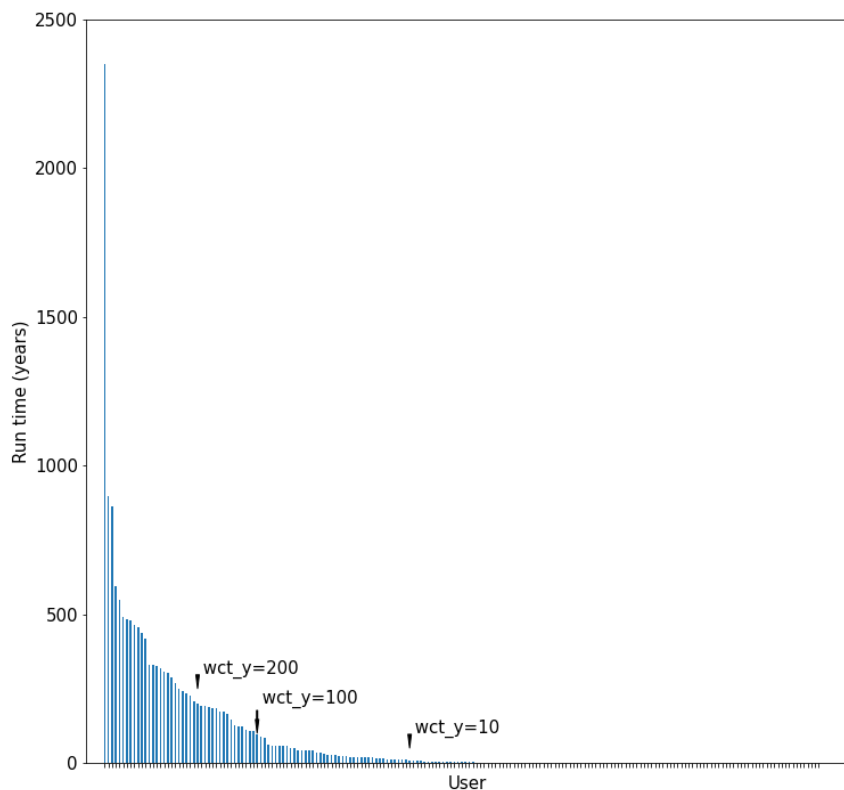
$wct_y > 1.0 \parallel (av_totcore * > 5000)$

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

CRESCO wall clock time (wct_y) 2021-2022

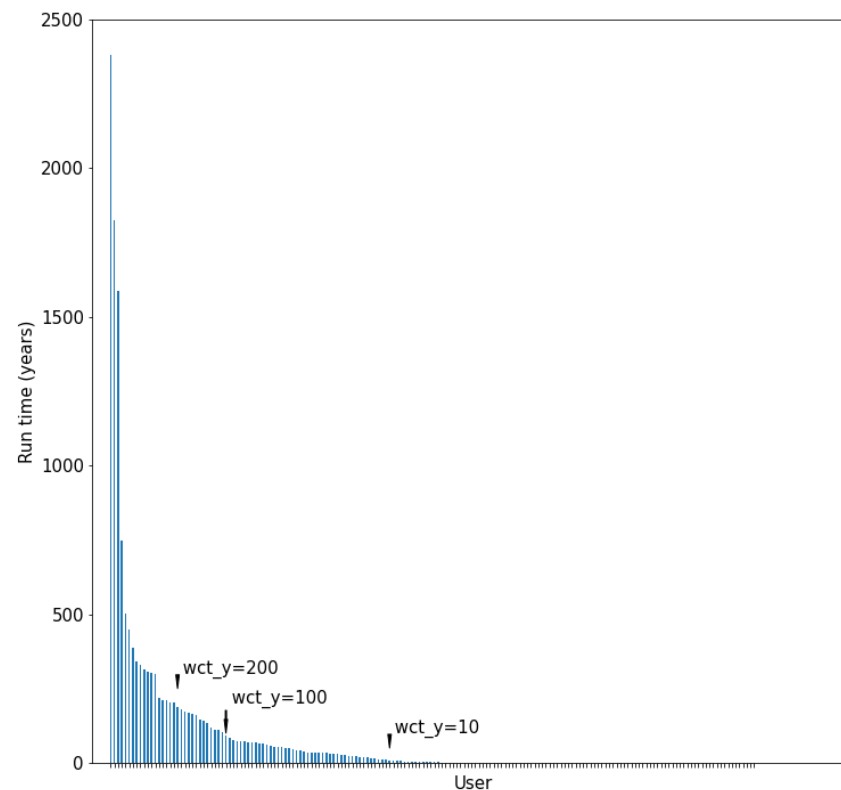
Wall clock time by user 2021-2022

Total run time by user 2021 (wct_y)



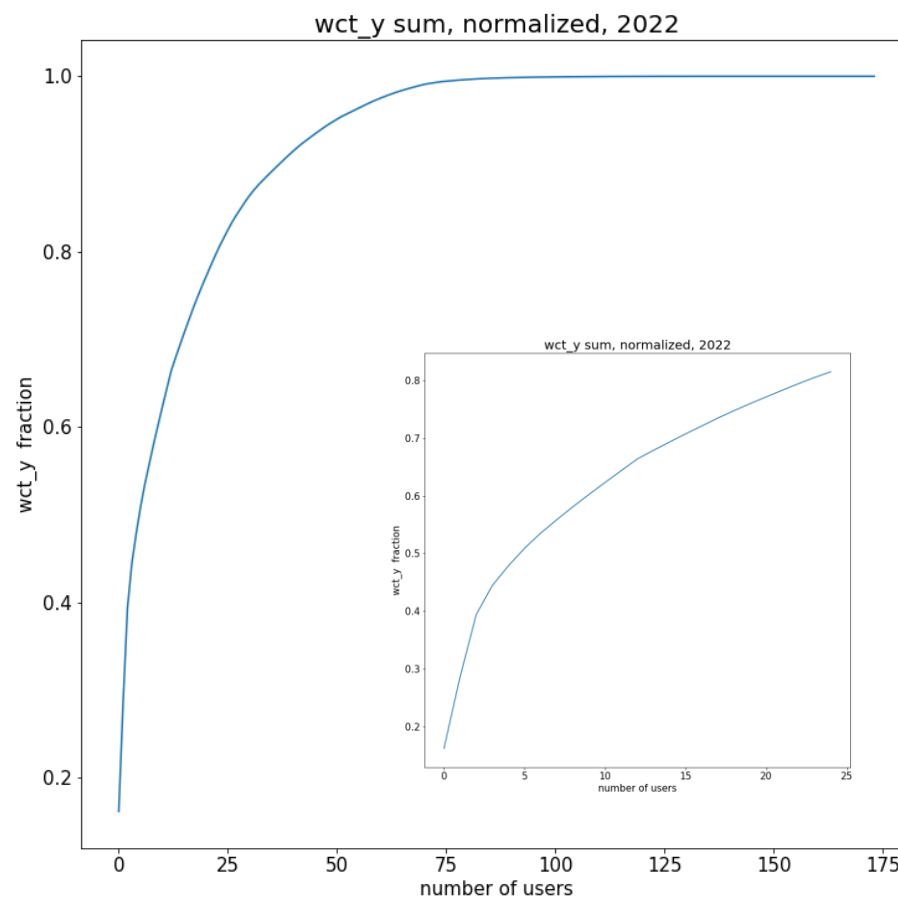
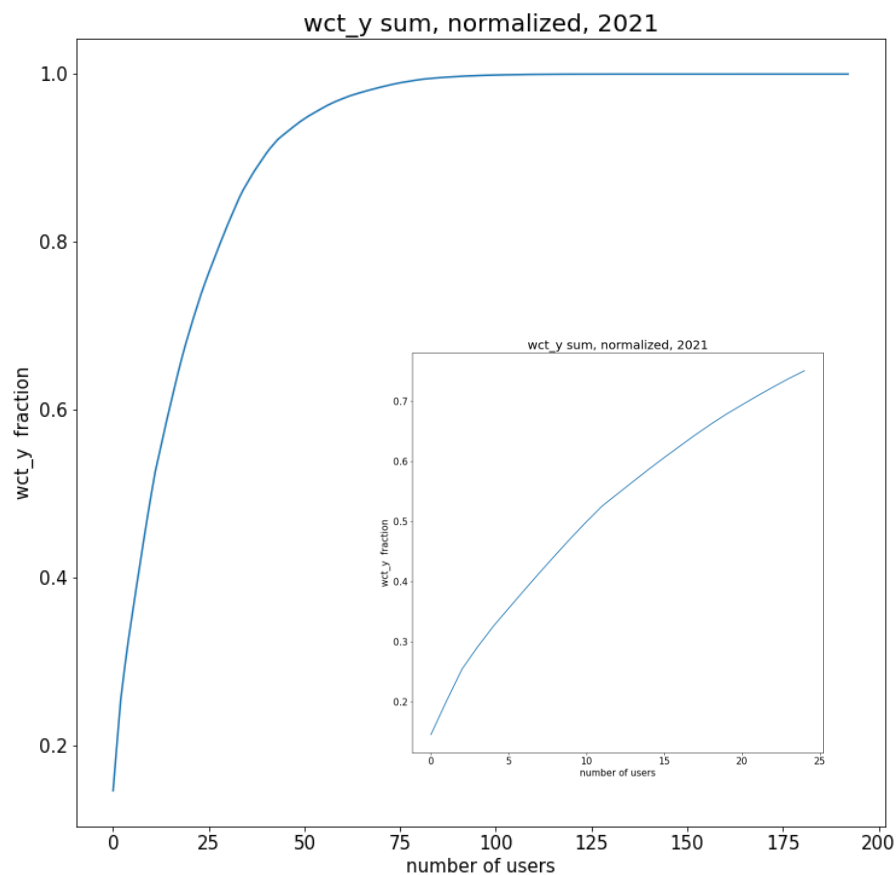
Tot. usage in 2021: 16130 years
wct_y > 200: 25 users
wct_y > 100: 41 users
wct_y > 10: 82 users

Total run time by user 2022 (wct_y)



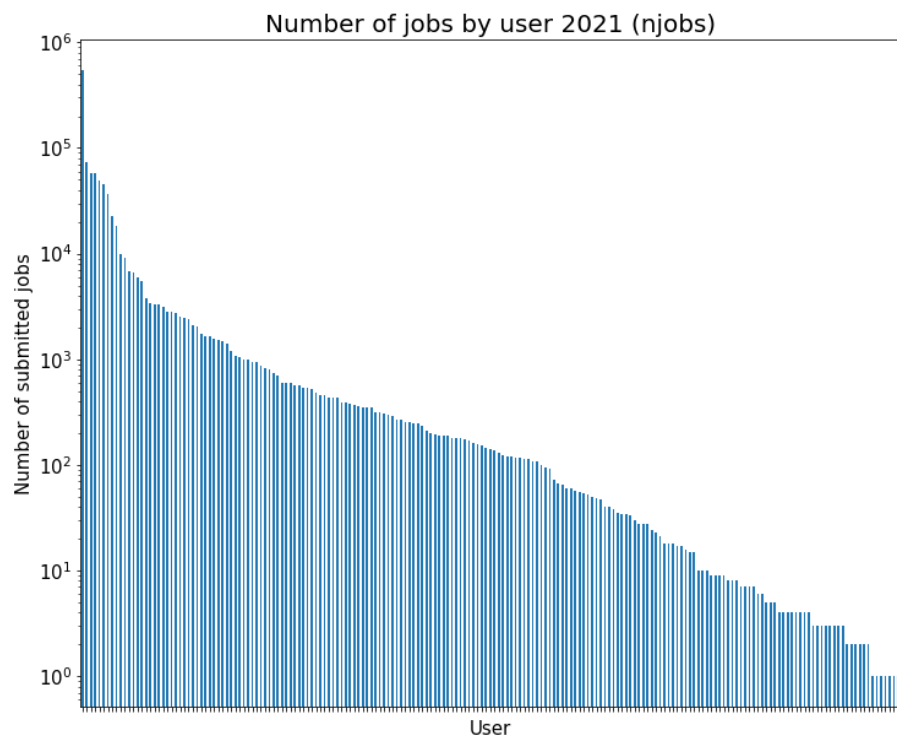
Tot usage in 2022: 14705 years
wct_y > 200: 18 users
wct_y > 100: 31 users
wct_y > 10: 75 users

Cumulative wall clock time distribution by user 2021-2022

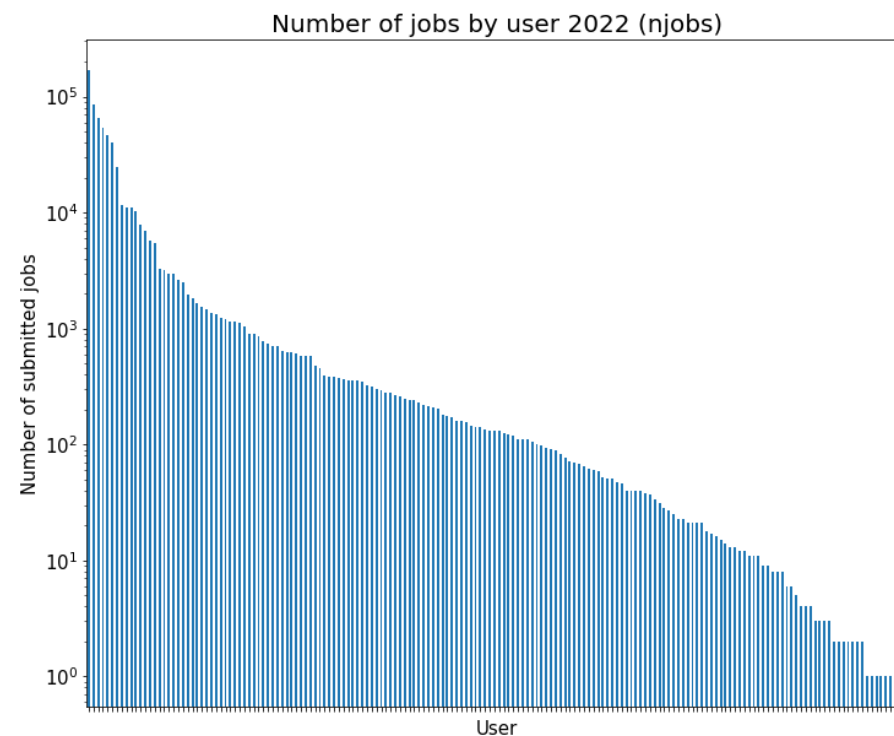


CRESCO number of jobs (njobs) 2021-2022

Total usage – njobs 2021-2022

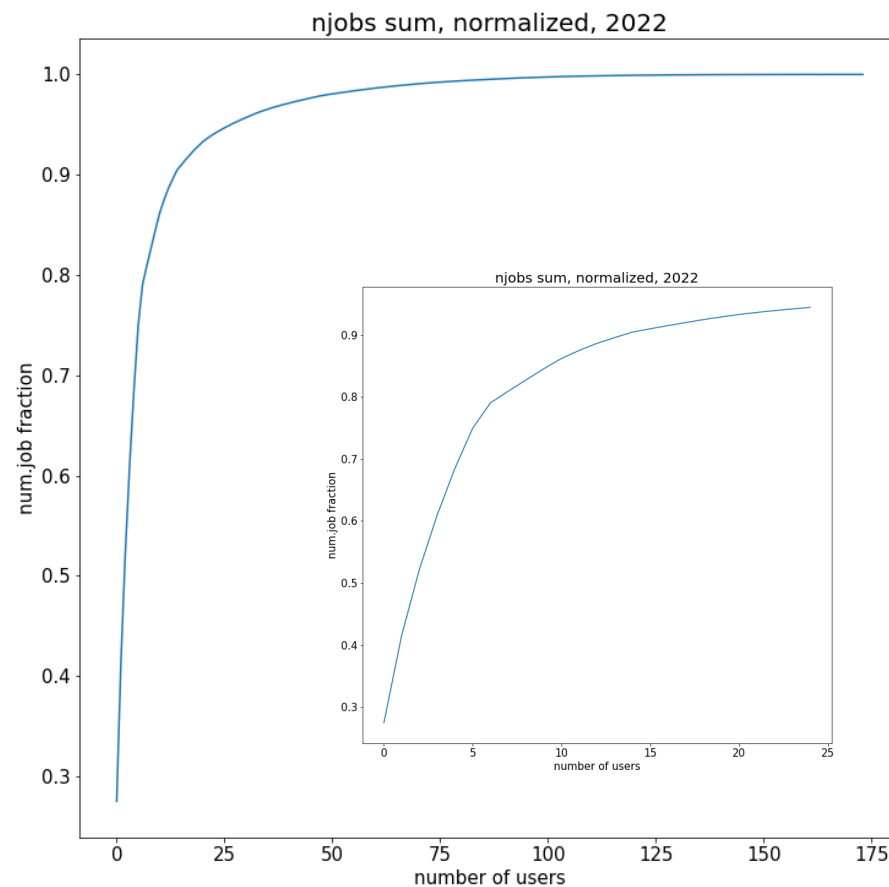
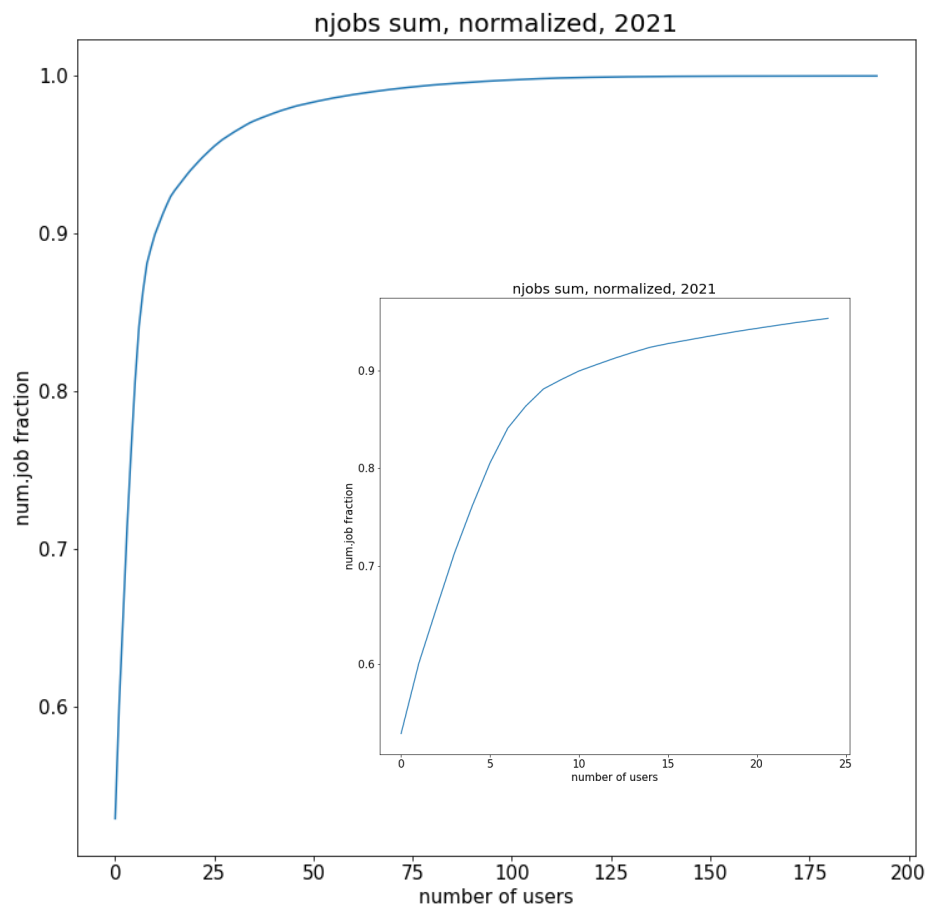


Tot. njobs 2021: 1.027.713



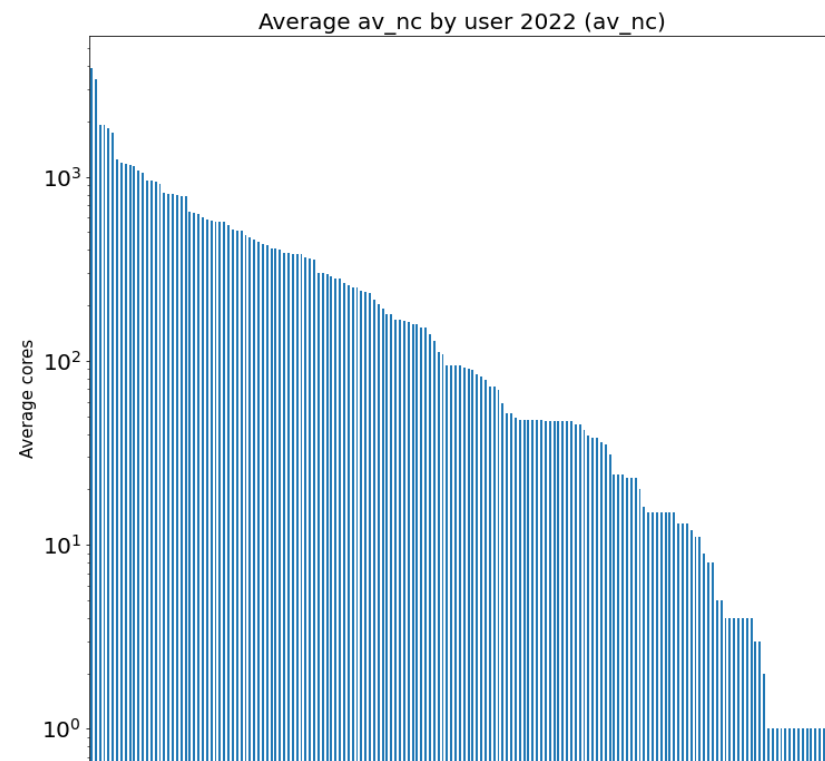
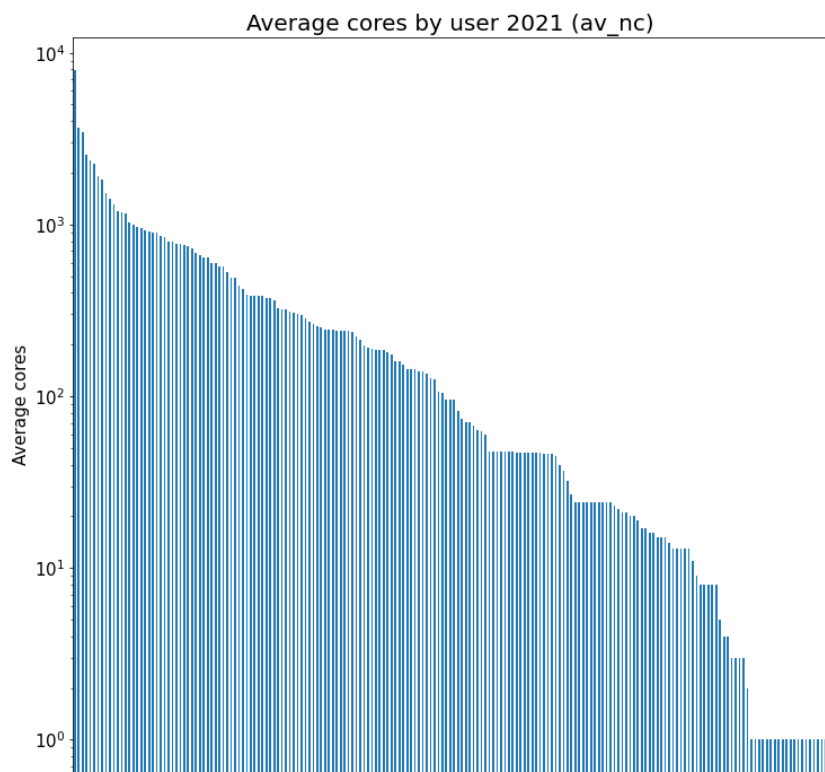
Tot. njobs 2022: 613.642

Cumulative njobs distribution by user 2021-2022



CRESCO average number of cores (nc_av) 2021-2022

Average number of cores by user 2021-2022



Average number of cores is 969 (2021) and 1020 (2022)
CRESCO6 has ~20000 cores but there is a limit on LSF: up to 6144 cores
(limit not valid for system queue only for admin).

Accounting details 2021-2022 ENEA and External Institutions

The 2021 CRESCO Users

Users 193

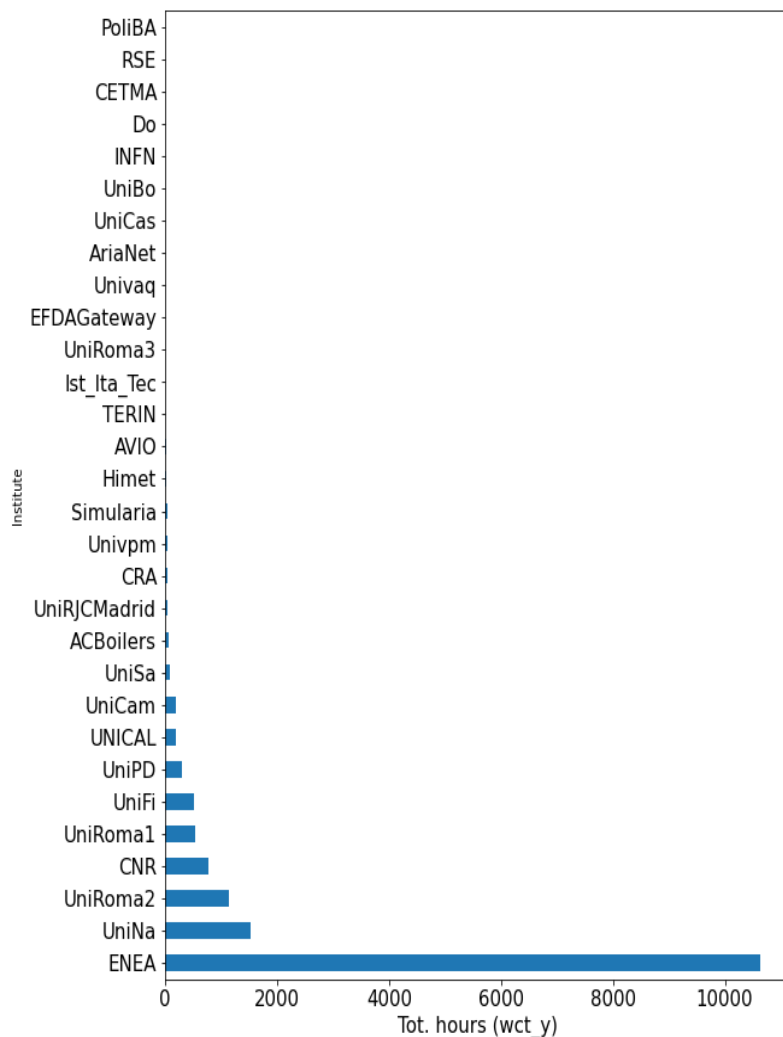
ENEA	129
TERIN	52
FSN	50
SSPT	22
other	5

External	64
UniNa	12
UniRoma1, Uniroma2	7
UNICAL, CNR, ACBoilers	3
UniSa, UniFi, UniCam, Simularia, AriaNet Ist_Ita_Tec, UniCas	2
UniBo, Uniroma3, PoliBA, Univpm, AVIO, UNIRCJMadrid, Himet, Do, CETMA, CRA, Univaq EFDAGateway, RSE, INFN, UniPD	1

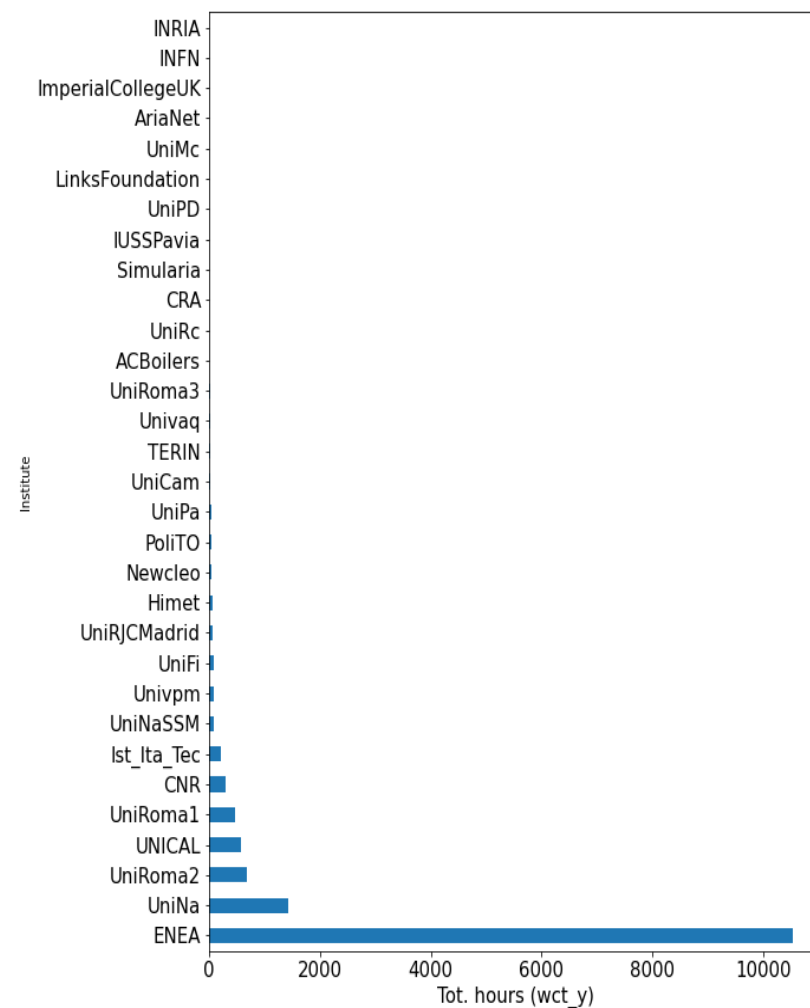
CRESCO wall clock time_years in details 2021-2022

ENEA and External usage wct_y 2021-2022

Total run time 2021 by Institute (wct_y)

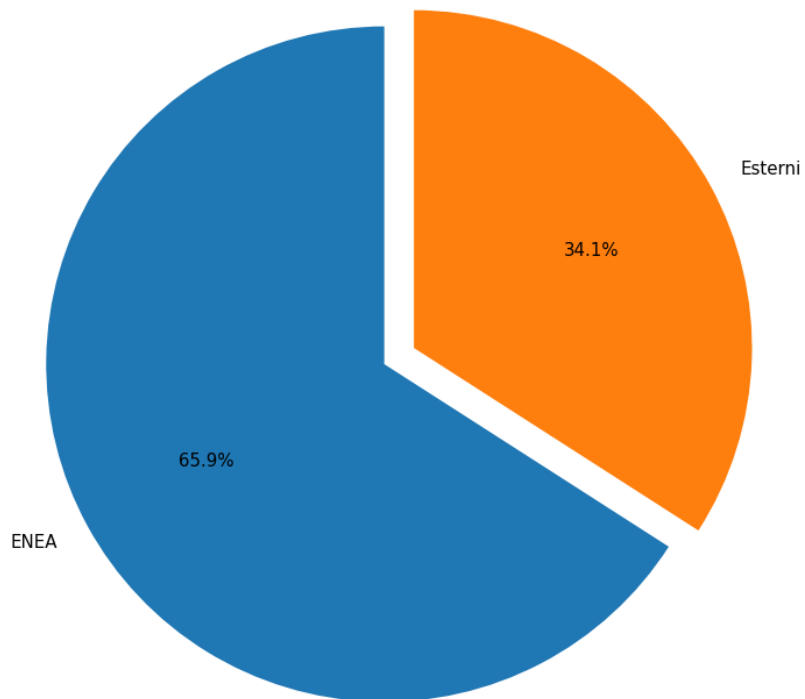


Total run time 2022 by Institute (wct_y)

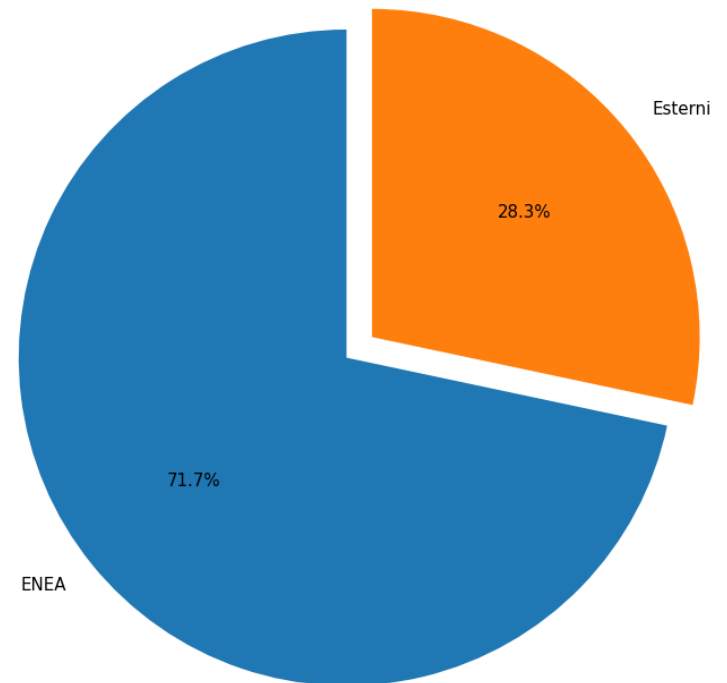


ENEA and External users usage (%wct_y) 2021-2022

Percentage run time 2021: ENEA and External Users

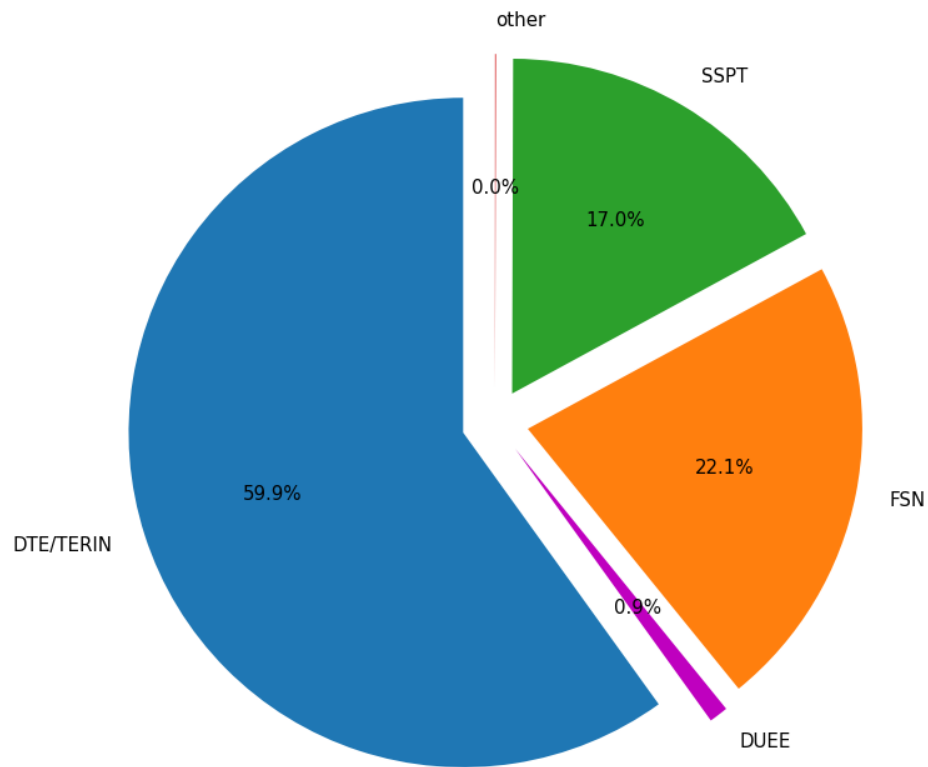


Percentage run time 2022: ENEA and External Users

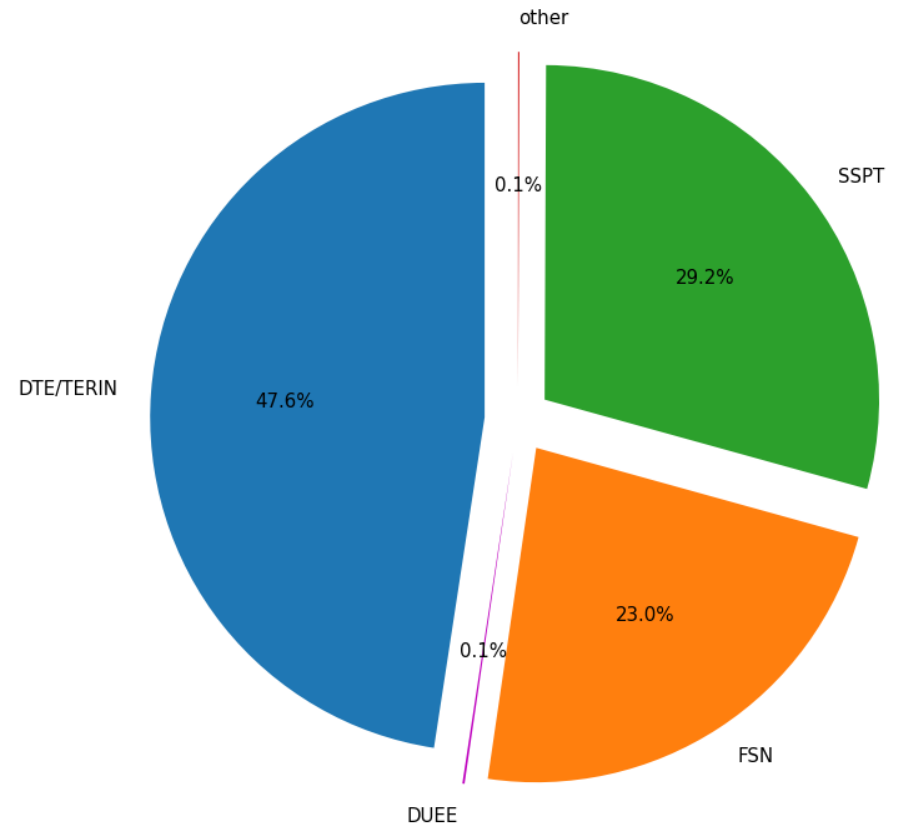


Percentage run time by ENEA department (internals) 2021-2022

Percentage run time 2021 for ENEA department (wct_y)

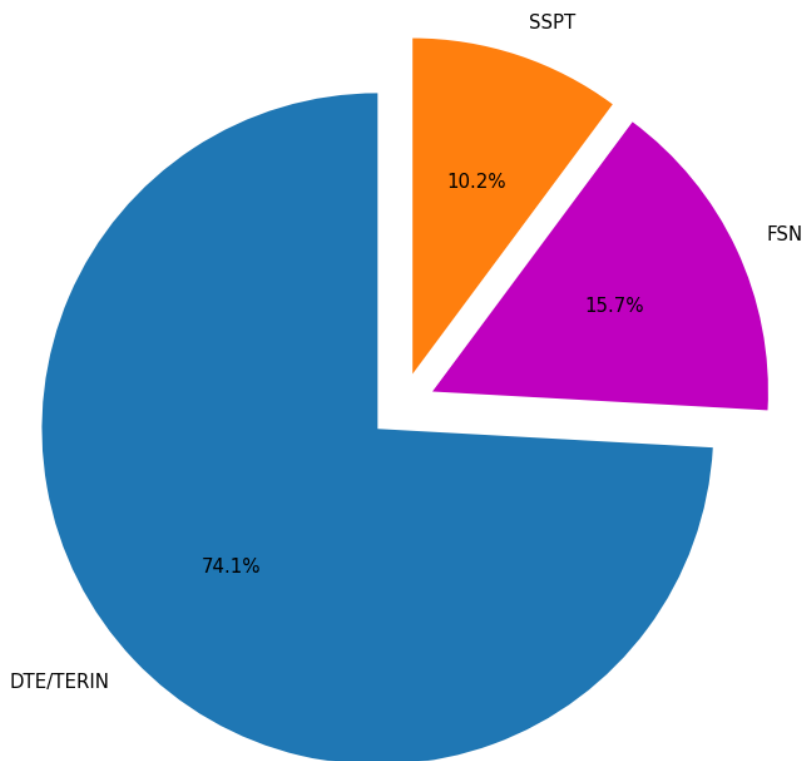


Percentage run time 2022 for ENEA department (wct_y)

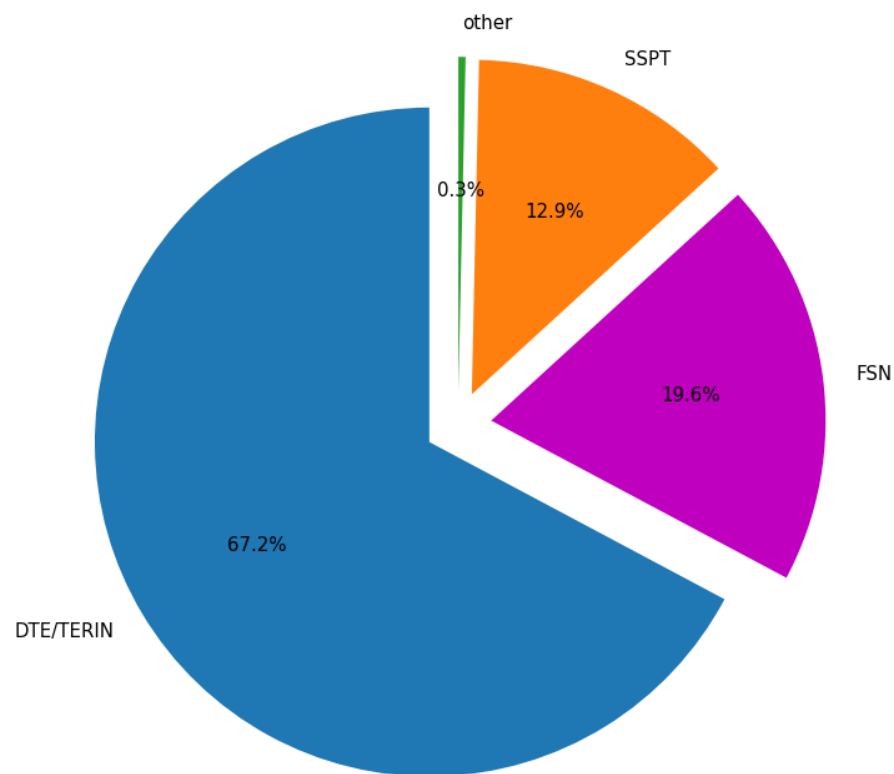


Percentage run time by ENEA department (collaboration) 2021-2022

Percentage run time 2021 for ENEA department-collaboration (wct_y)



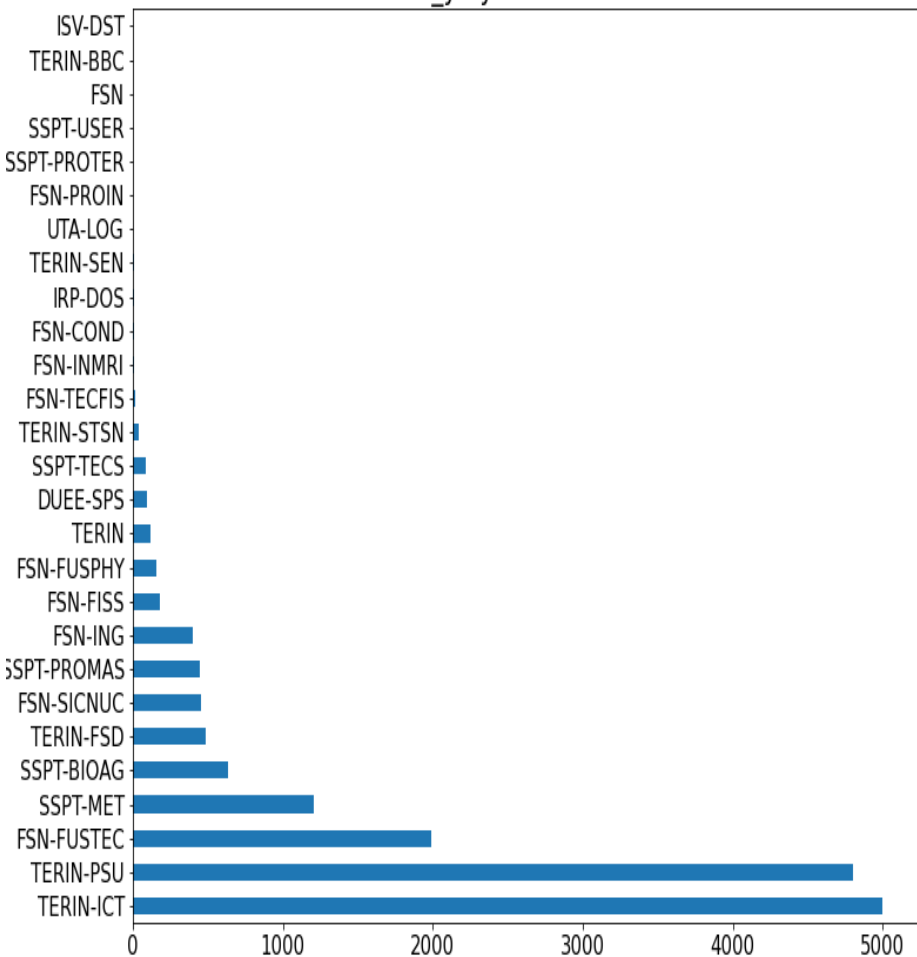
Percentage run time 2022 for ENEA department-collaboration (wct_y)



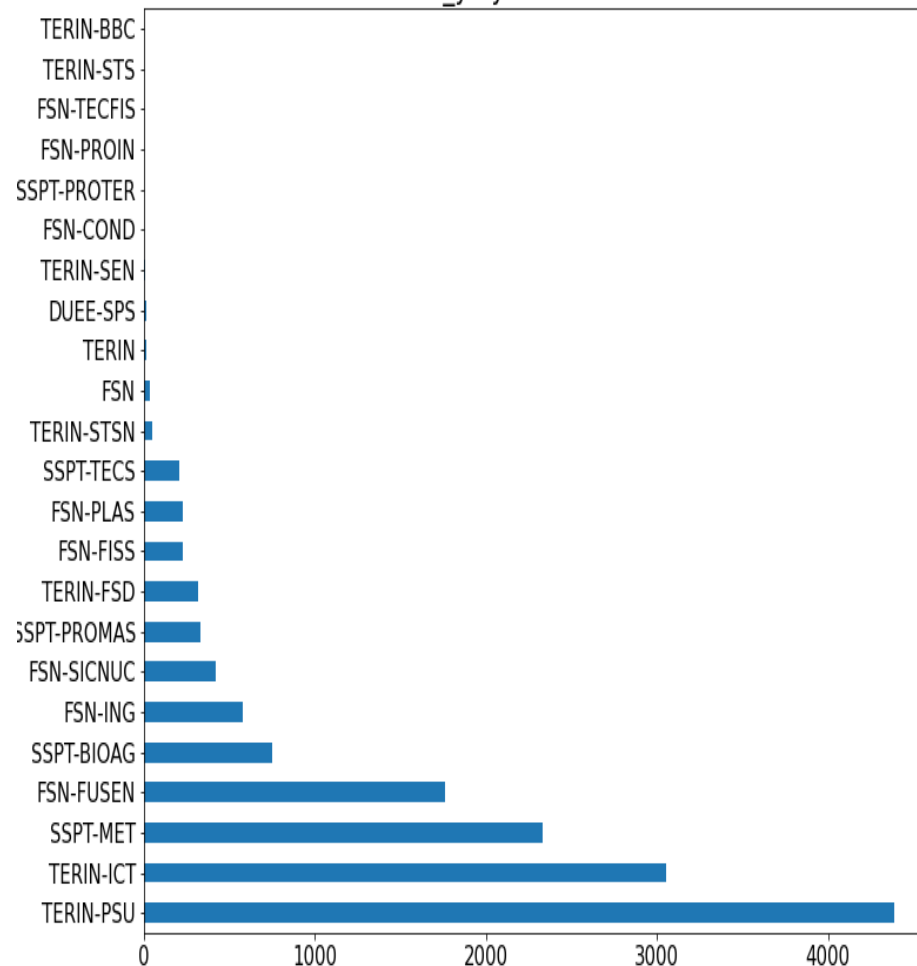
ENEA usage by Division (wct_y)

2021-2022

wct_y by Division 2021



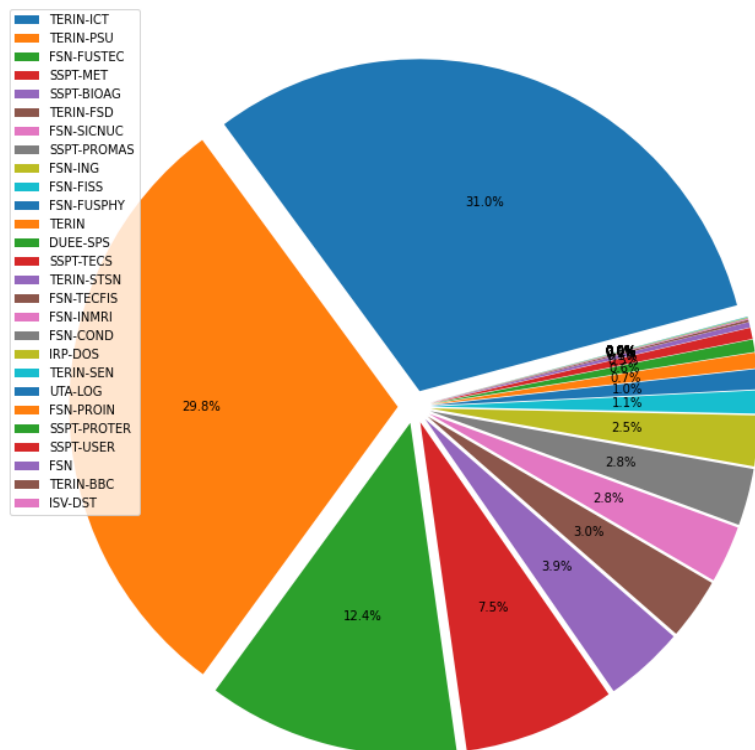
wct_y by Division 2022



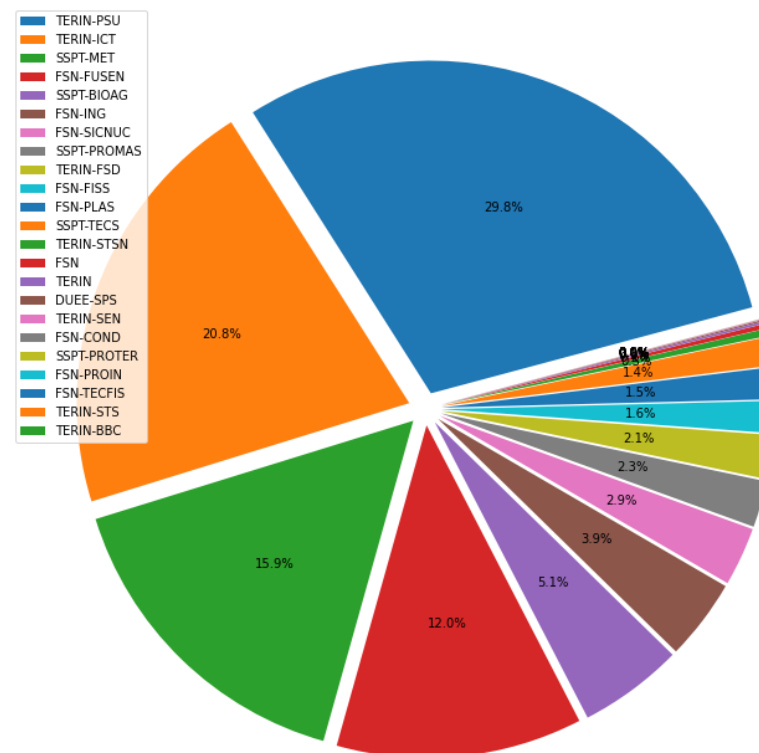
ENEA usage by Division (%wct_y)

2021-2022

ENEA-Division wct_y-percentage 2021



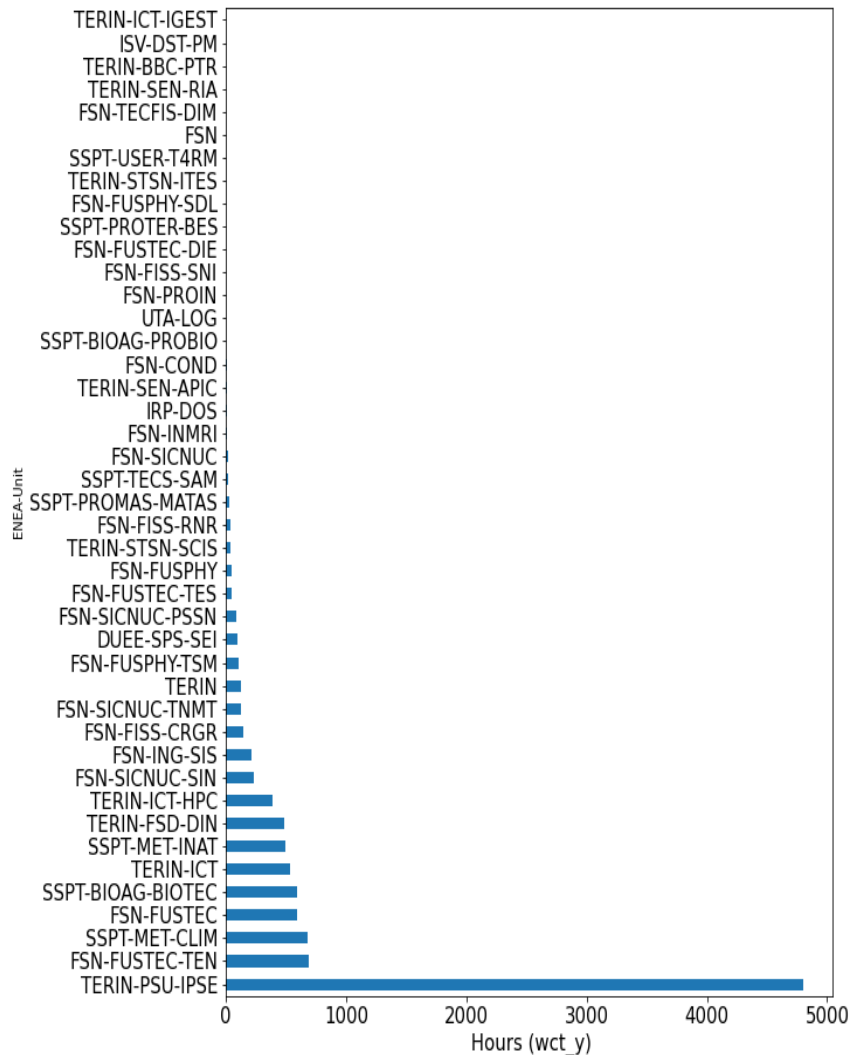
ENEA-Division wct_y-percentage 2022



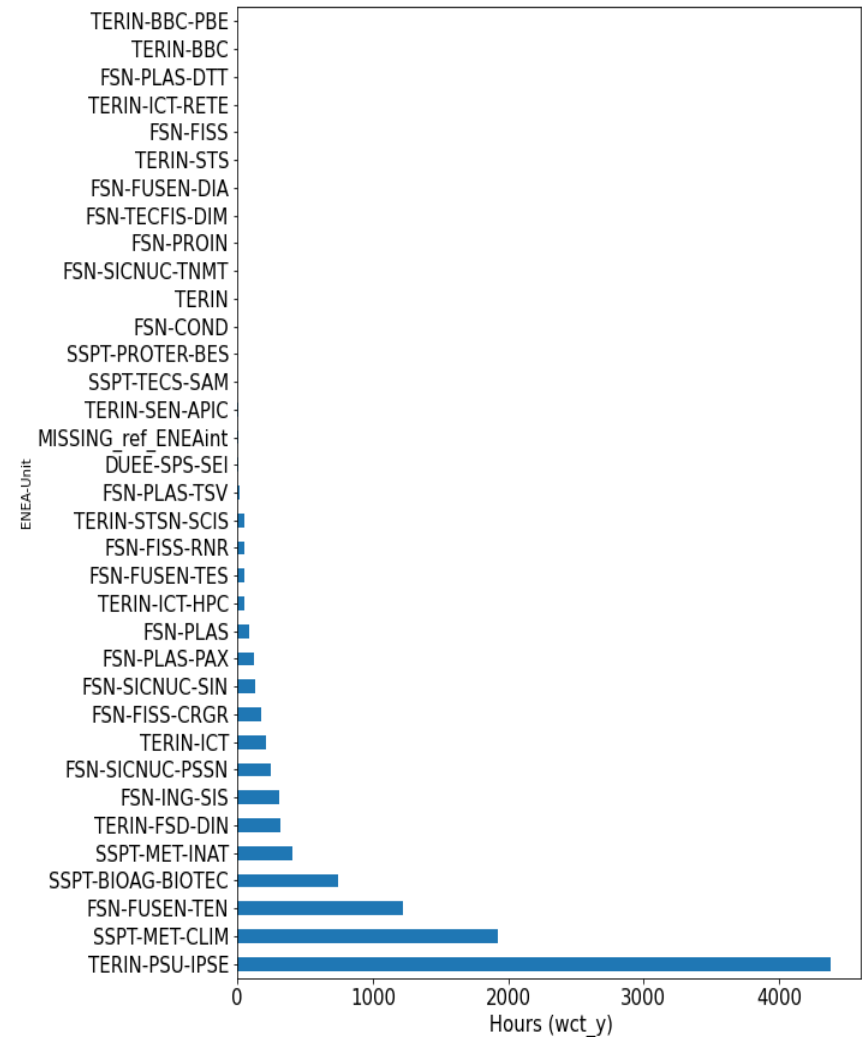
ENEA usage laboratories (internals) wct_y

2021-2022

Total run time 2021 for ENEA laboratories (wct_y)

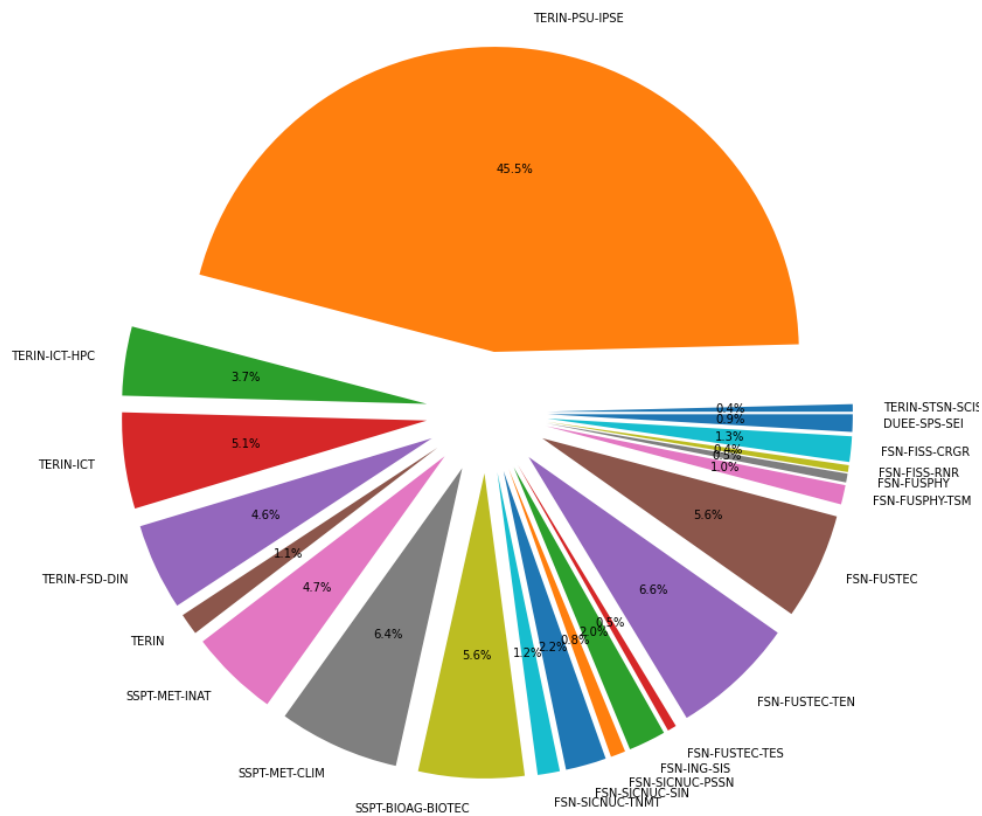


Total run time 2022 for ENEA laboratories (wct_y)

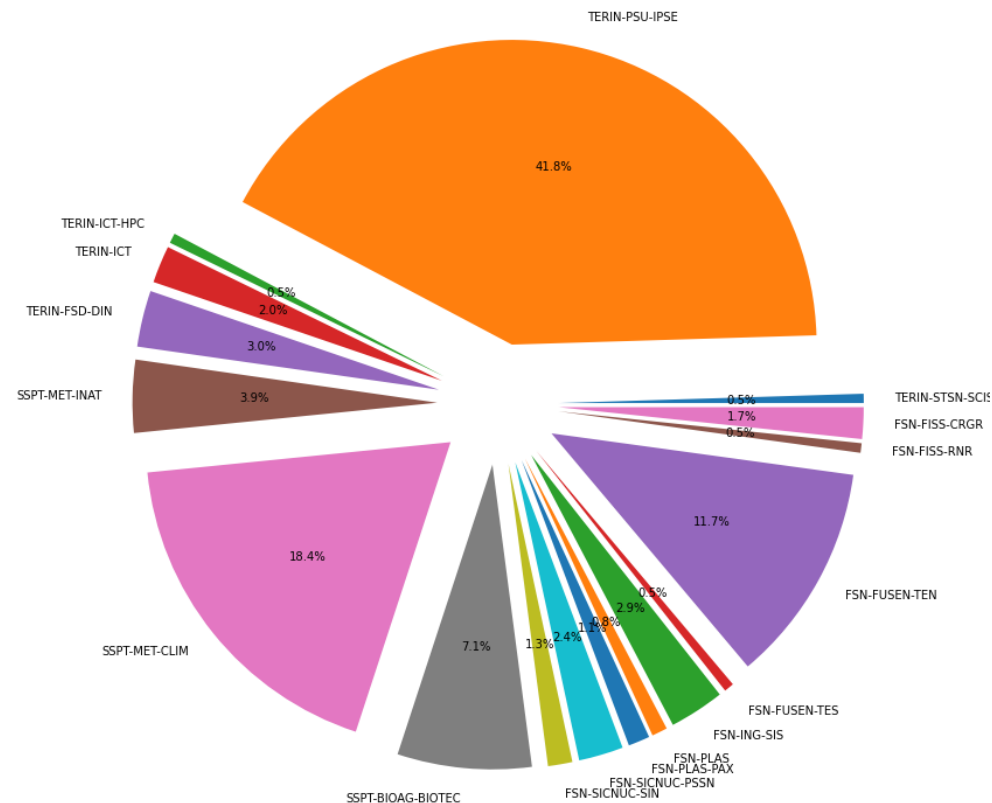


Percentage run time by ENEA laboratories (internals) 2021-2022

ENEA-lab percentage wct_y 2021



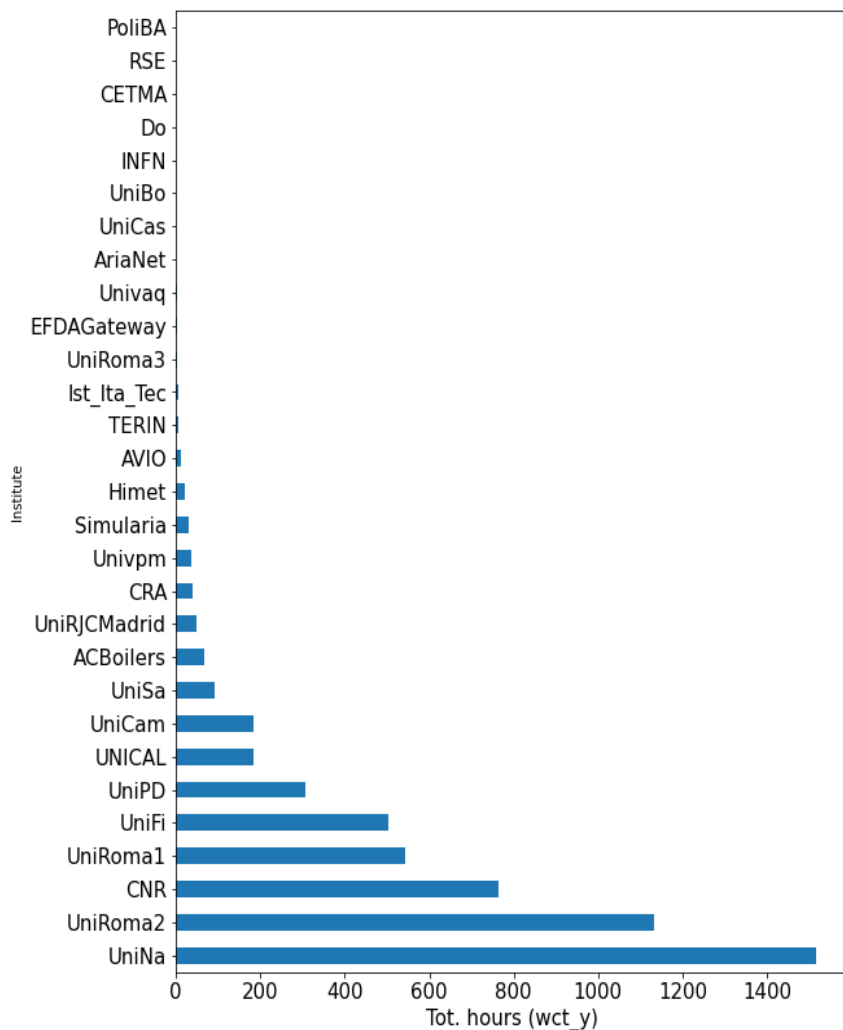
ENEA-lab percentage wct_y 2022



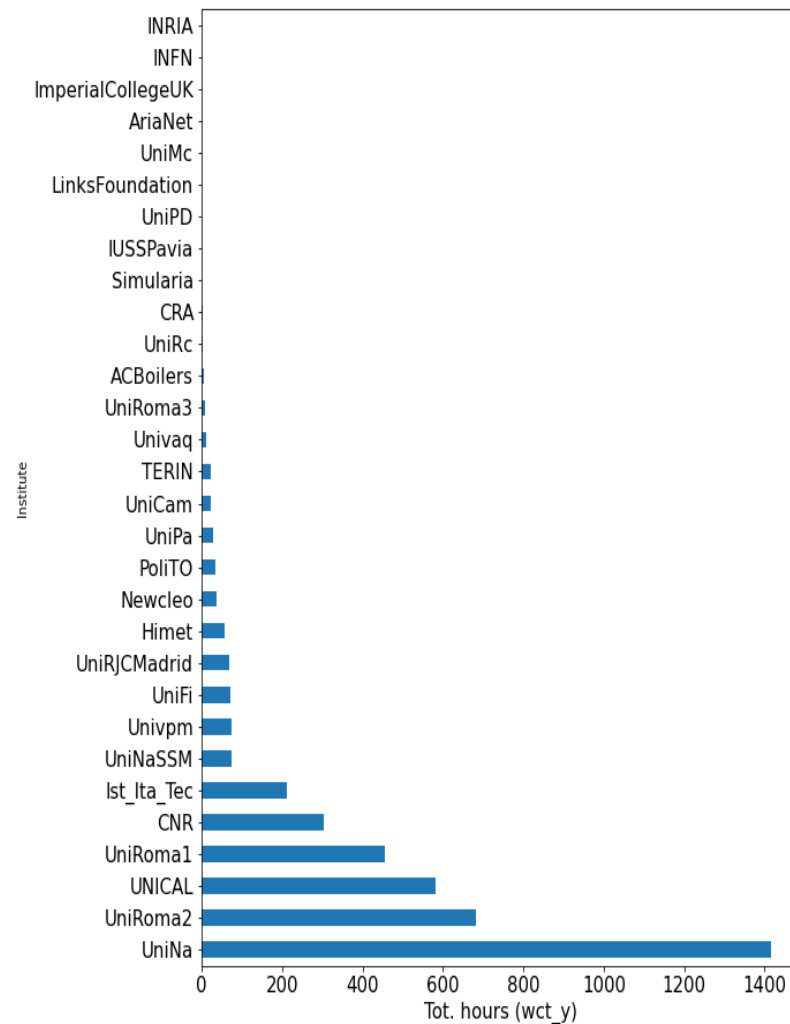
Usage by external institute (wct_y)

2021-2022

Total run time 2021 for external institutes (wct_y)

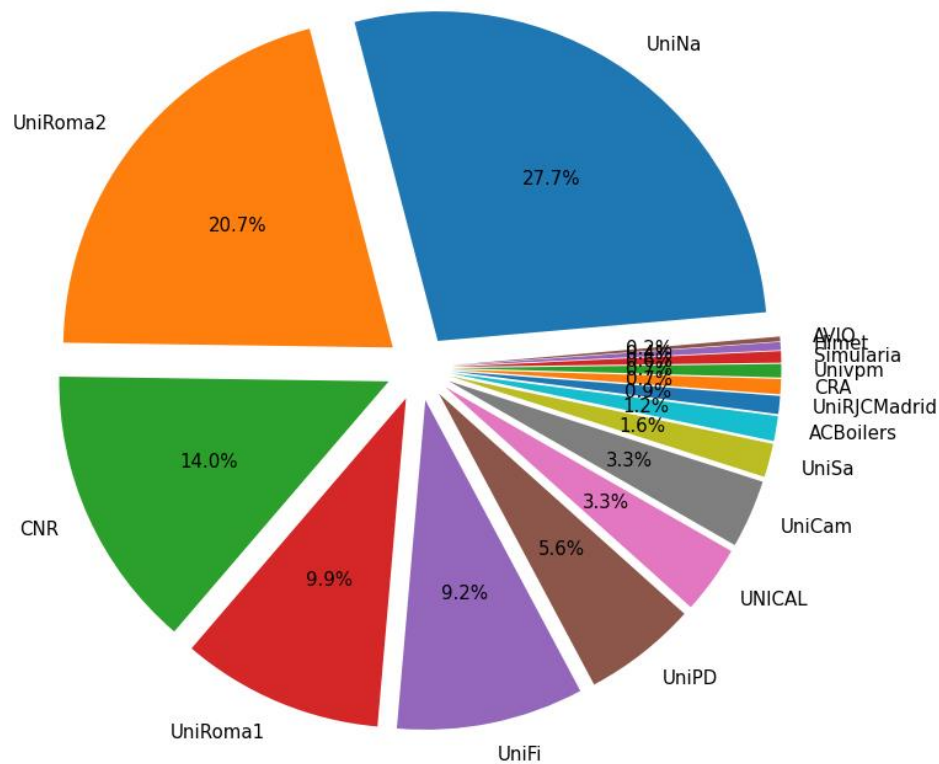


Total run time 2022 for external institutes (wct_y)

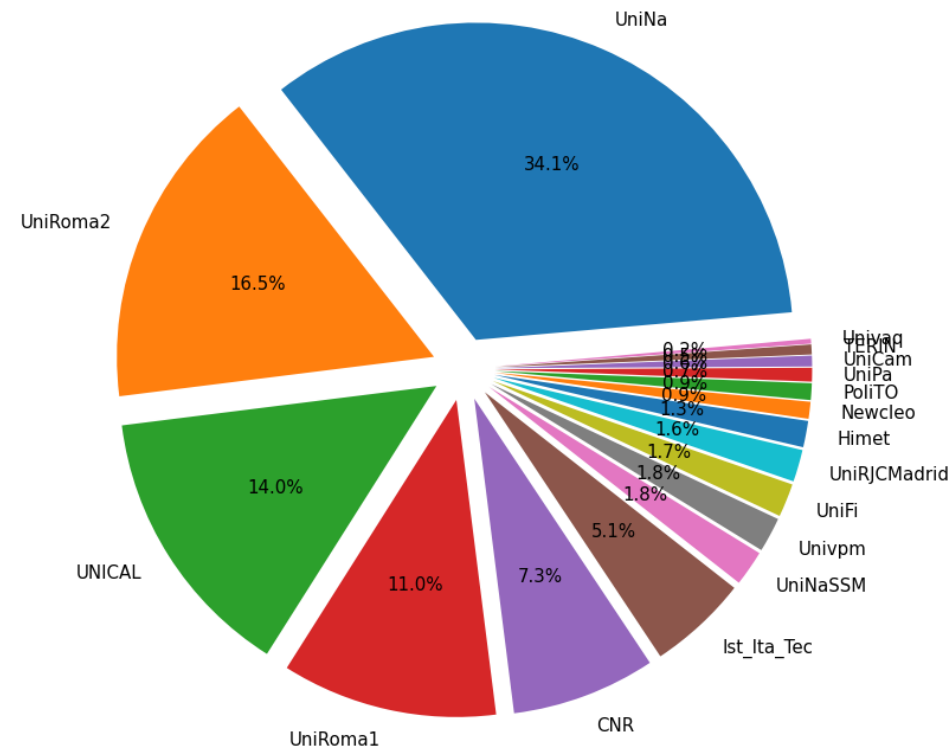


Usage by external institute (%wct_y) 2021-2022

Percentage run time 2021 for external institutes (wct_y>10)

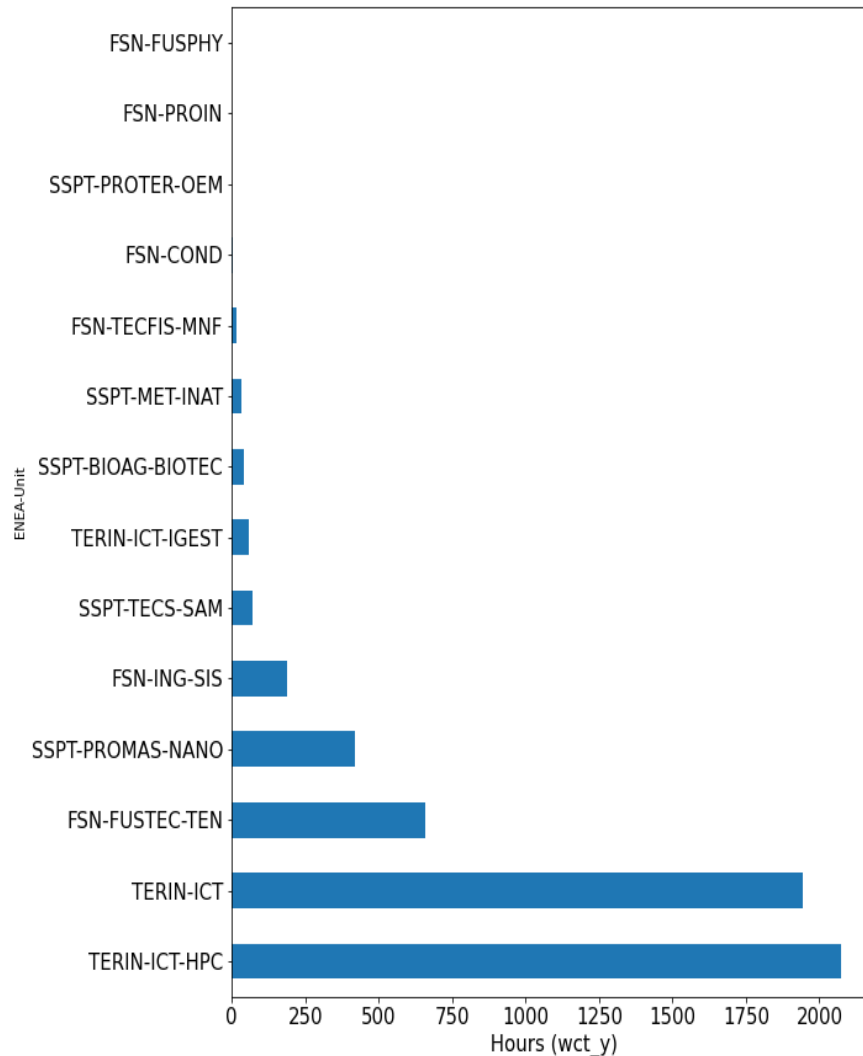


Percentage run time 2022 for external institutes (wct_y>10)

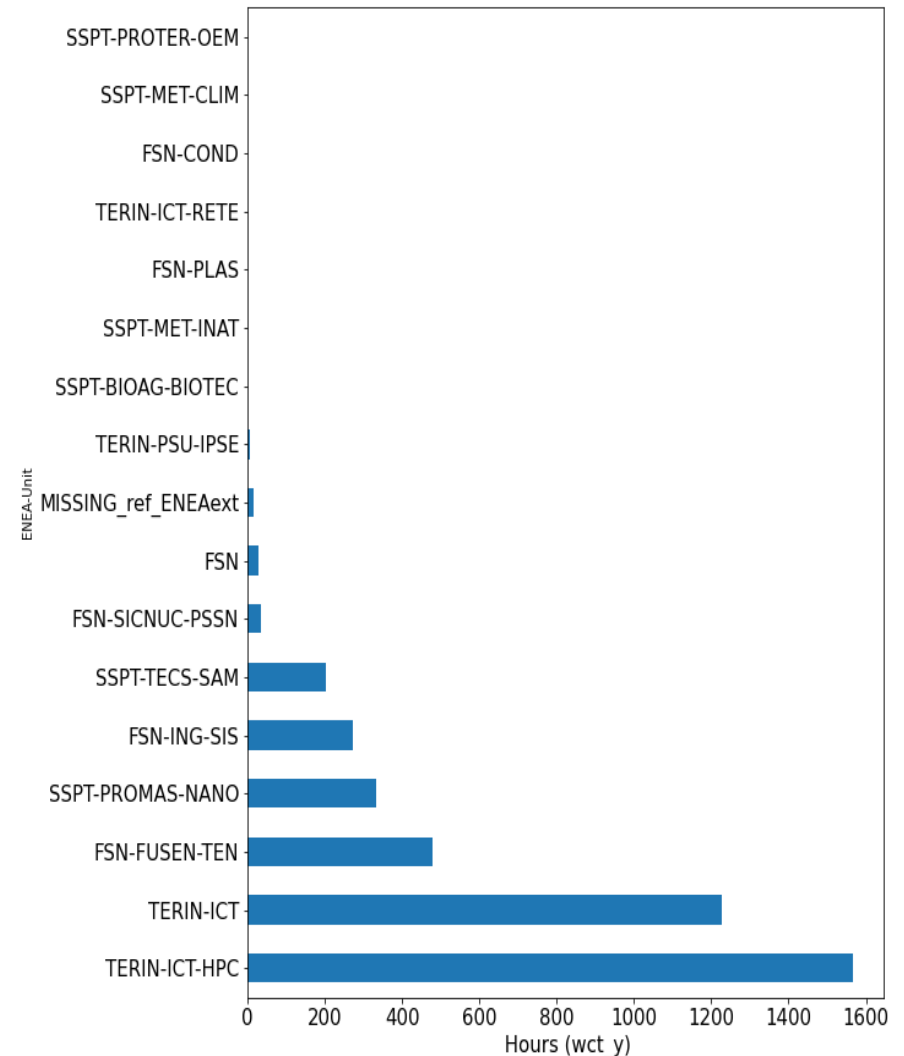


Usage by External Institute-ENEA lab collaboration (wct_y) 2021-2022

Total run time 2021 for ENEA laboratories collaboration (wct_y)

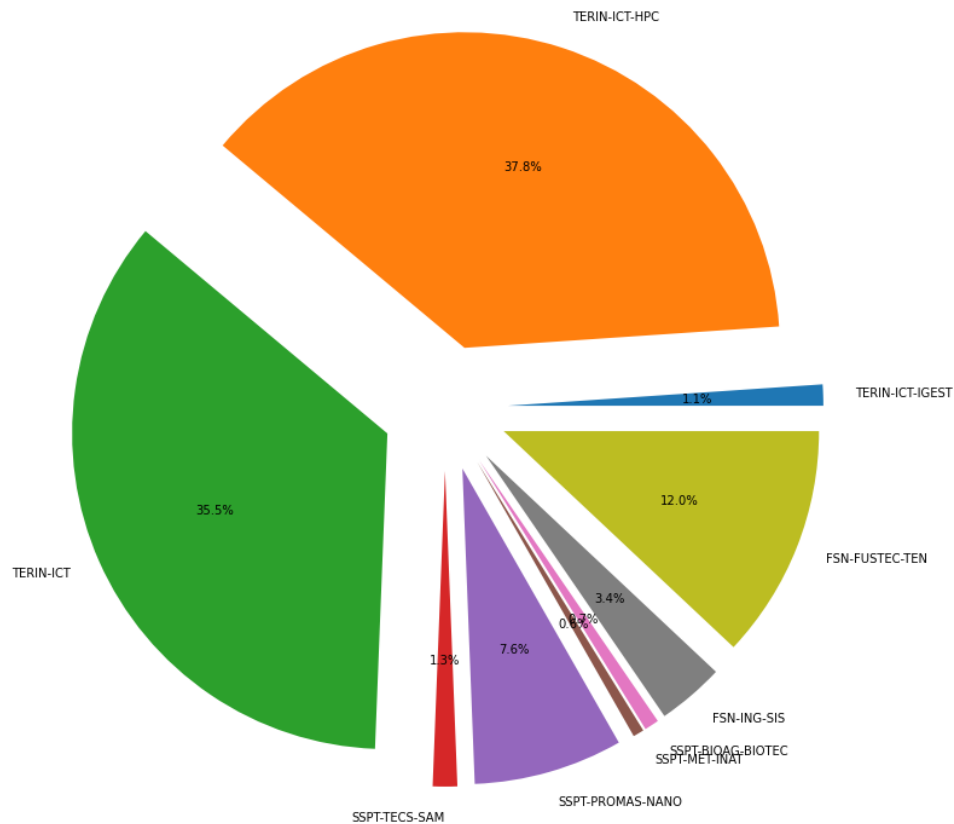


Total run time 2022 for ENEA laboratories collaboration (wct_y)

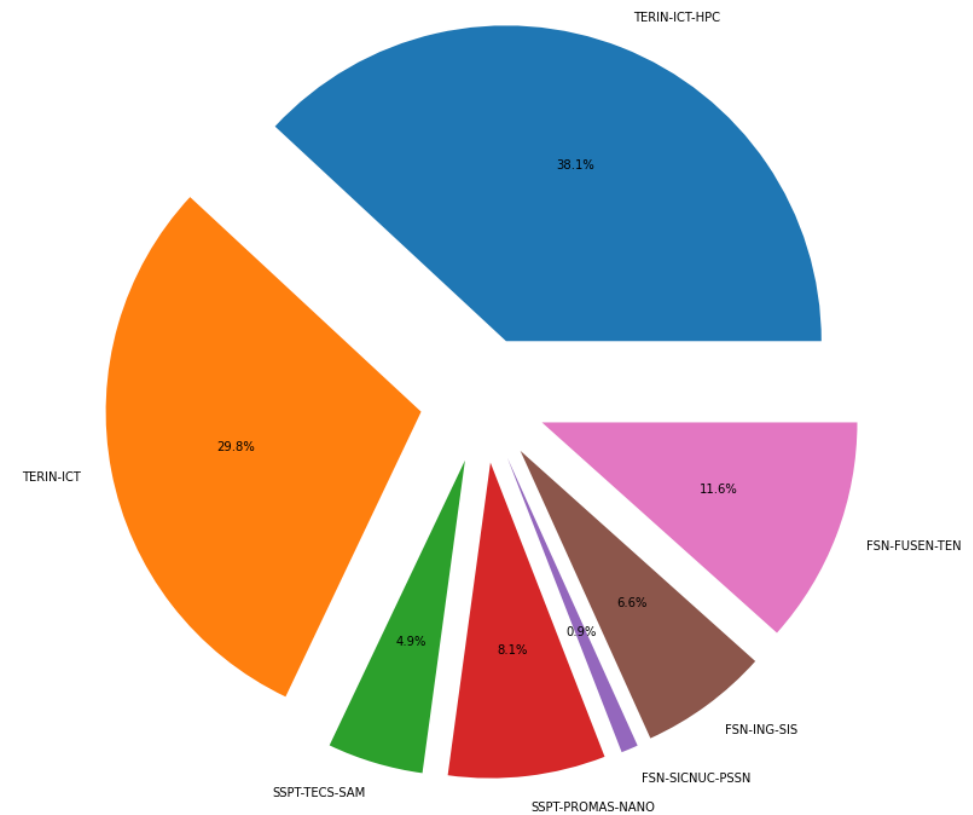


Usage by External Institute-ENEA lab collaboration (%wct_y) 2021-2022

ENEA-lab-collaboration percentage wct_y 2021



ENEA-lab-collaboration percentage wct_y 2022

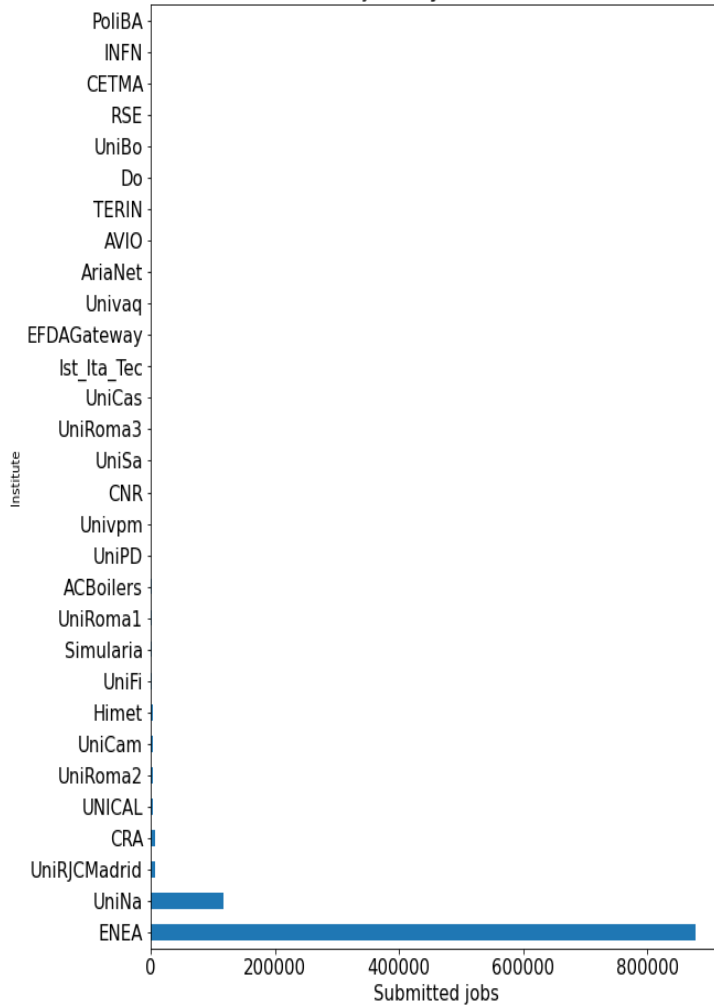


Detailed CRESCO usage

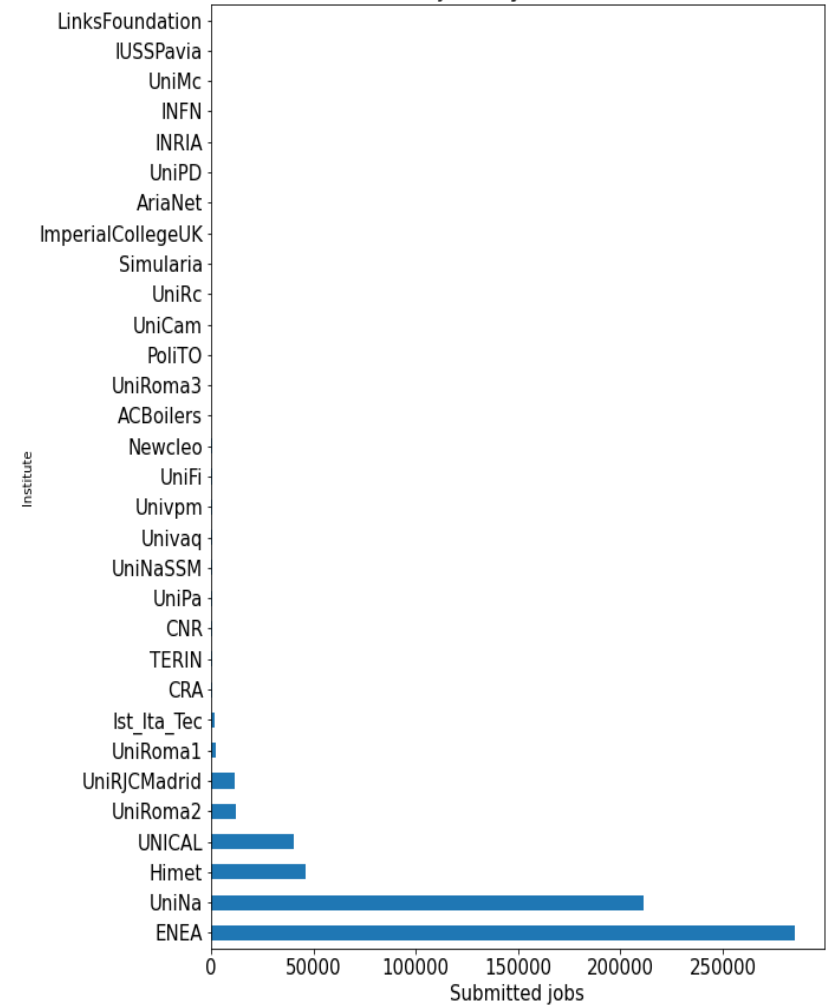
CRESCO jobs in details 2021-2022

Usage by Institute (njobs) 2021-2022

Submitted jobs by Institute in 2021

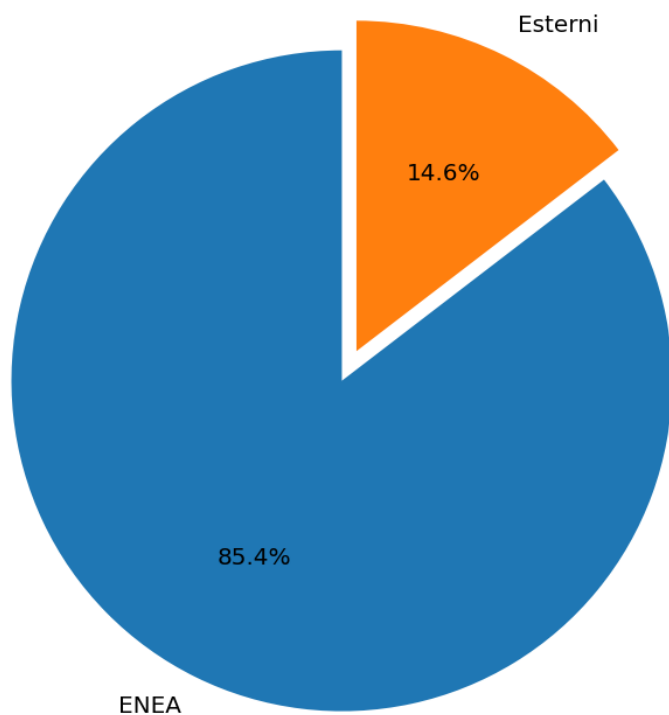


Submitted jobs by Institute in 2022

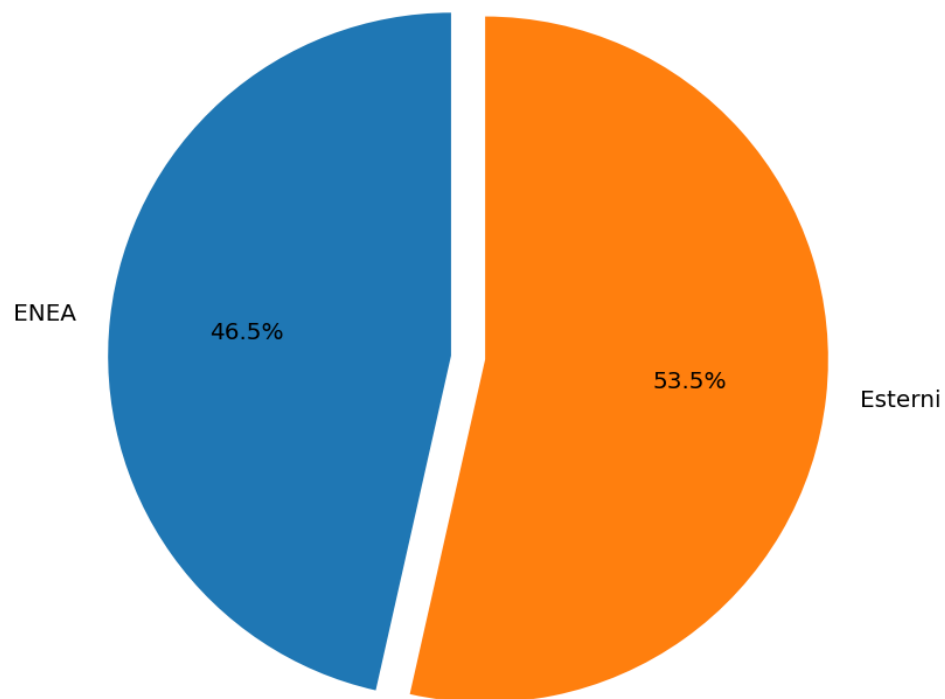


Usage by Institute (%njobs) 2021-2022

Submitted jobs 2021: ENEA and External Users

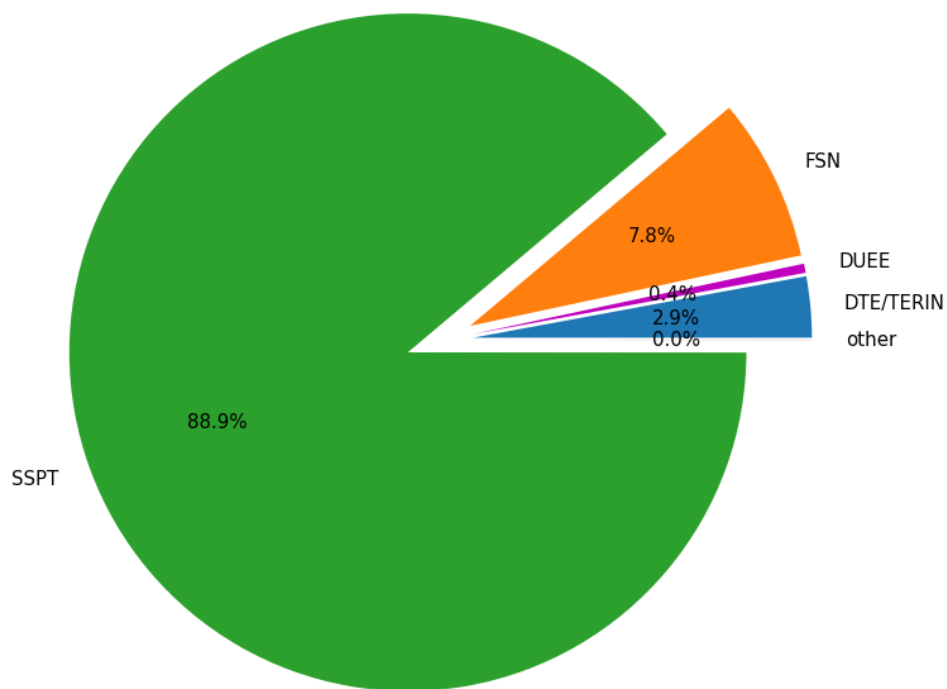


Submitted jobs 2022: ENEA and External Users

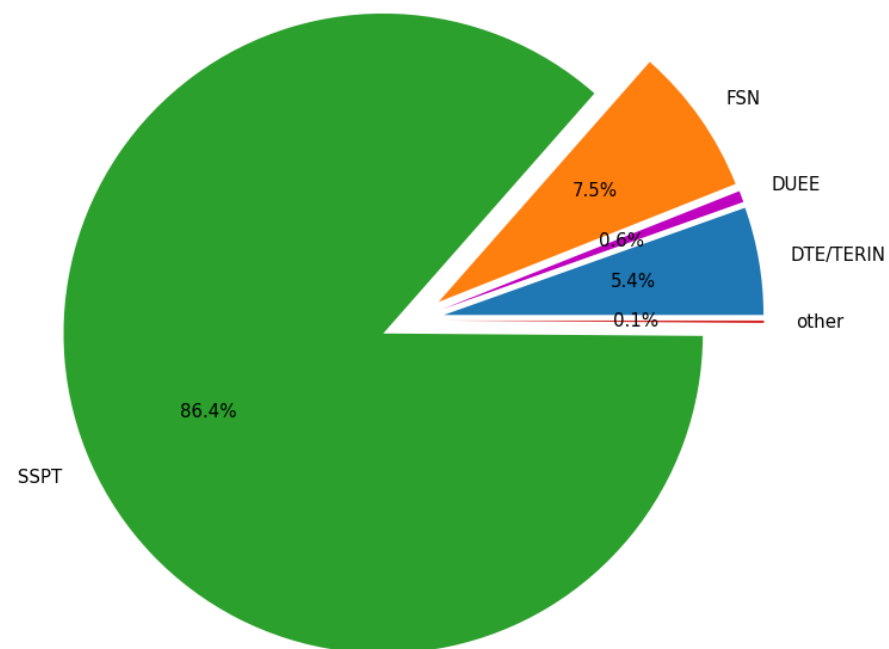


Usage by ENEA department-internals (%njobs) 2021-2022

Jobs 2021 for ENEA department internals (njobs)

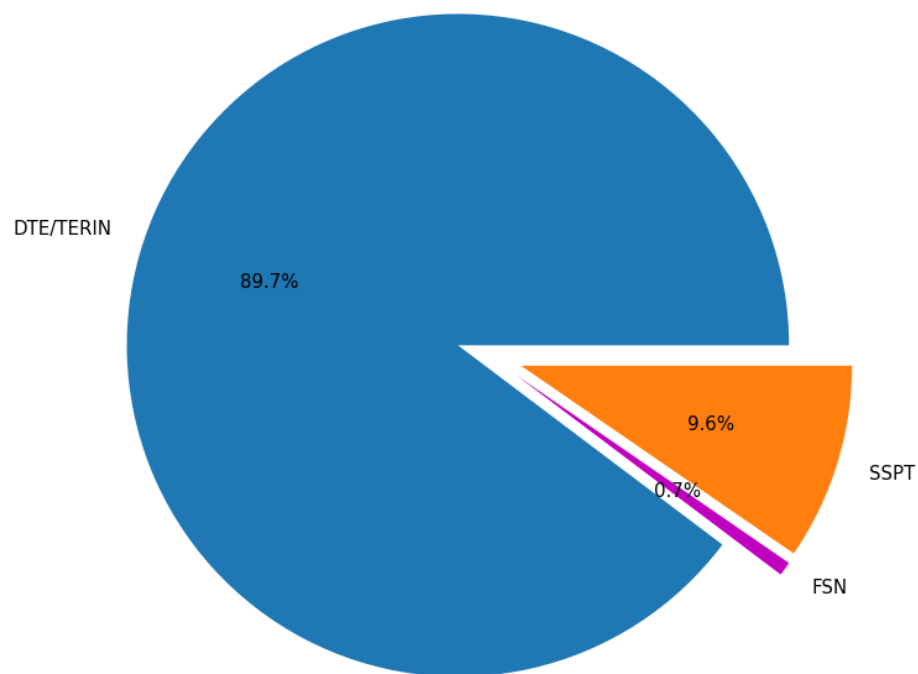


Jobs 2022 for ENEA department internals (njobs)

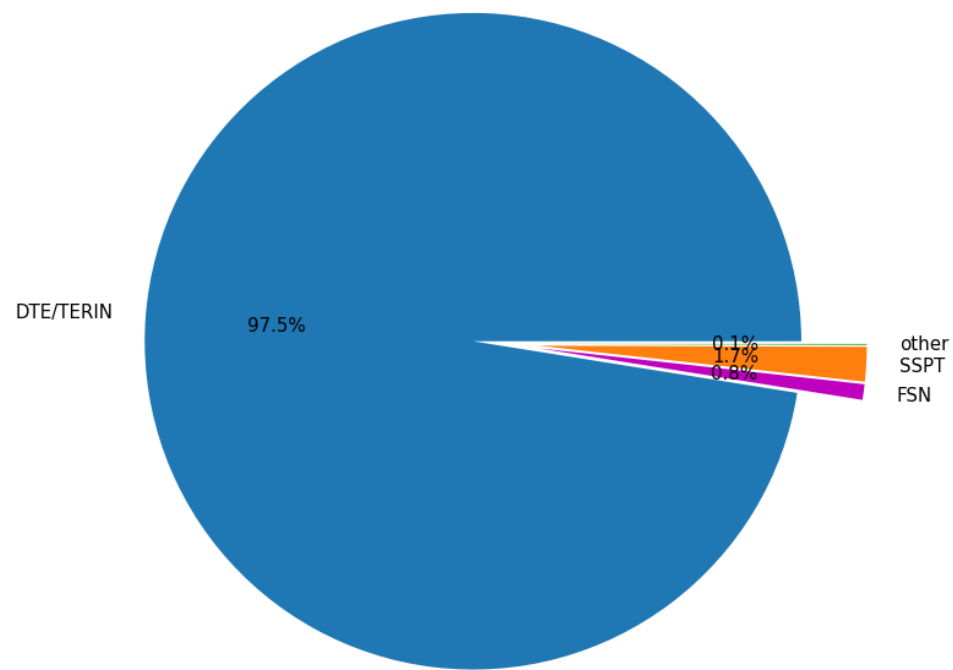


Usage by ENEA department-collaboration (%njobs) 2021-2022

Jobs 2021 for ENEA department collaboration (njobs)



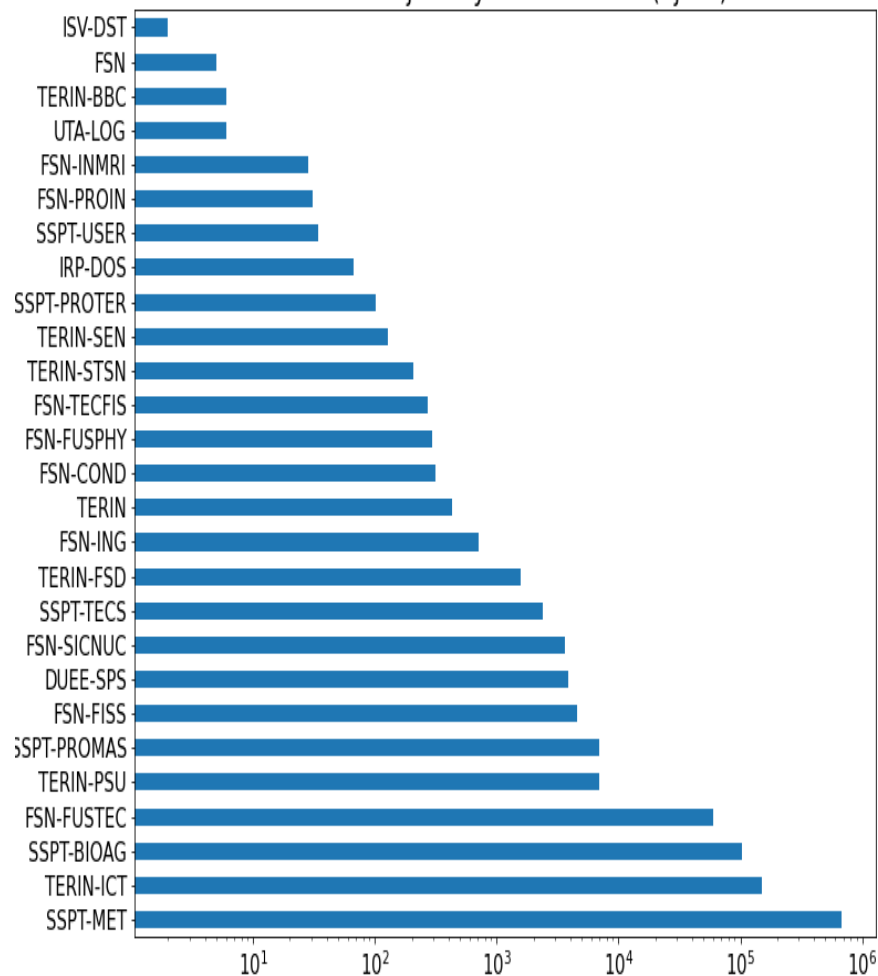
Jobs 2022 for ENEA department collaboration (njobs)



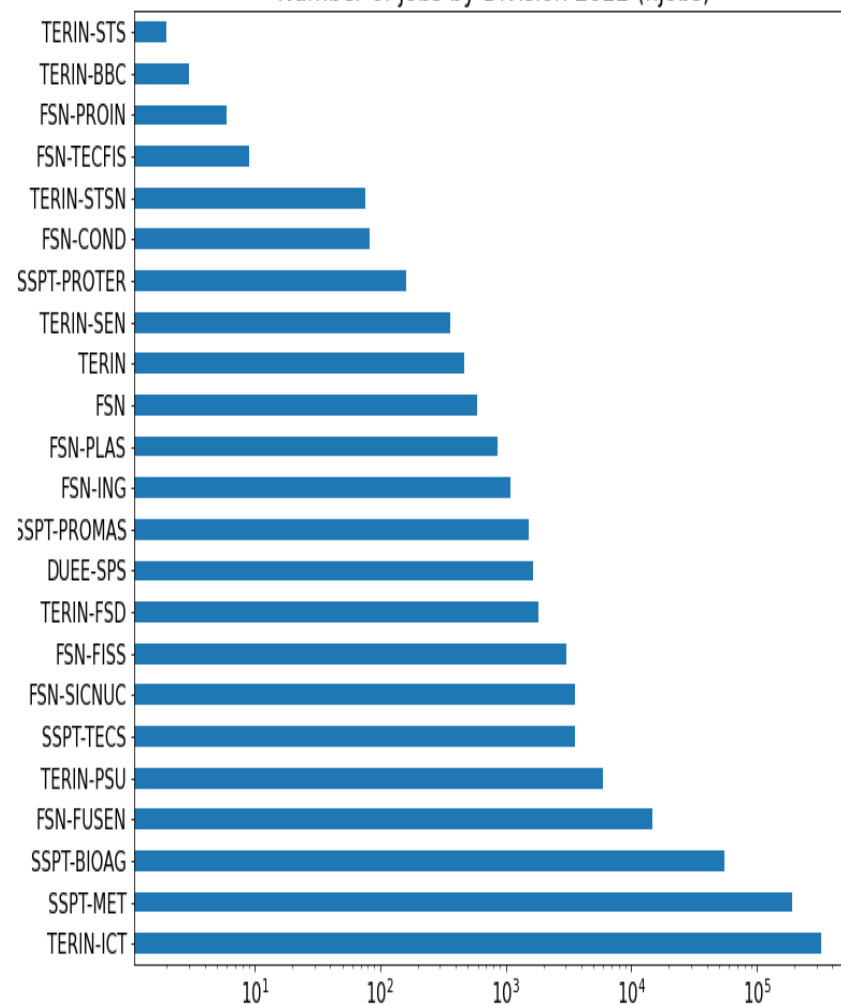
Usage by ENEA Division (njobs)

2021-2022

Number of jobs by Division 2021 (njobs)

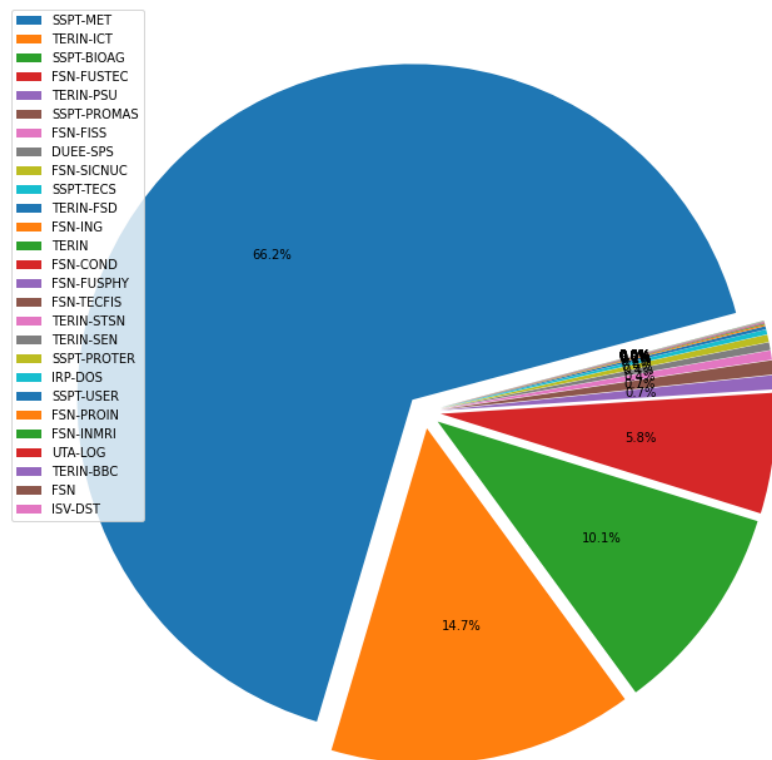


Number of jobs by Division 2022 (njobs)

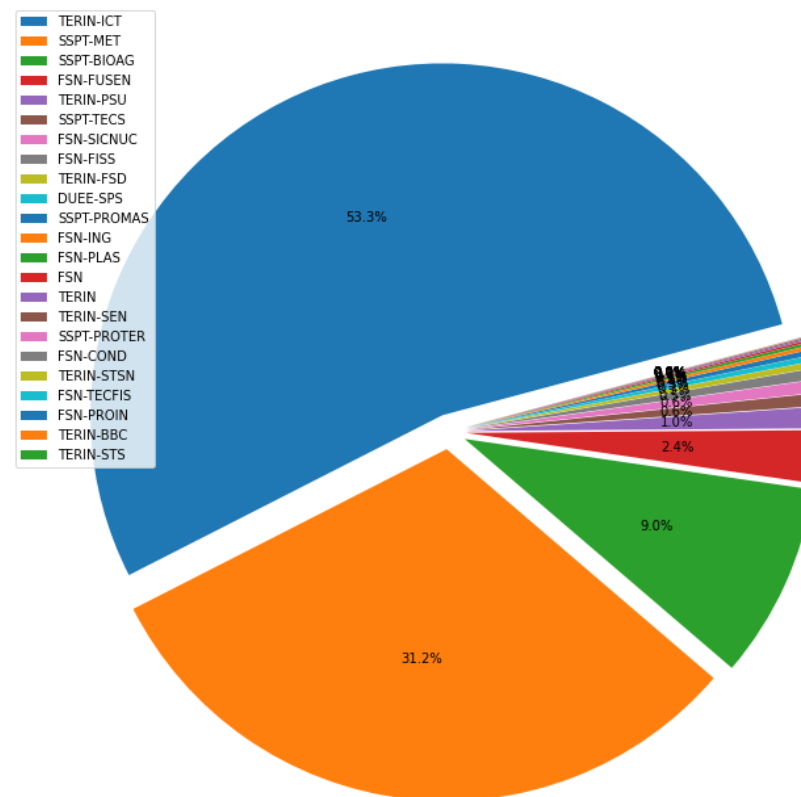


Usage by ENEA Division (%njobs) 2021-2022

ENEA-Division njobs-percentage 2021



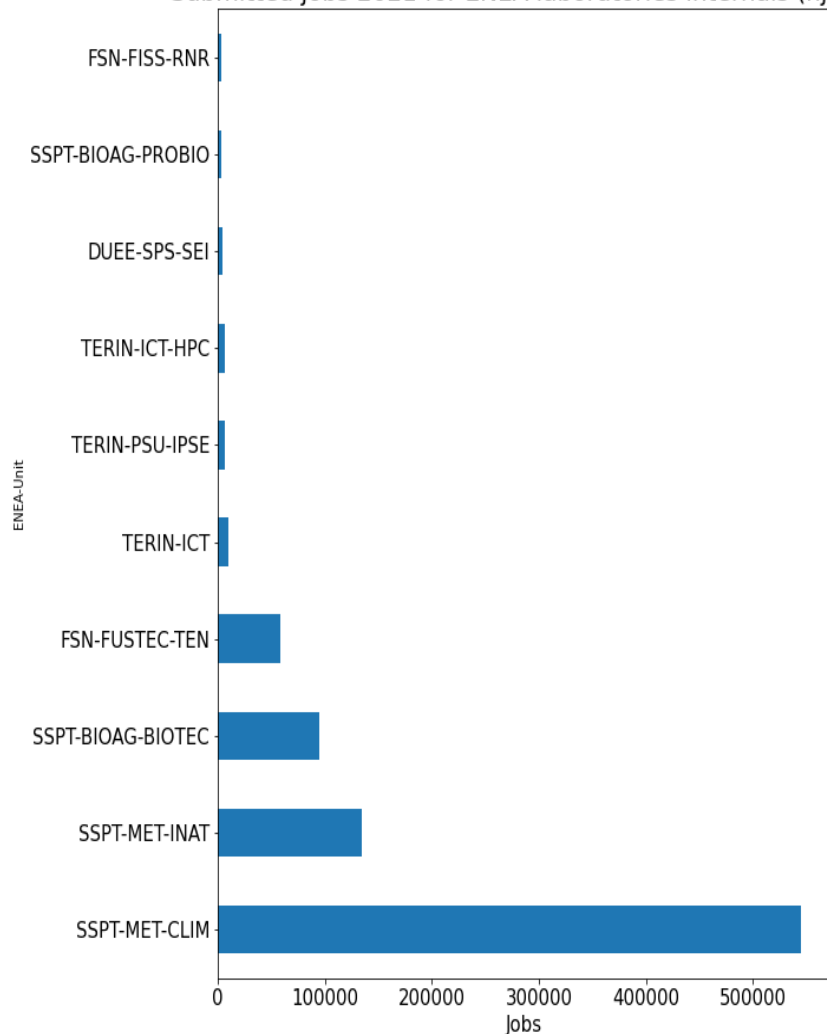
ENEA-Division njobs-percentage 2022



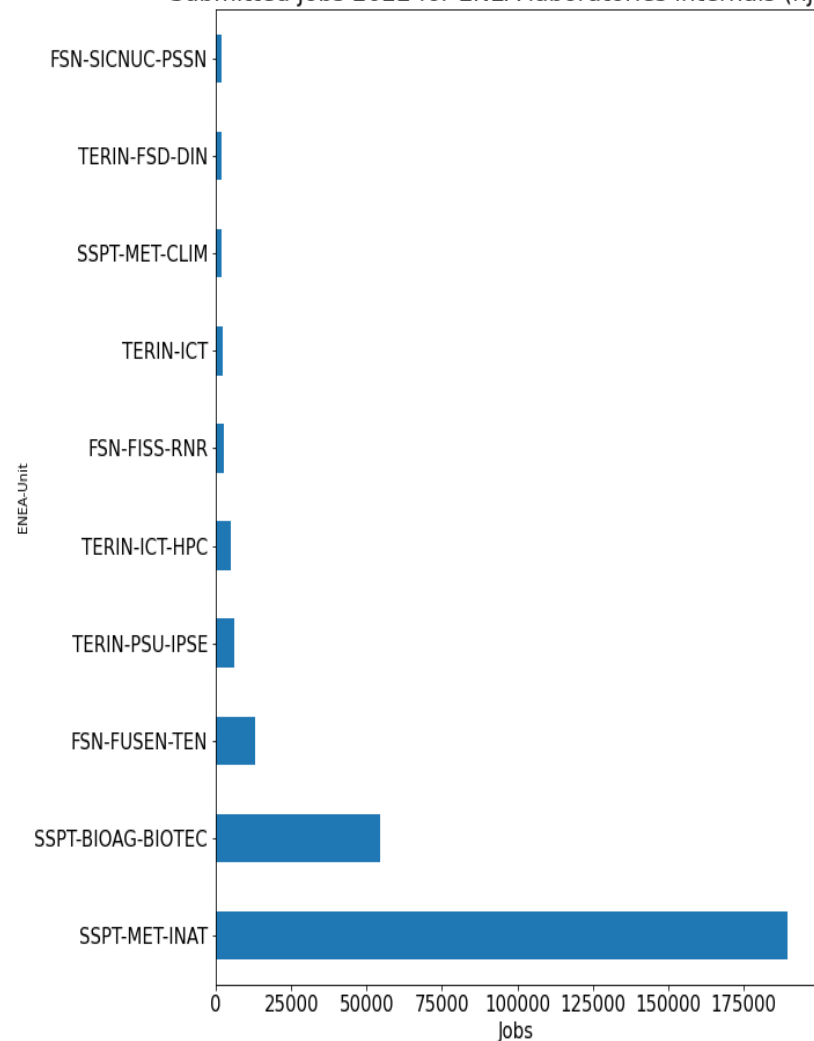
Usage by ENEA laboratories-internals (njobs)

2021-2022

Submitted jobs 2021 for ENEA laboratories internals (njobs)

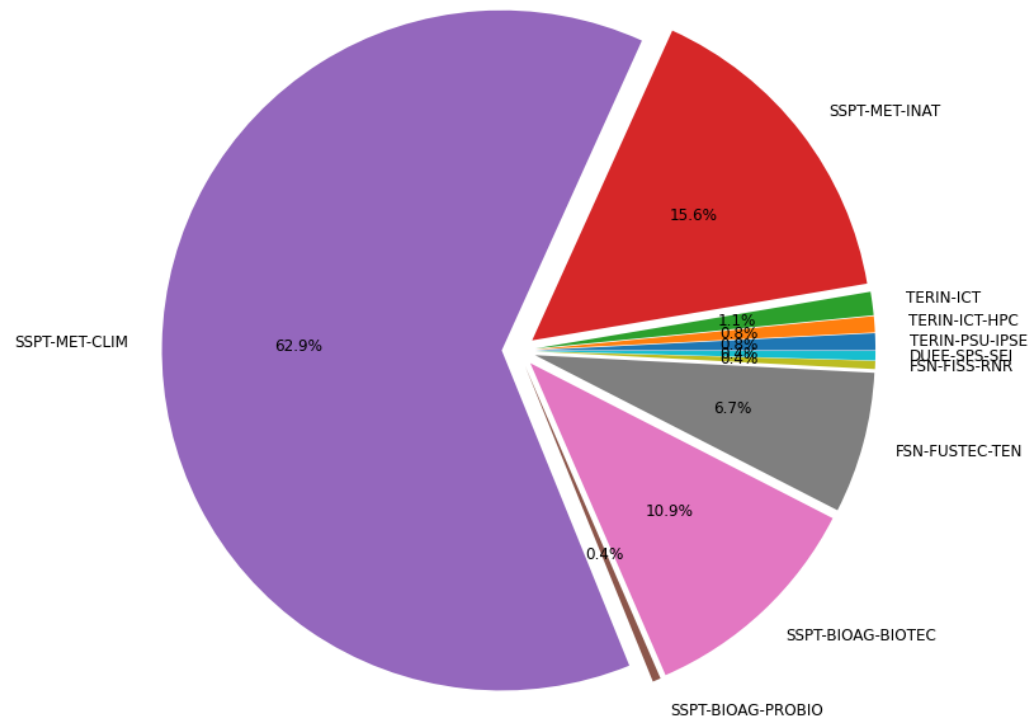


Submitted jobs 2022 for ENEA laboratories internals (njobs)

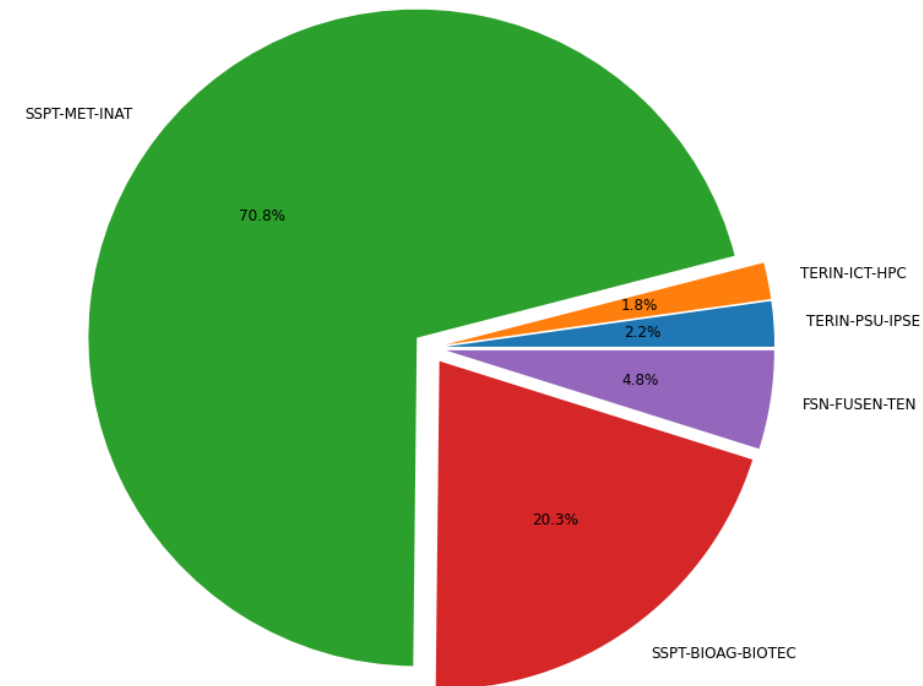


Usage by ENEA laboratories-internals (%njobs) 2021-2022

Submitted jobs 2021 for ENEA laboratories internals (njobs>3000)

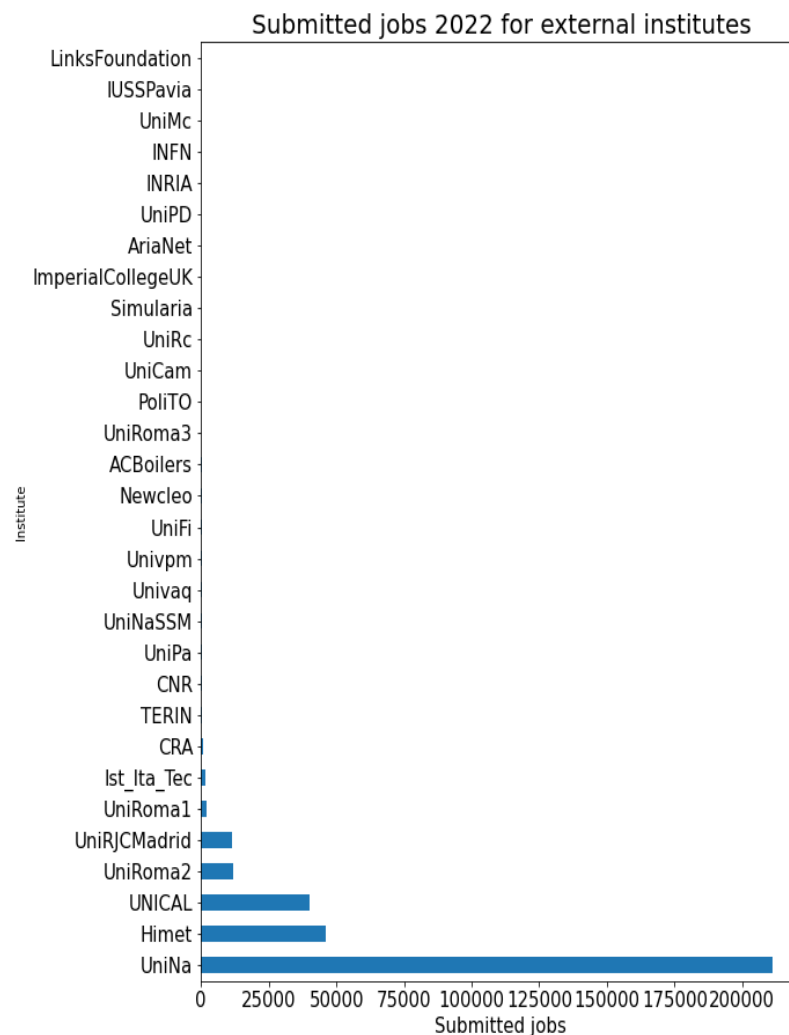
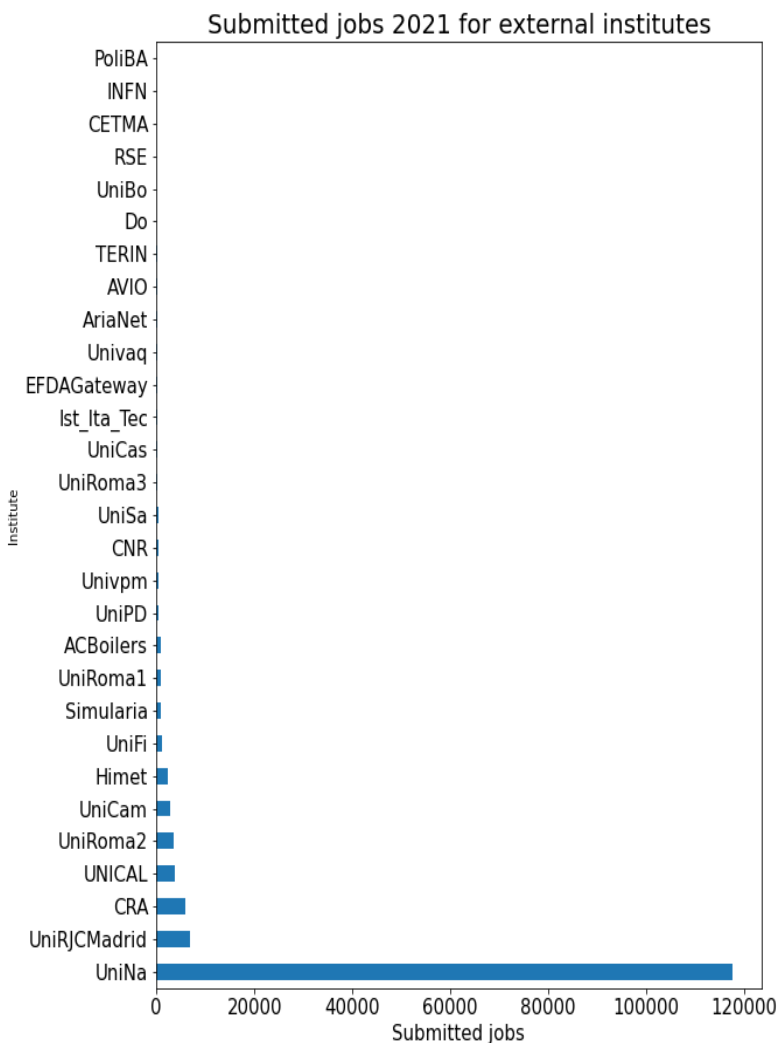


Submitted jobs 2022 for ENEA laboratories internals (njobs>3000)



Usage by external Institute (njobs)

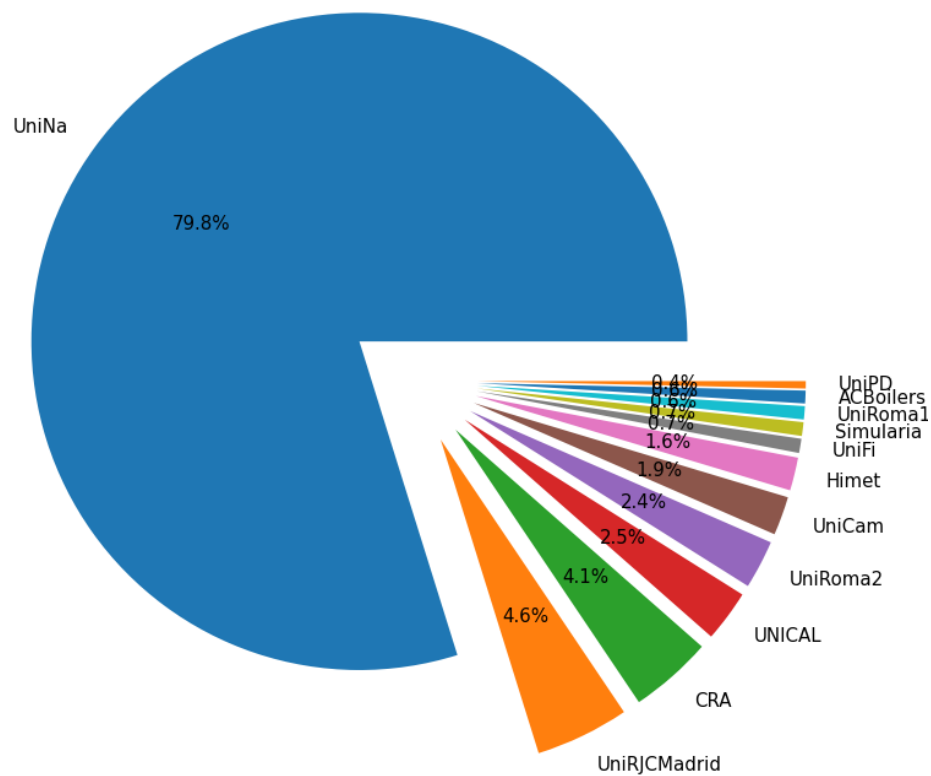
2021-2022



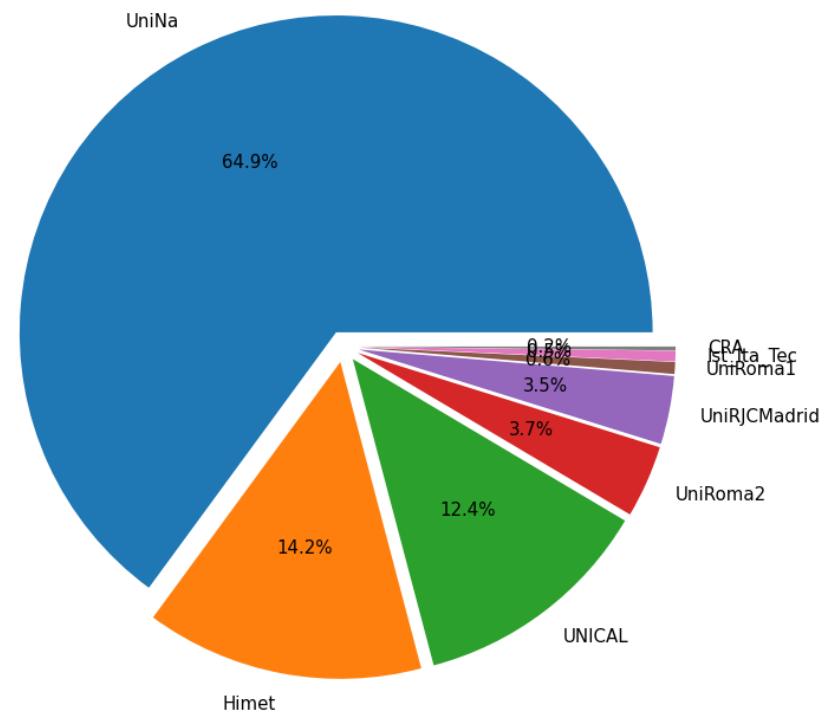
Usage by external Institute (%njobs)

2021-2022

Jobs (njobs>500) for external institutes 2021

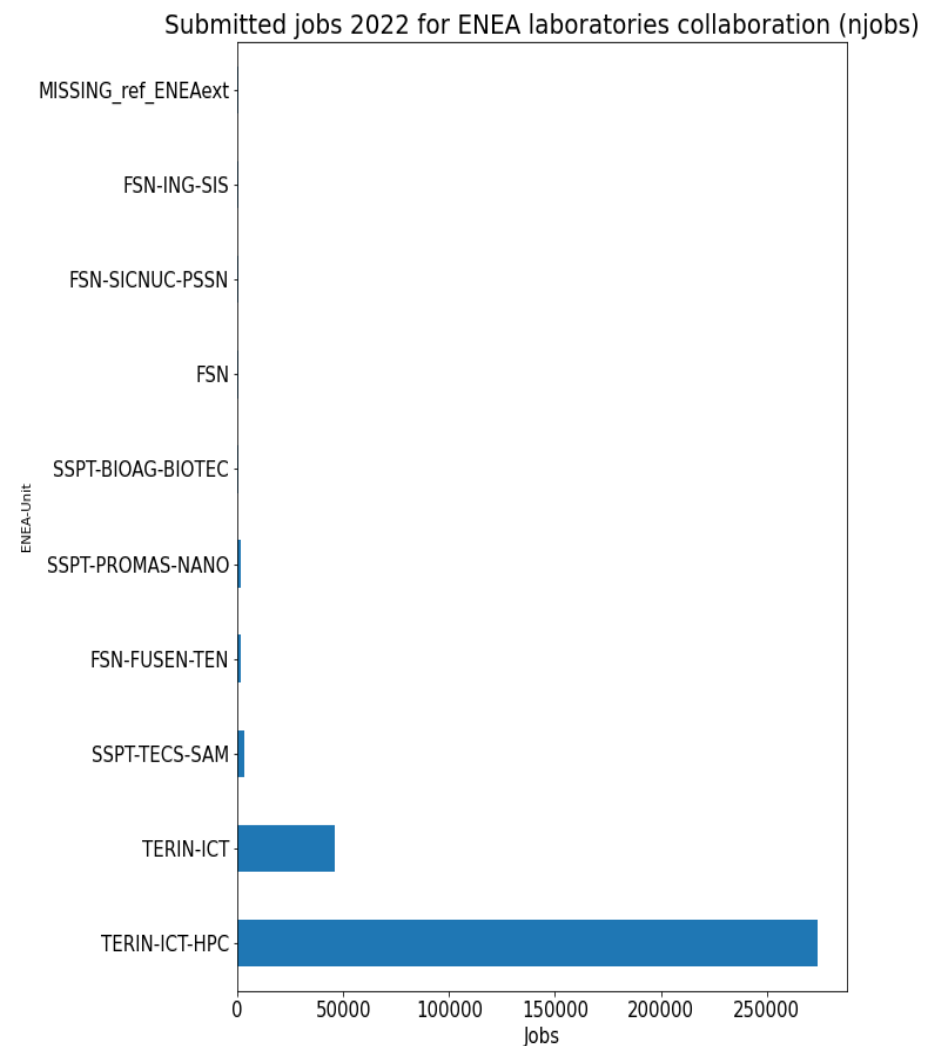
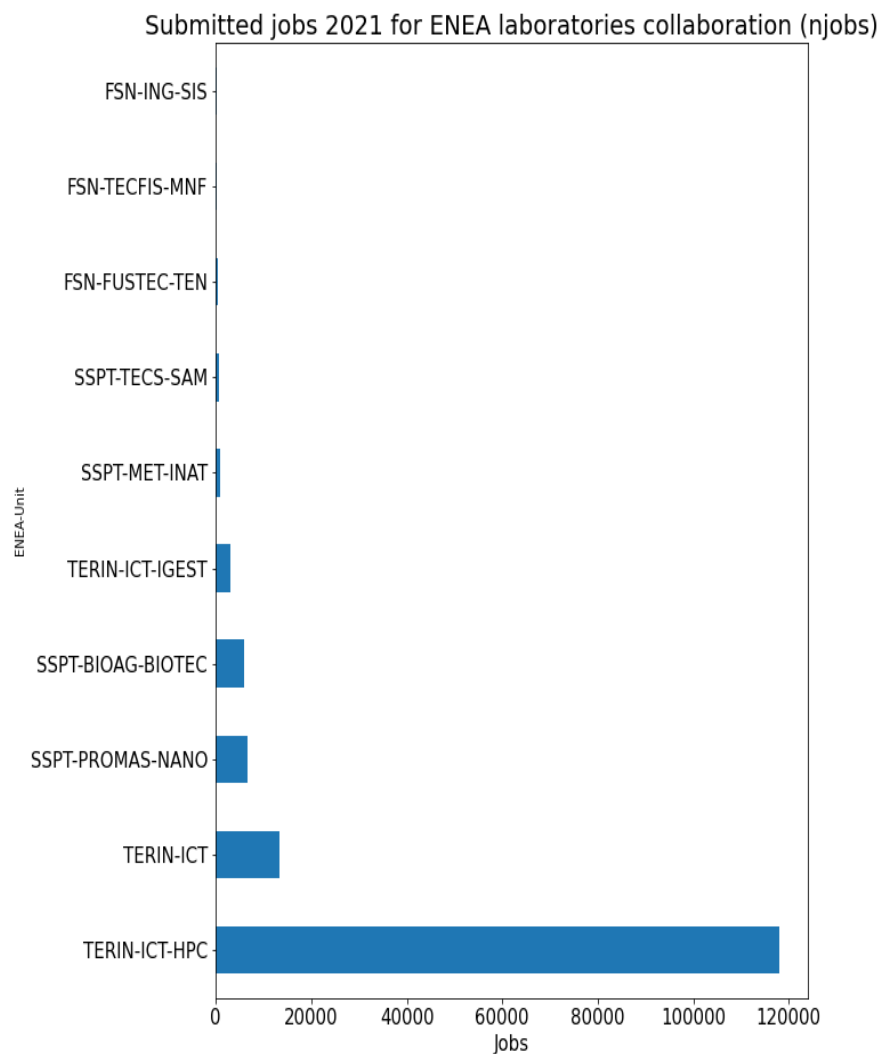


Jobs (njobs>500) for external institutes 2022



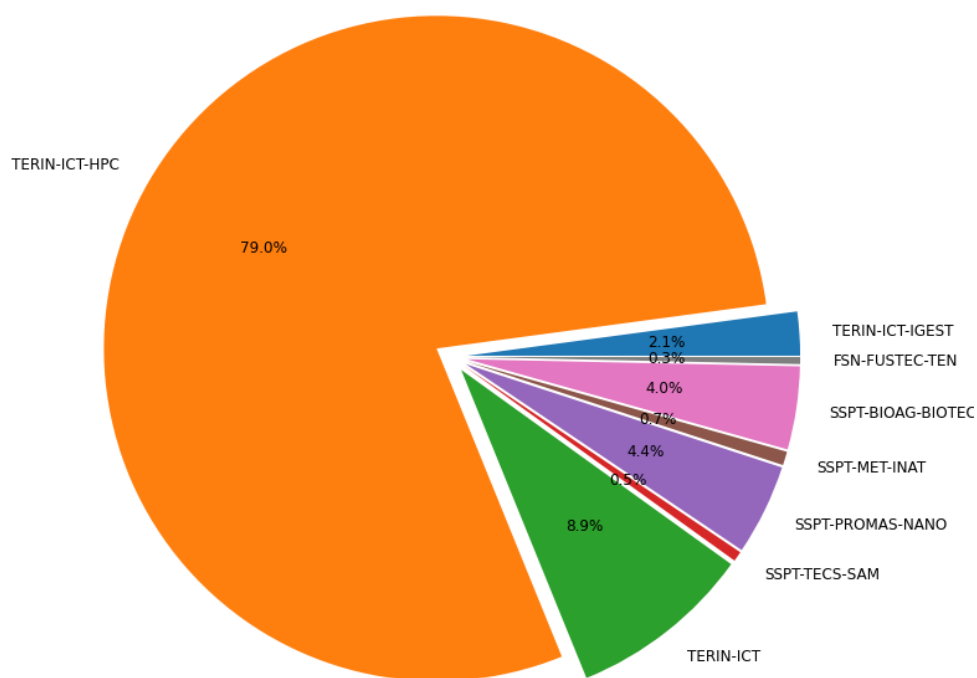
Usage by ENEA laboratories-collaboration (njobs)

2021-2022

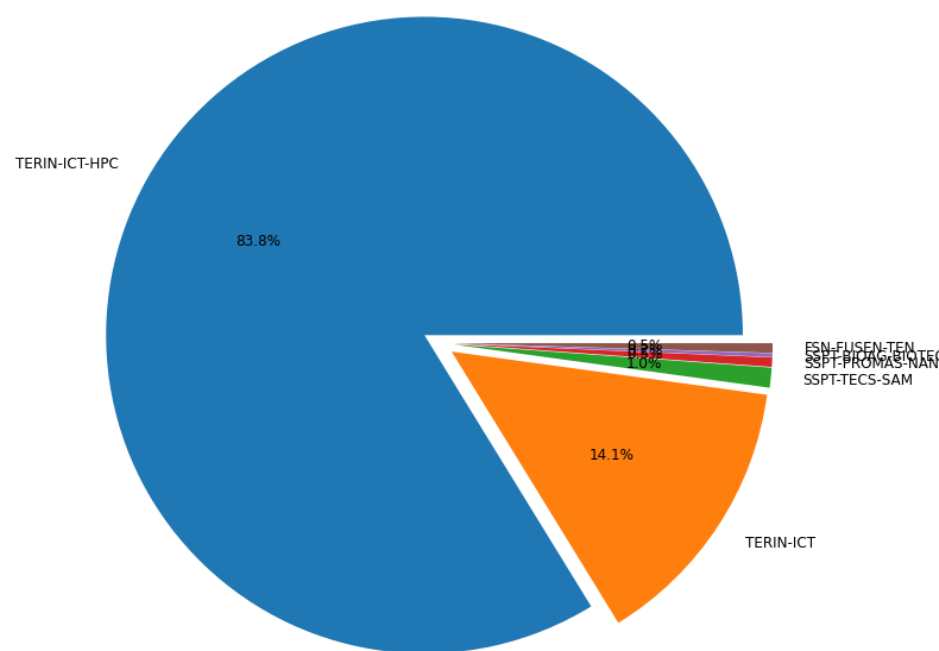


Usage by ENEA laboratories-collaboration (%njobs) 2021-2022

Submitted jobs 2021 for ENEA laboratories collaboration(njobs)



Submitted jobs 2022 for ENEA laboratories collaboration(njobs)



CRESCO Report

2021 report statistics

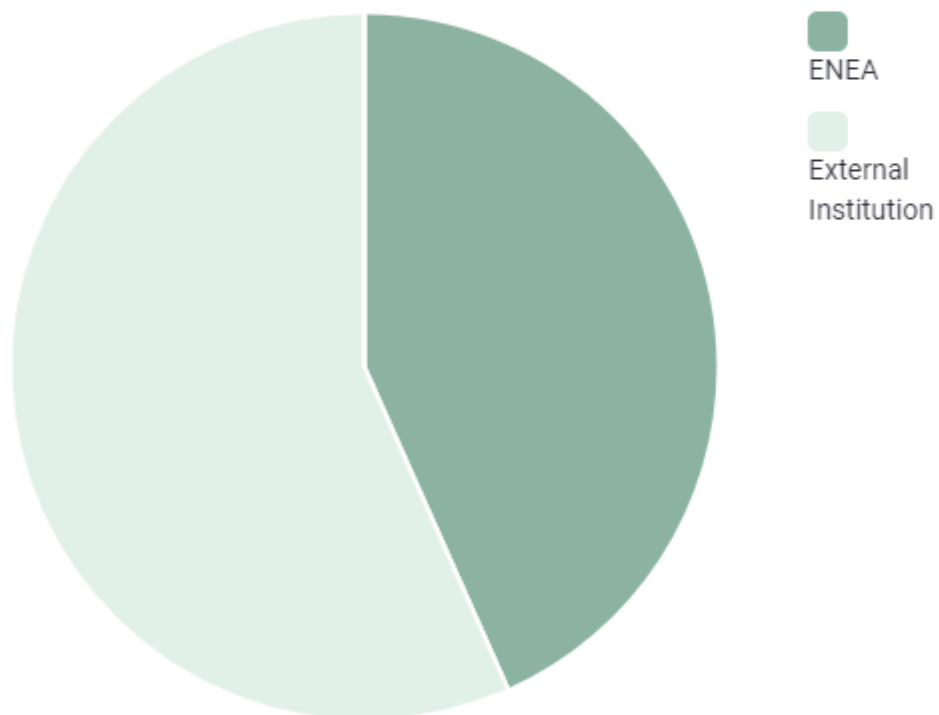
Contributed papers: statistics

- ✓ Invited users: 115/193
 - ✓ $wct_y > 1.0 \parallel (njobs * av_nc > 5000)$
- ✓ Survey responses: 30
- ✓ Papers : 33 (156 authors, ~ 5 authors/paper)
- ✓ Missing authors with $wct_y > 100$: 14 (on top 41)
- ✓ 2021: we had 33 papers (L. Bucci)
- ✓ 2020: we had 52 papers (D. De Chiara, S. Giusepponi)
- ✓ 2019: we had 42 papers (G. Santomauro, G. Guarnieri)
- ✓ 2018: we had 44 papers (G. Santomauro)
- ✓ 2017: we had 38 papers (M. Galli)
- ✓ 2016: we had 45 papers (M. Gusso)
- ✓ 2015: we had 46 papers (G. Ponti)
- ✓ 2014: we had 28 papers (F. Ambrosino)

ENEA and external Users

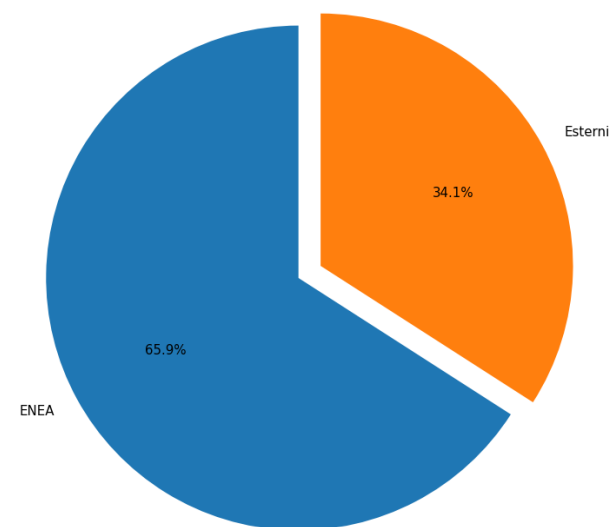
Affiliation

Risposta	Conteggio	Percentuale
ENEA (A1)	13	43.33%
External Institution (A2)	17	56.67%
Nessuna risposta	0	0.00%
Non visualizzato	0	0.00%

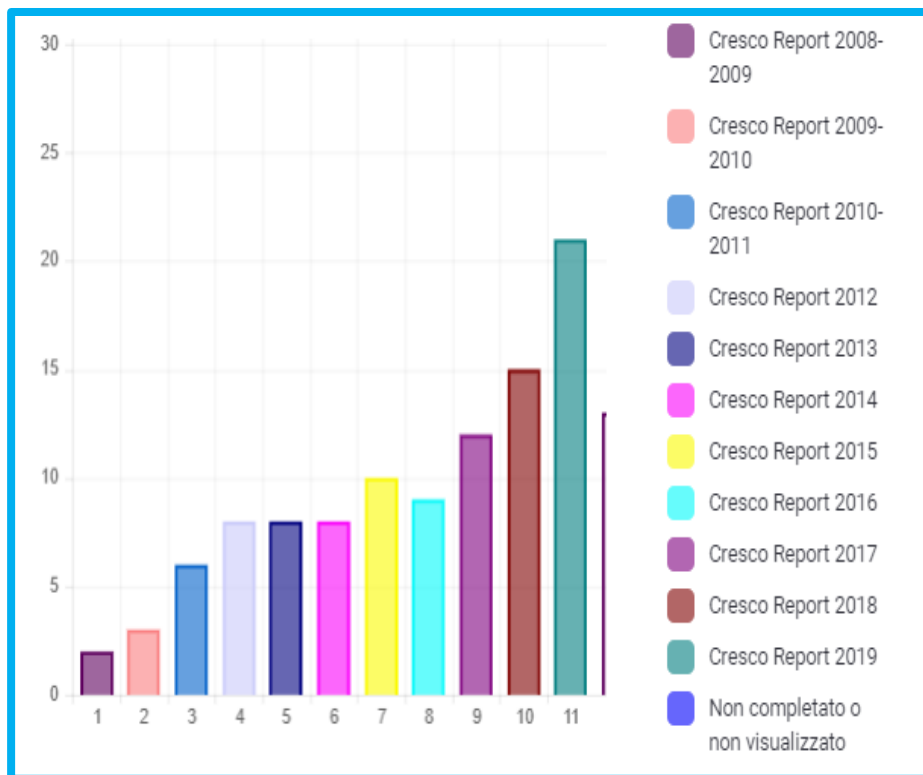


External Institutions are more responsive to contribute to the Report!!!

Percentage run time 2021: ENEA and External Users



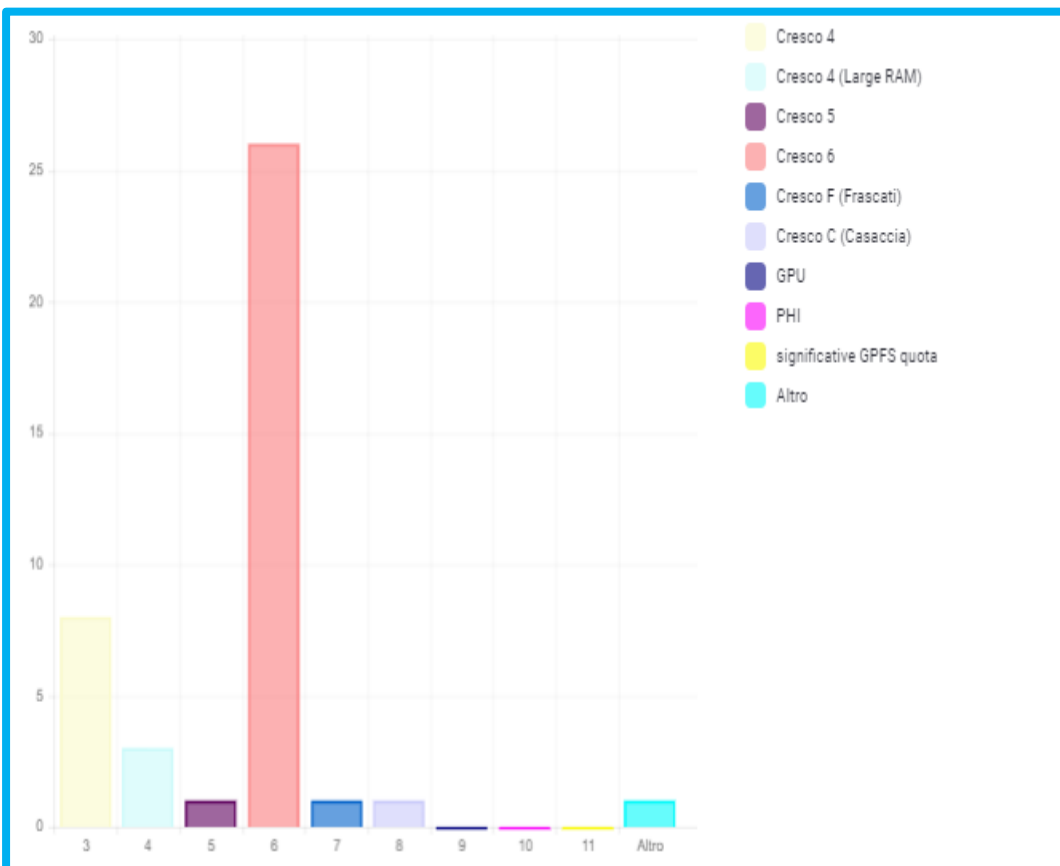
Contribution to a previous CRESCO Report



Select the reports:		
	Conteggio	Percentuale
Cresco Report 2008-2009 (1)	2	5.00%
Cresco Report 2009-2010 (2)	3	7.50%
Cresco Report 2010-2011 (3)	6	15.00%
Cresco Report 2012 (4)	8	20.00%
Cresco Report 2013 (5)	8	20.00%
Cresco Report 2014 (6)	8	20.00%
Cresco Report 2015 (7)	10	25.00%
Cresco Report 2016 (8)	9	22.50%
Cresco Report 2017 (9)	12	30.00%
Cresco Report 2018 (10)	15	37.50%
Cresco Report 2019 (11)	21	52.50%
Non completato o non visualizzato	13	32.50%

Contribution to Report 2020: 24 user account
(31 if all authors are considered)

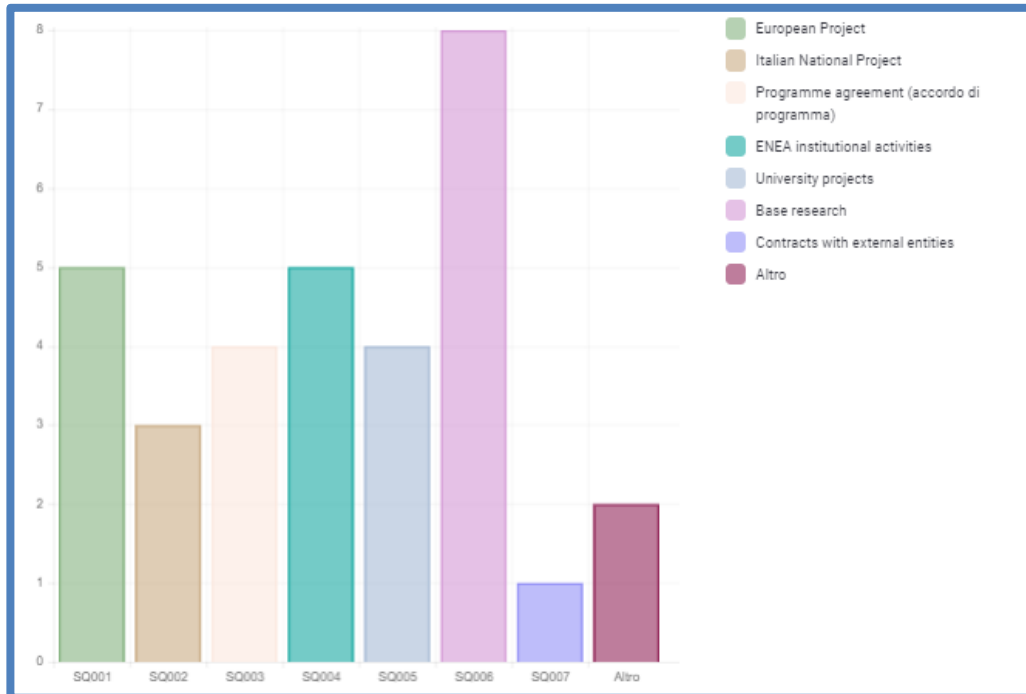
Clusters



Hardware		
Risposta	Conteggio	Percentuale
Cresco 4 (3)	8	26.67%
Cresco 4 (Large RAM) (4)	3	10.00%
Cresco 5 (5)	1	3.33%
Cresco 6 (6)	26	86.67%
Cresco F (Frascati) (7)	1	3.33%
Cresco C (Casaccia) (8)	1	3.33%
GPU (9)	0	0.00%
PHI (10)	0	0.00%
significative GPFS quota (11)	0	0.00%
Altro Sfogliare	1	3.33%

Cresco6 is the most used cluster: not a surprise!

Context of the Activity



Risposta	Conteggio	Percentuale
European Project Sfogliare	5	16.67%
Italian National Project Sfogliare	3	10.00%
Programme agreement (accordo di programma) Sfogliare	4	13.33%
ENEA institutional activities Sfogliare	5	16.67%
University projects Sfogliare	4	13.33%
Base research Sfogliare	8	26.67%
Contracts with external entities Sfogliare	1	3.33%
Altro Sfogliare	2	6.67%

Many works on base research

EU projects

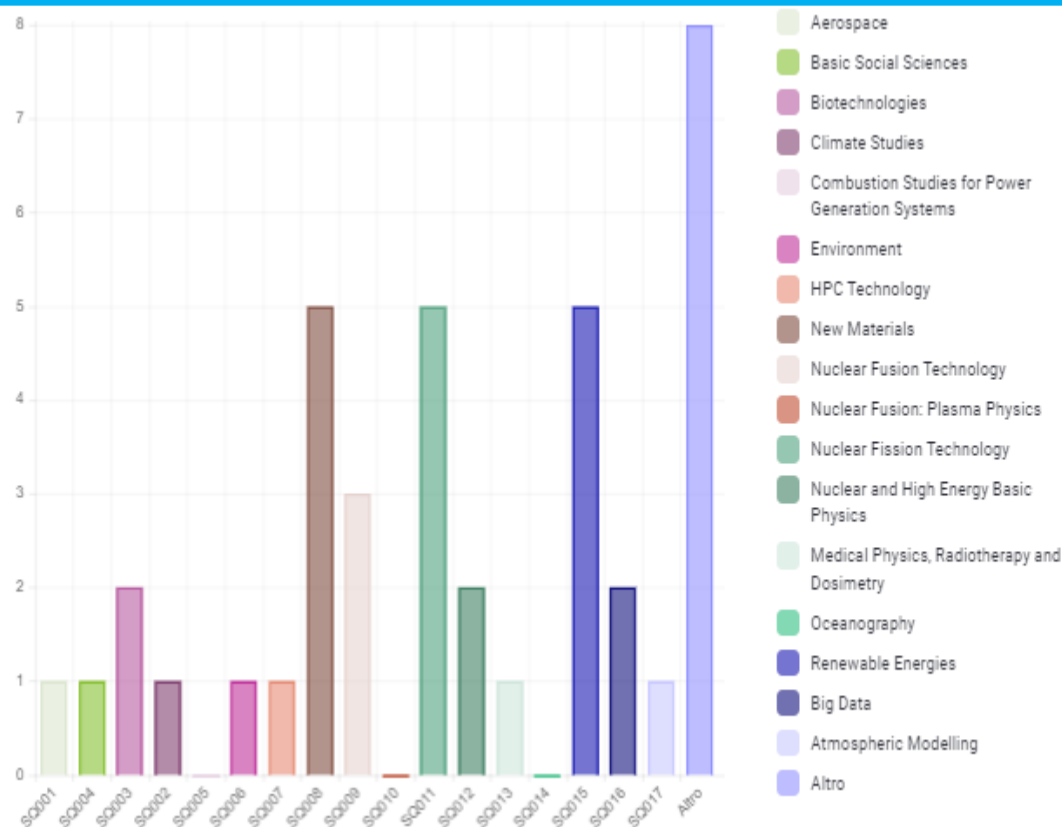
ENEA institutional activities

Programme agreement

Contracts with external entities

Italian National Project

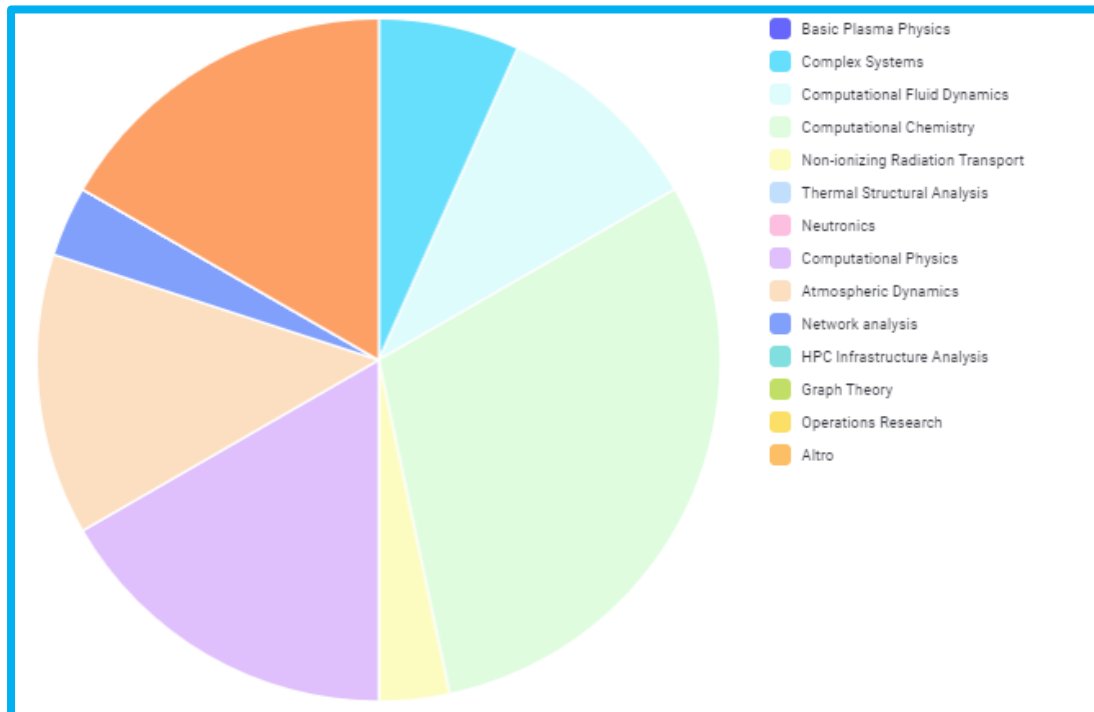
Research Domains



Main Domains
 Renewable Energies
 New Materials
 Nuclear Fission Technology

Research & Development Domain			
Risposta	Conteggio	Percentuale	
Aerospace (SQ001)	1	3.33%	
Basic Social Sciences (SQ004)	1	3.33%	
Biotechnologies (SQ003)	2	6.67%	
Climate Studies (SQ002)	1	3.33%	
Combustion Studies for Power Generation Systems (SQ005)	0	0.00%	
Environment (SQ006)	1	3.33%	
HPC Technology (SQ007)	1	3.33%	
New Materials (SQ008)	5	16.67%	
Nuclear Fusion Technology (SQ009)	3	10.00%	
Nuclear Fusion: Plasma Physics (SQ010)	0	0.00%	
Nuclear Fission Technology (SQ011)	5	16.67%	
Nuclear and High Energy Basic Physics (SQ012)	2	6.67%	
Medical Physics, Radiotherapy and Dosimetry (SQ013)	1	3.33%	
Oceanography (SQ014)	0	0.00%	
Renewable Energies (SQ015)	5	16.67%	
Big Data (SQ016)	2	6.67%	
Atmospheric Modelling (SQ017)	1	3.33%	
Altro Sfogliare	8	26.67%	

Modeling & Simulation Background



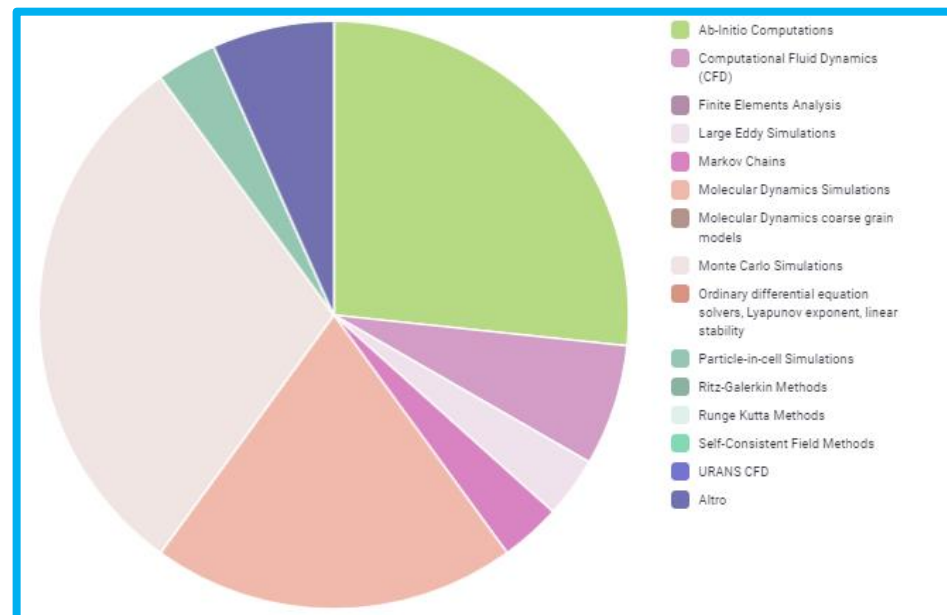
Computational Chemistry (9), Neutronics (5) and Computational Physics (4) are the main actors

Modeling & Simulation Background			
	Conteggio	Percentuale	
Basic Plasma Physics (1)	0	0.00%	
Complex Systems (2)	2	6.67%	
Computational Fluid Dynamics (3)	3	10.00%	
Computational Chemistry (4)	9	30.00%	
Non-ionizing Radiation Transport (5)	1	3.33%	
Non-ionizing Radiation Transport (6)	0	0.00%	
Thermal Structural Analysis (7)	0	0.00%	
Neutronics (8)	5	16.67%	
Computational Physics (9)	4	13.33%	
Atmospheric Dynamics (10)	1	3.33%	
Network analysis (11)	0	0.00%	
HPC Infrastructure Analysis (12)	0	0.00%	
Graph Theory (13)	0	0.00%	
Operations Research (14)	0	0.00%	
Altro Sfogliare	5	16.67%	
Nessuna risposta	0	0.00%	
Non visualizzato	0	0.00%	

Computational Methodology

Computational Methodology:

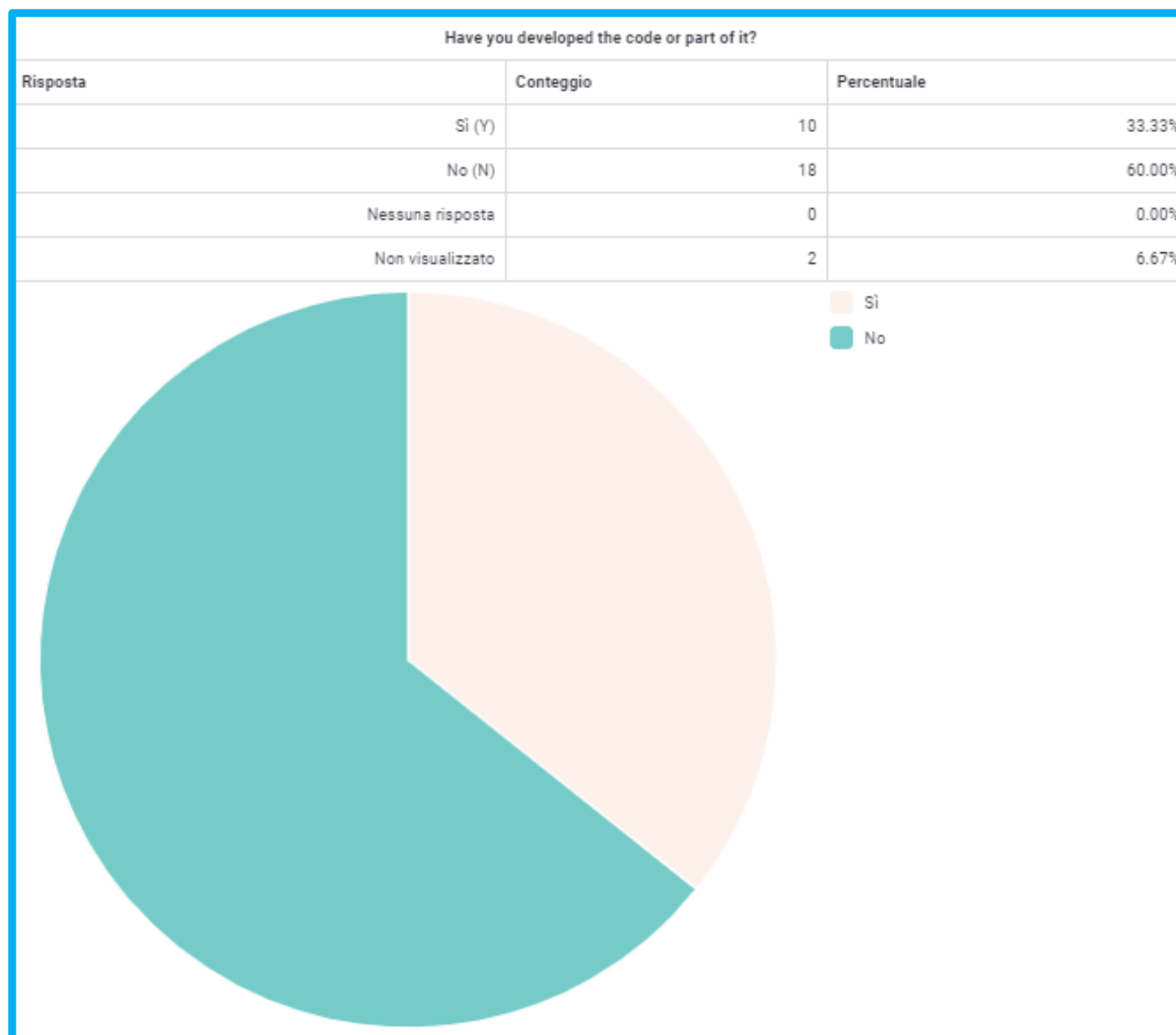
	Conteggio	Percentuale
Ab-Initio Computations (1)	8	26.67%
Computational Fluid Dynamics (CFD) (2)	2	6.67%
Finite Elements Analysis (3)	0	0.00%
Large Eddy Simulations (4)	1	3.33%
Markov Chains (5)	1	3.33%
Molecular Dynamics Simulations (6)	6	20.00%
Molecular Dynamics coarse grain models (7)	0	0.00%
Monte Carlo Simulations (8)	9	30.00%
Ordinary differential equation solvers, Lyapunov exponent, linear stability (9)	0	0.00%
Particle-in-cell Simulations (10)	1	3.33%
Ritz-Galerkin Methods (11)	0	0.00%
Runge Kutta Methods (12)	0	0.00%
Self-Consistent Field Methods (13)	0	0.00%
URANS CFD (14)	0	0.00%
Altro Sfogliare	2	6.67%
Nessuna risposta	0	0.00%
Non visualizzato	0	0.00%



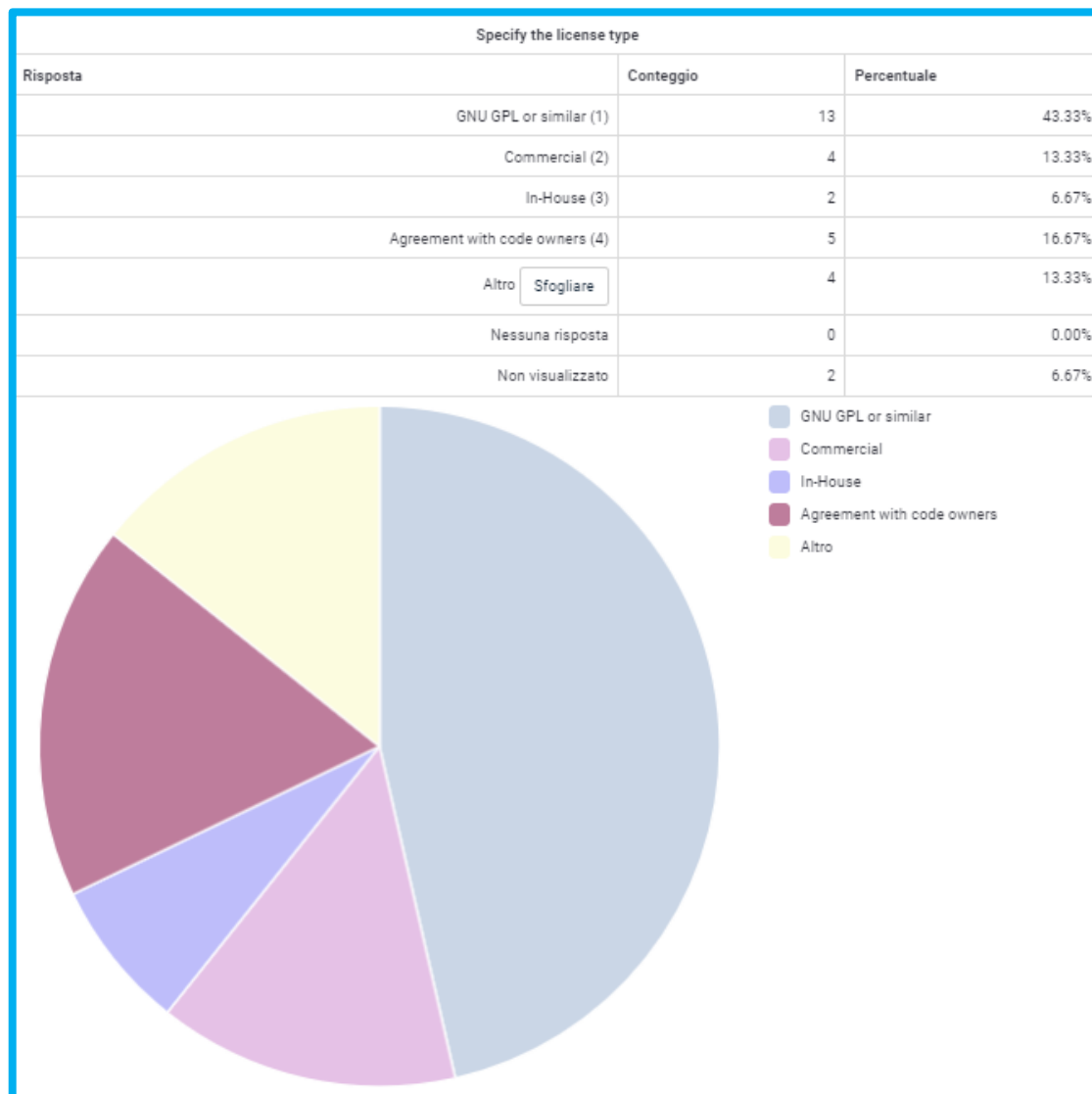
Montecarlo papers (9) Ab-Initio (8) and Molecular Dynamics (6)

Code Development

1/3 of contributors works on software codes

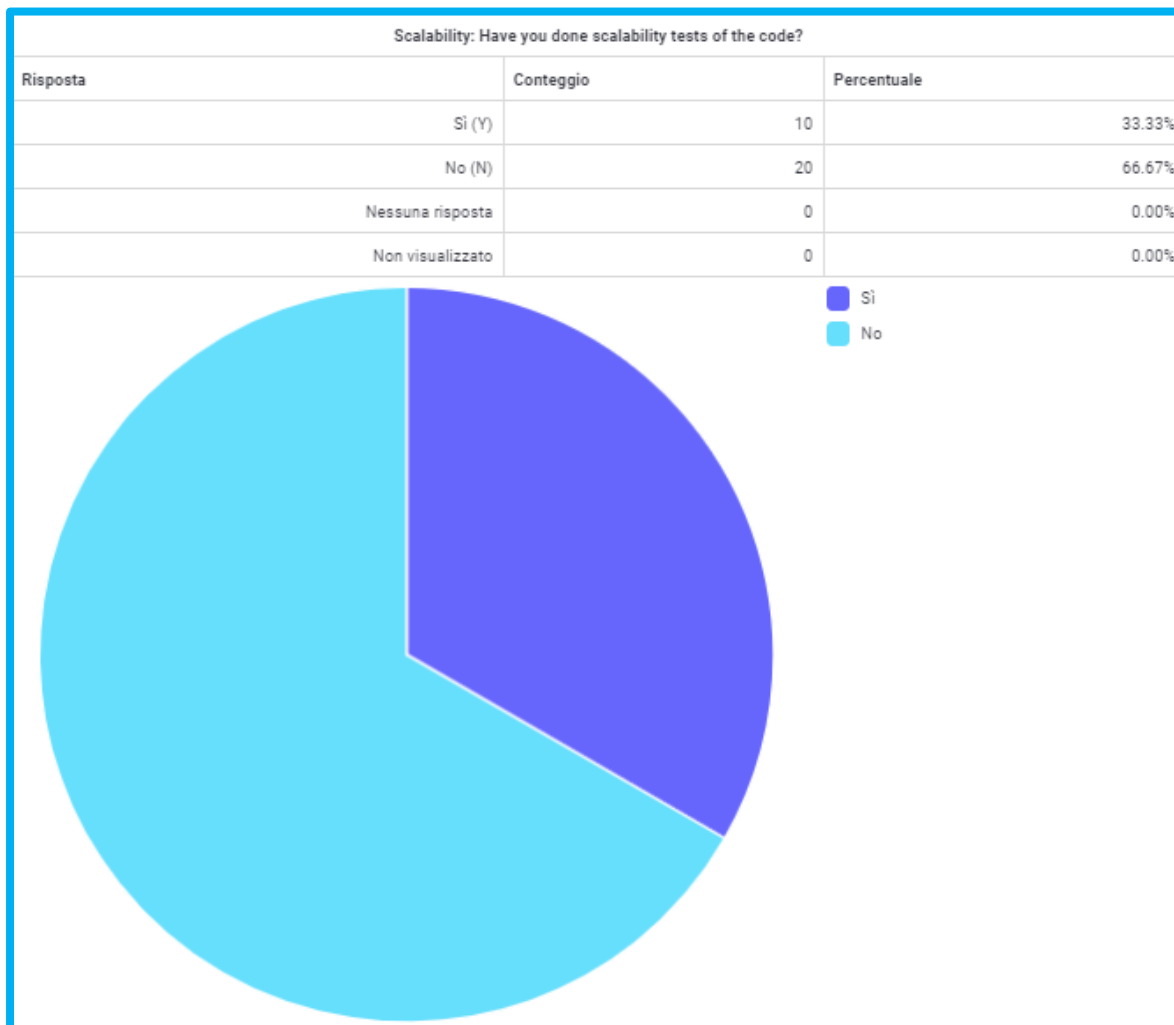


License type



- Most of code has a free-type license,
- 16% agreement with code owners
- 13% cases of commercial software use

Scalability tests?

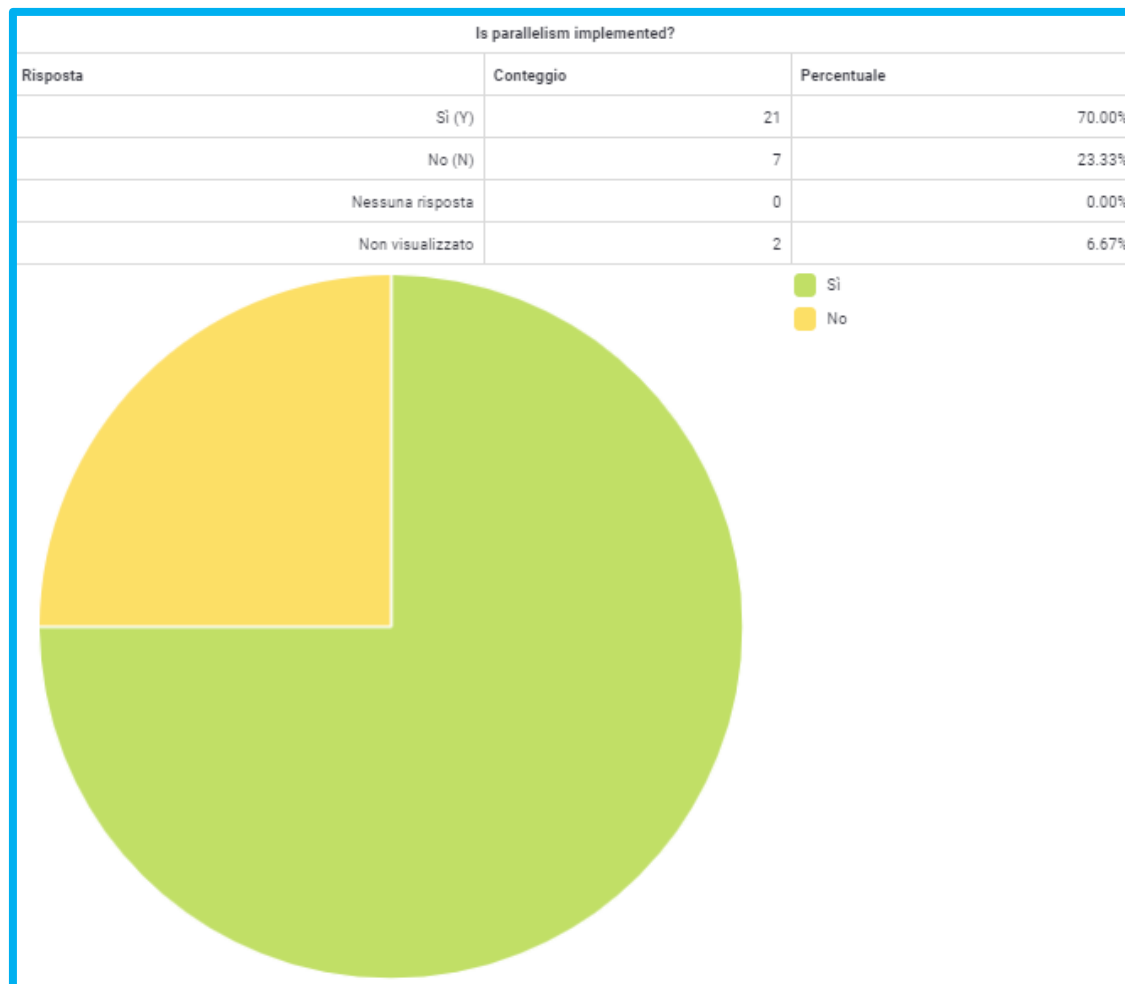


~33% of users do perform scalability tests

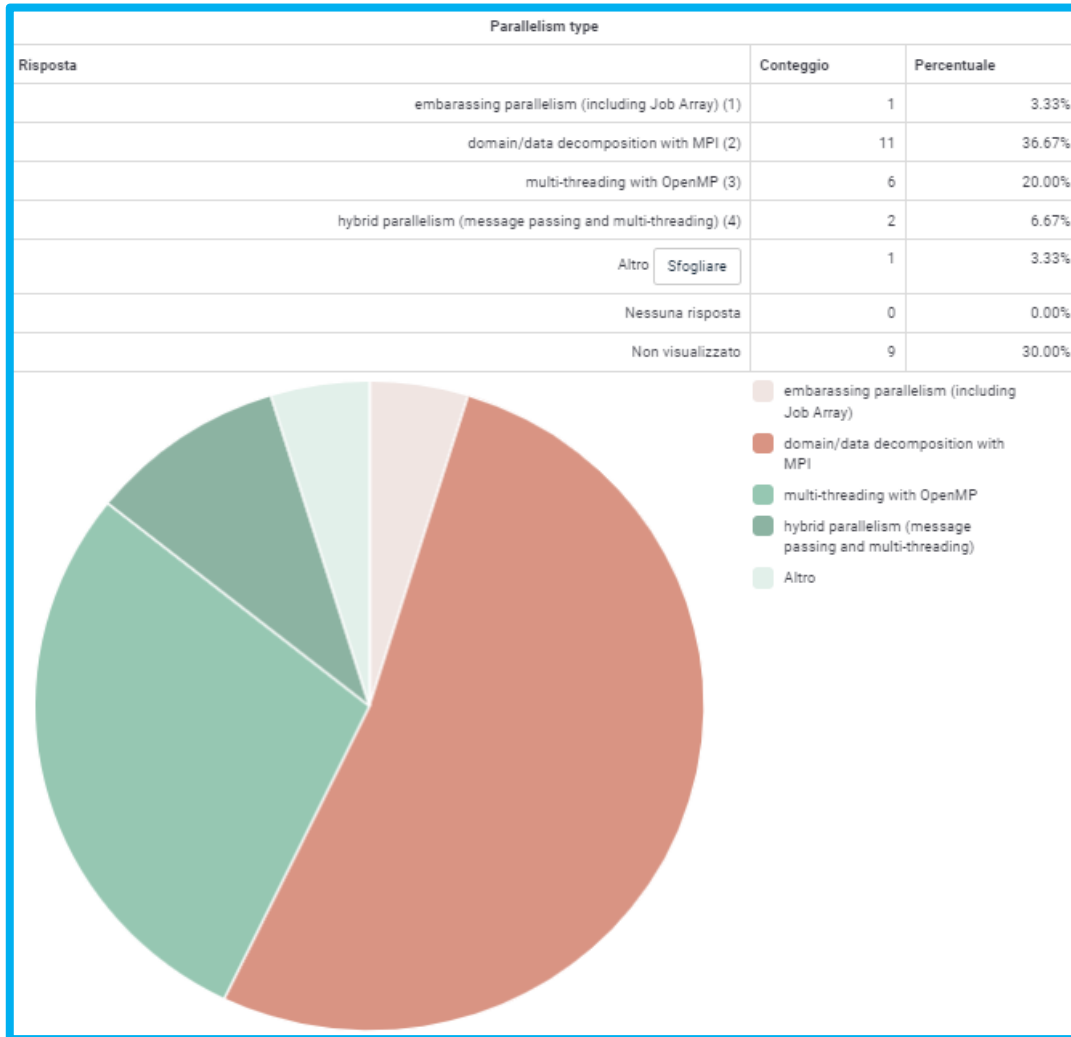
67% of users do not

Parallelism implemented

70 % of parallel code

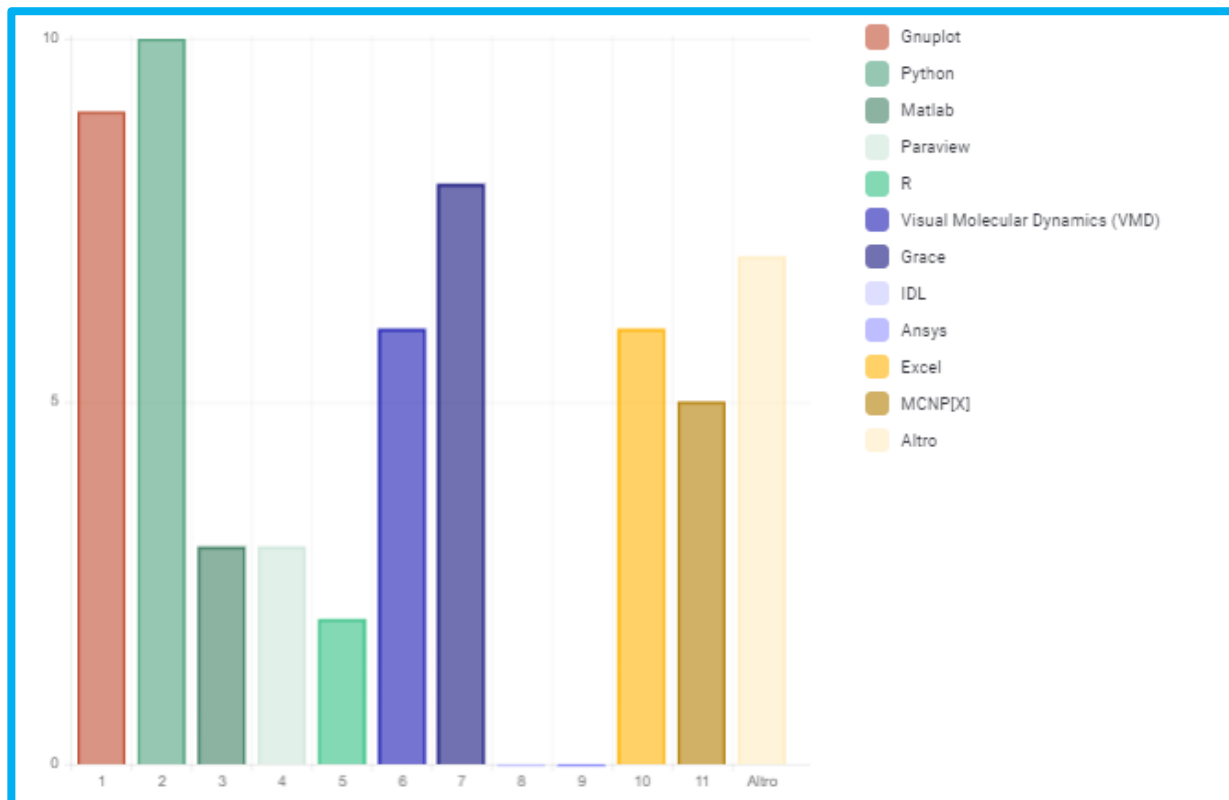


Type of parallelism implemented



Most users use MPI and OpenMP
a fraction of 7% uses hybrid code

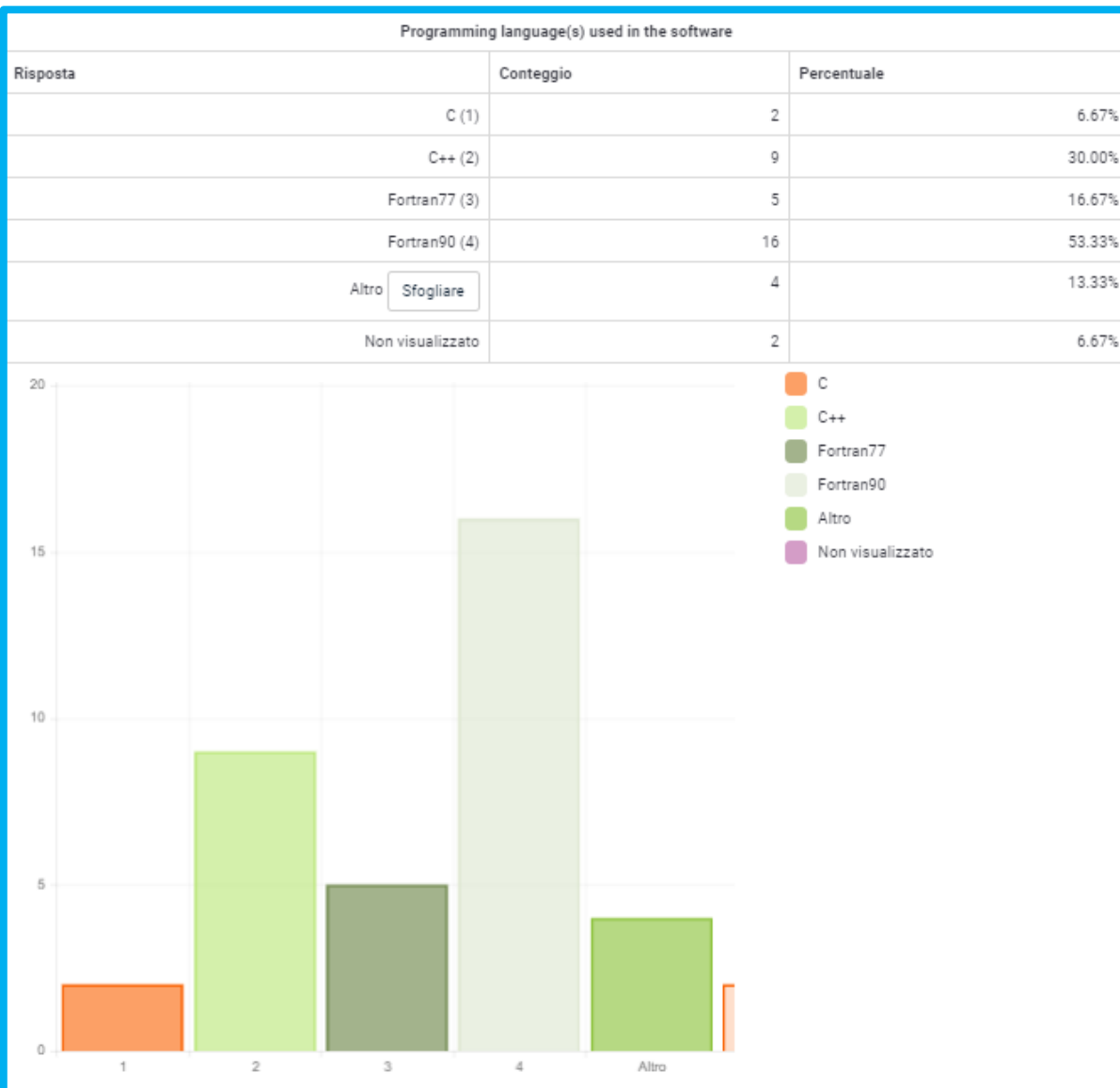
Data Visualization software



Data Visualization: Specify the tools you used to view simulation results			
	Conteggio	Percentuale	
Gnuplot (1)	9	30.00%	
Python (2)	10	33.33%	
Matlab (3)	3	10.00%	
Paraview (4)	3	10.00%	
R (5)	2	6.67%	
Visual Molecular Dynamics (VMD) (6)	6	20.00%	
Grace (7)	8	26.67%	
IDL (8)	0	0.00%	
Ansys (9)	0	0.00%	
Excel (10)	6	20.00%	
MCNP[X] (11)	5	16.67%	
Altro Sfogliare	7	23.33%	

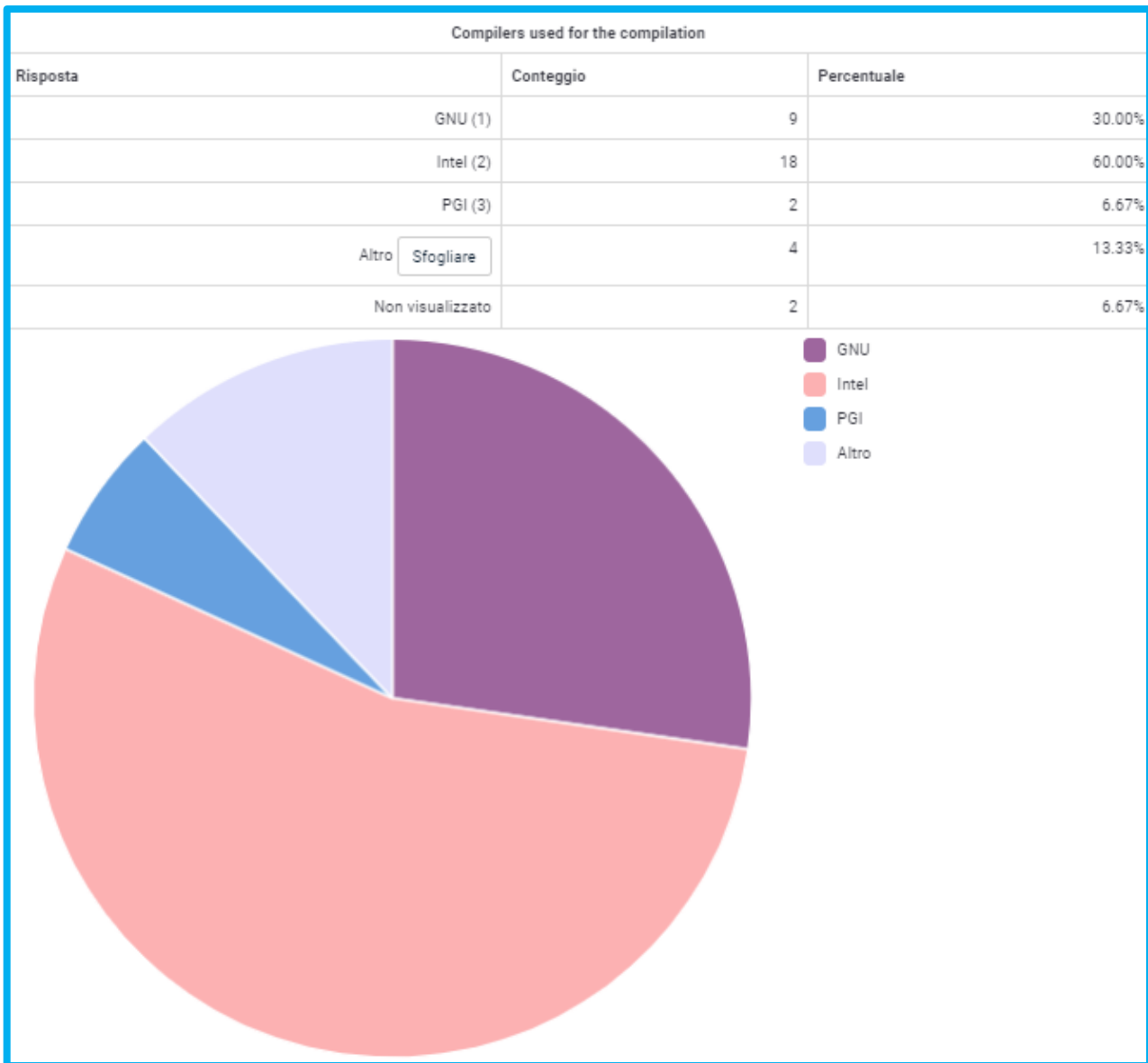
Python is the preferred visualization tool followed by Grace, VMD ...

Computer Languages



The most used language is Fortran, followed by C++ and C

Compilers



The Intel compiler is the most used, followed by GNU

Some Used Software and libraries

Softwares:

- **Nuclear:** MCNP, FLUKA, GEANT4.
- **MD:** GROMACS, LAMMPS, NAMD, AMBER.
- **Ab-Initio:** Quantum Espresso, VASP, CP2K, Siesta.
- **CFD:** OpenFOAM.
- **Environment:** WRF (Weather Research and Forecasting).
- **Other:** HeaRT, Python ...

Libraries

- BLAS (Basic Linear Algebra Subprograms)
- LAPACK (Linear Algebra PACKage)
- ScaLAPACK (Scalable Linear Algebra PACKage)
- MKL (Math Kernel Library)

CRESCO usage 2014-2021

Trends 2014-2022

Cresco major events

Some major events			
YEAR	CLUSTER	PEAK TFlops	CORES
2008-15	CRESCO1 CRESCO2	25	672 2048->2720
2013-17	CRESCO3	20	2016
2014	CRESCO4	100	4864
2015-18	CRESCO5	24	640
2018	CRESCO6	700	10416->
2019	CRESCO6+	1.400	->20832

Cresco in numbers in recent years

Year	jobs	wct_y
2014	756428	5529
2015	162698	5314
2016	847184	4857
2017	571258	3895
2018	1321623	4853
2019	1675438	9992
2020	1637704	12277

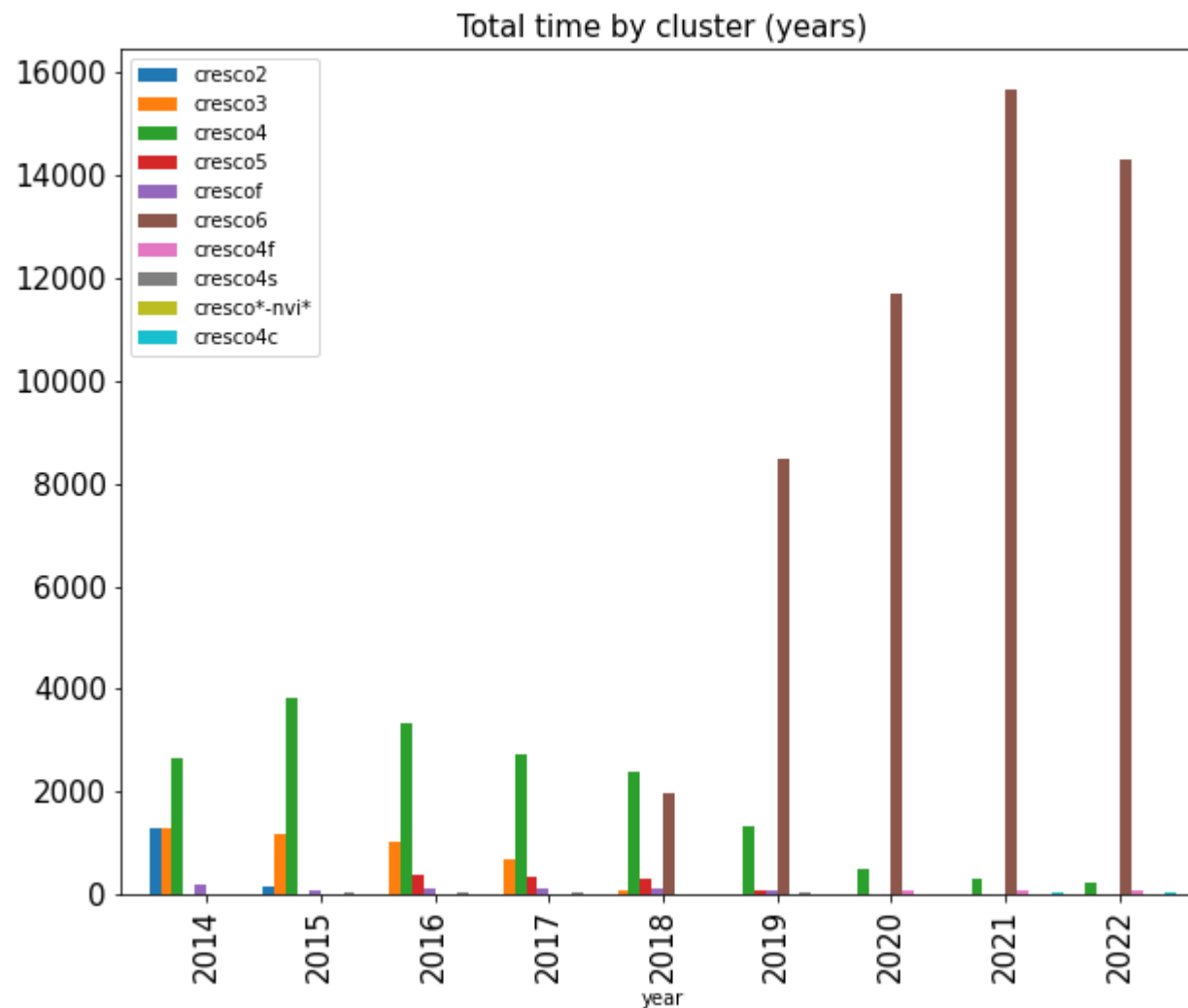
2021	1027713	16130
2022	613642	14705

There is any correlation between njobs and the n. of contributions to the Report???

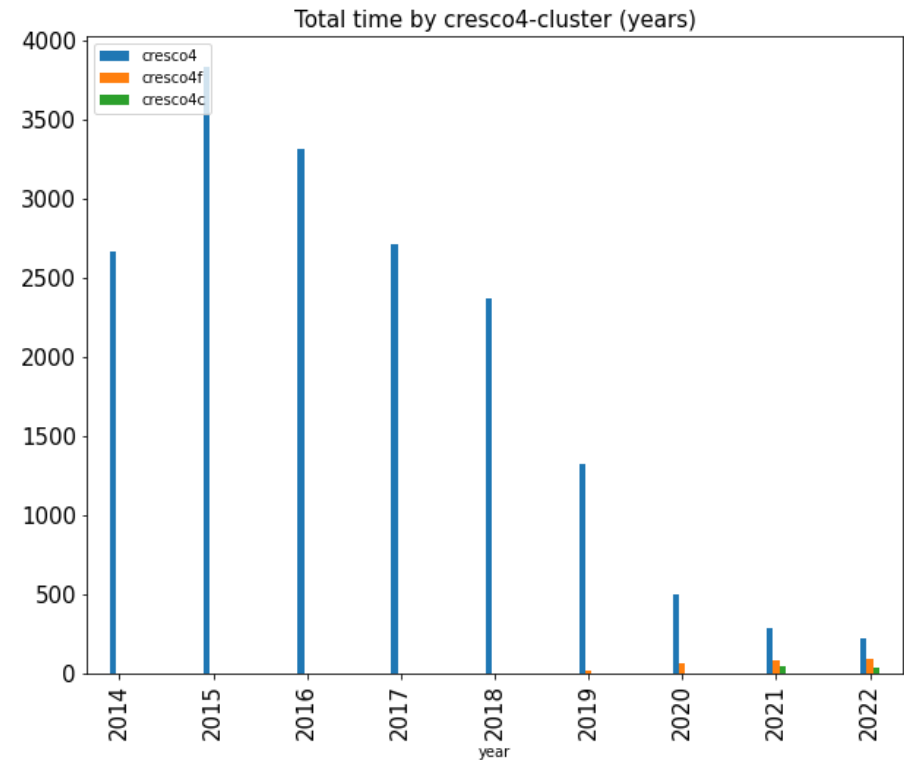
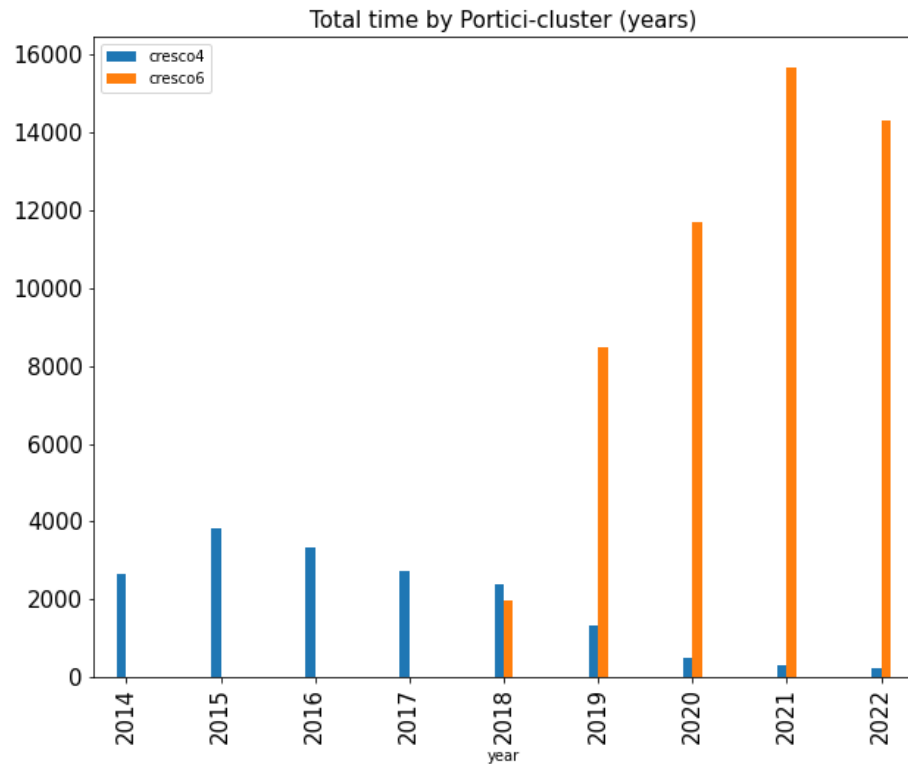


$$1027713/1637704 \times 52 = 32,5$$

Usage (wct_y) by clusters in recent years

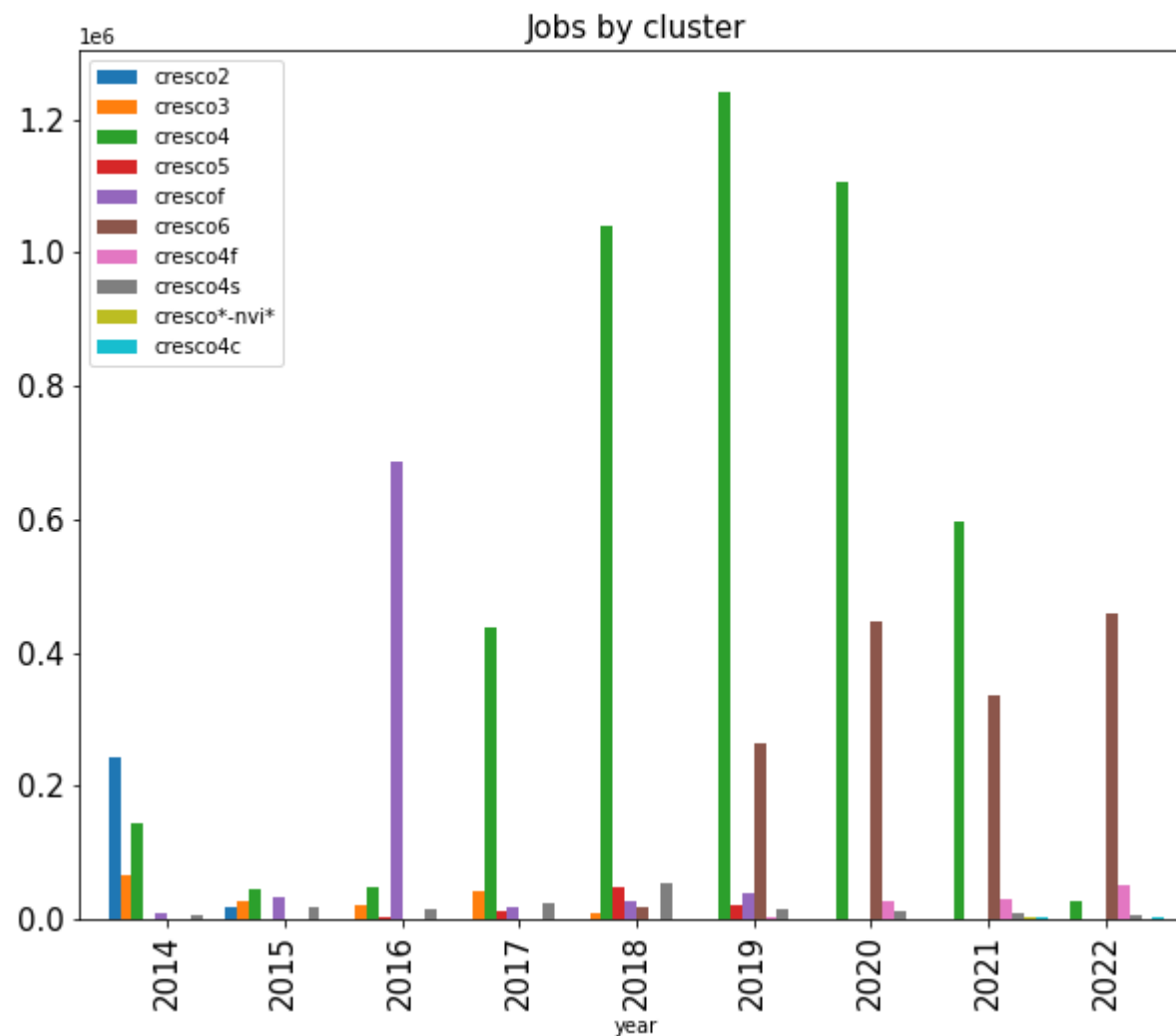


Usage (wct_y) by Portici and cresco4 clusters in recent years

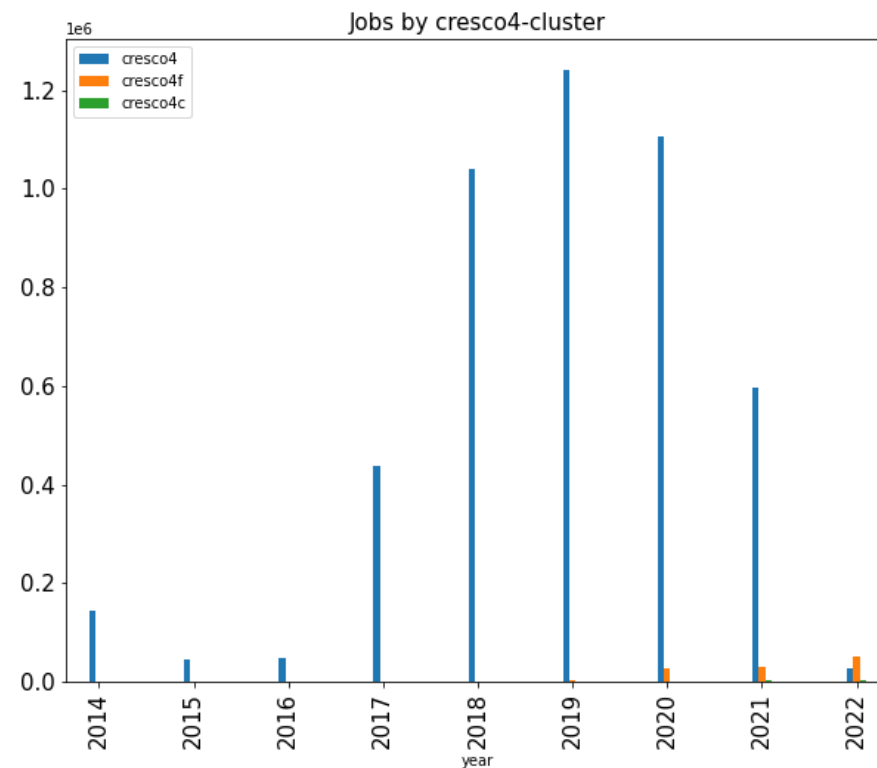
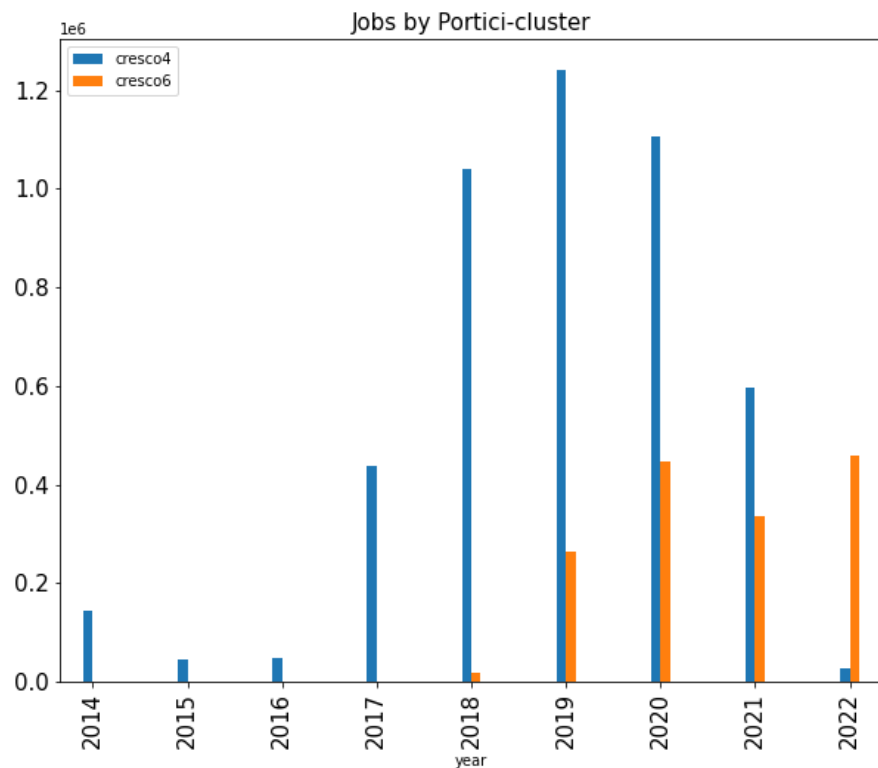


- CRESCO6 wct_y in:
 - 2021: 15680 years
 - 2022: 14329 years

Usage (jobs) by clusters in recent years



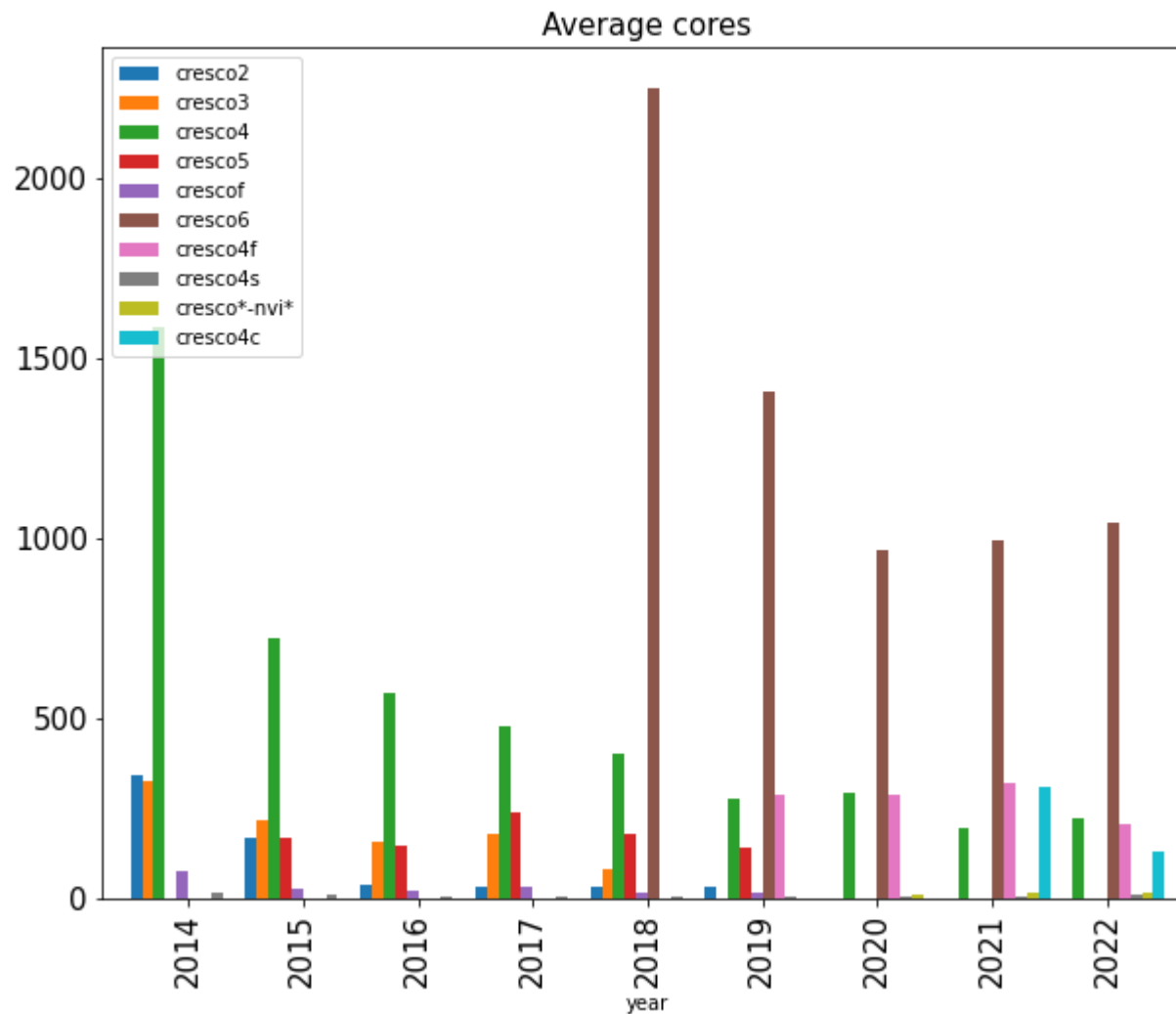
Usage (jobs) by Portici and cresco4 clusters in recent years



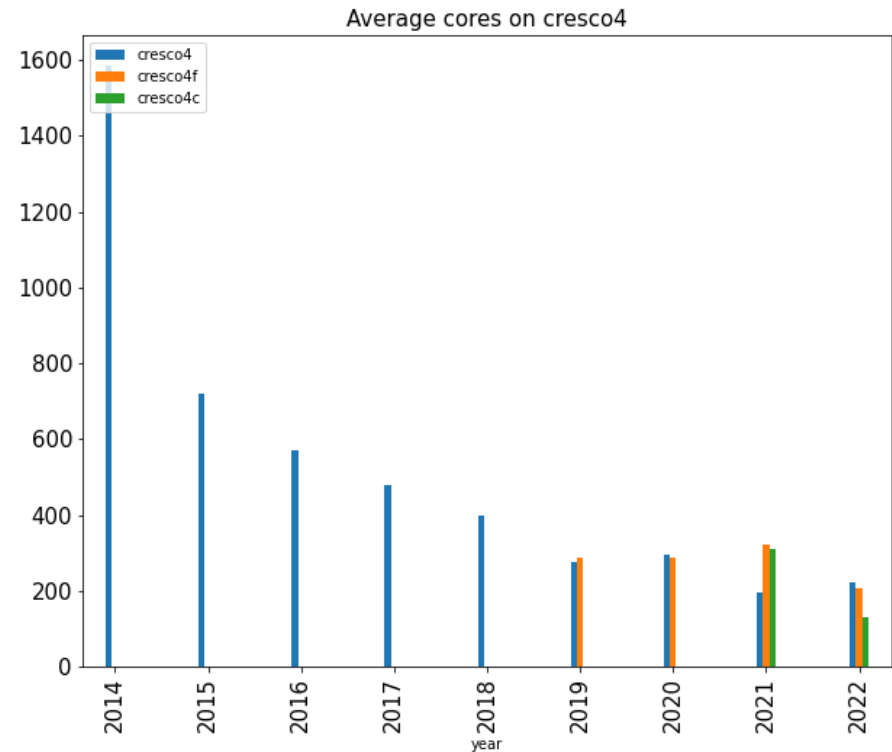
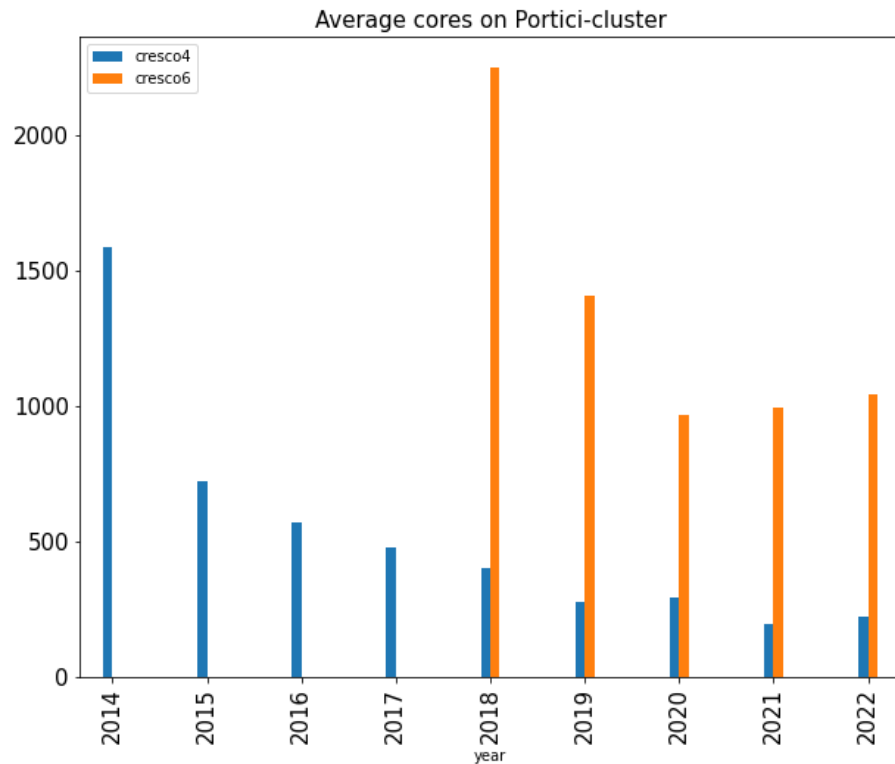
CRESCO6 jobs in:

- 2021: 334430
- 2022: 459073

Parallelism



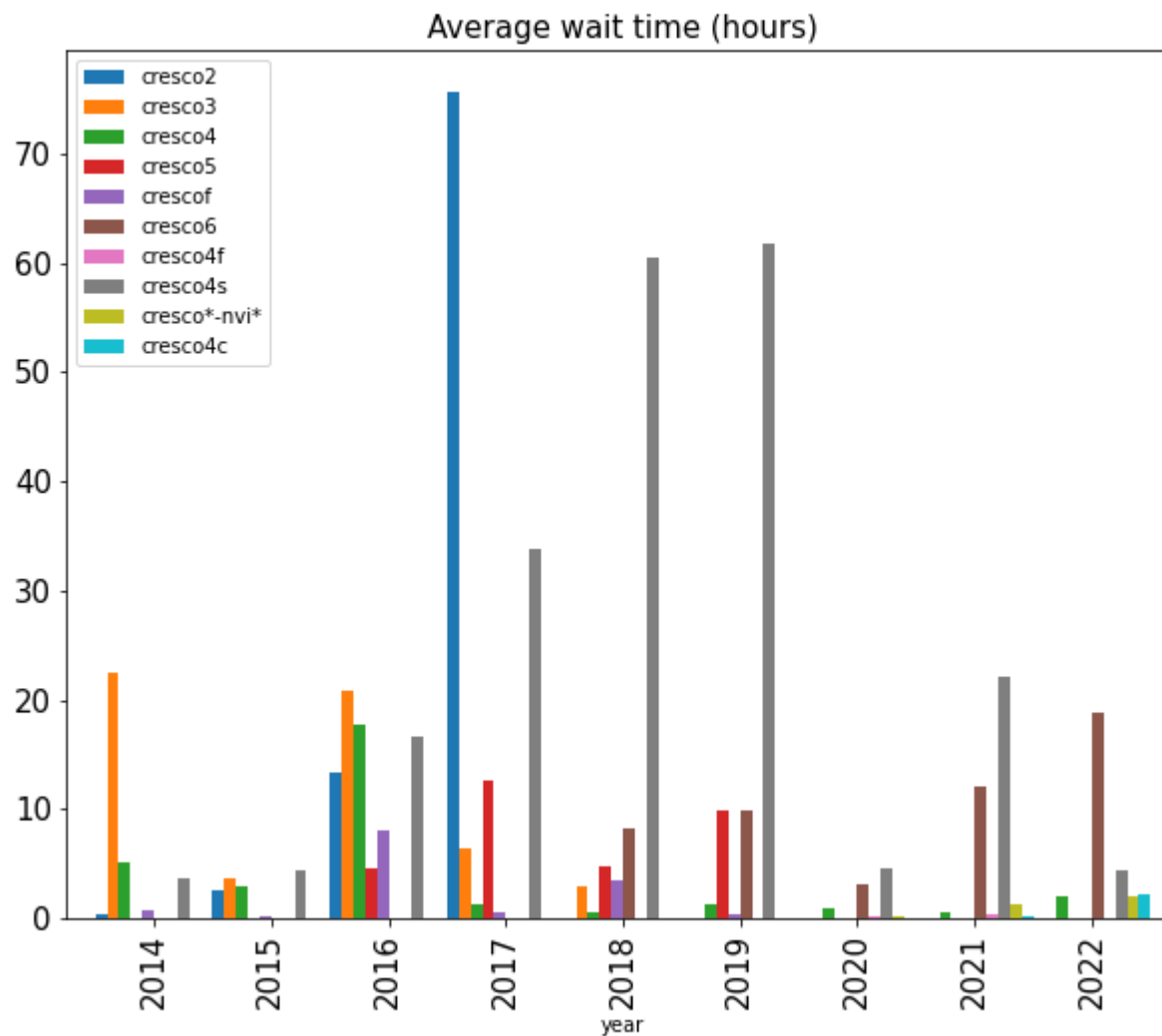
Parallelism on Portici and cresco4 clusters



CRESCO6 av_nc:

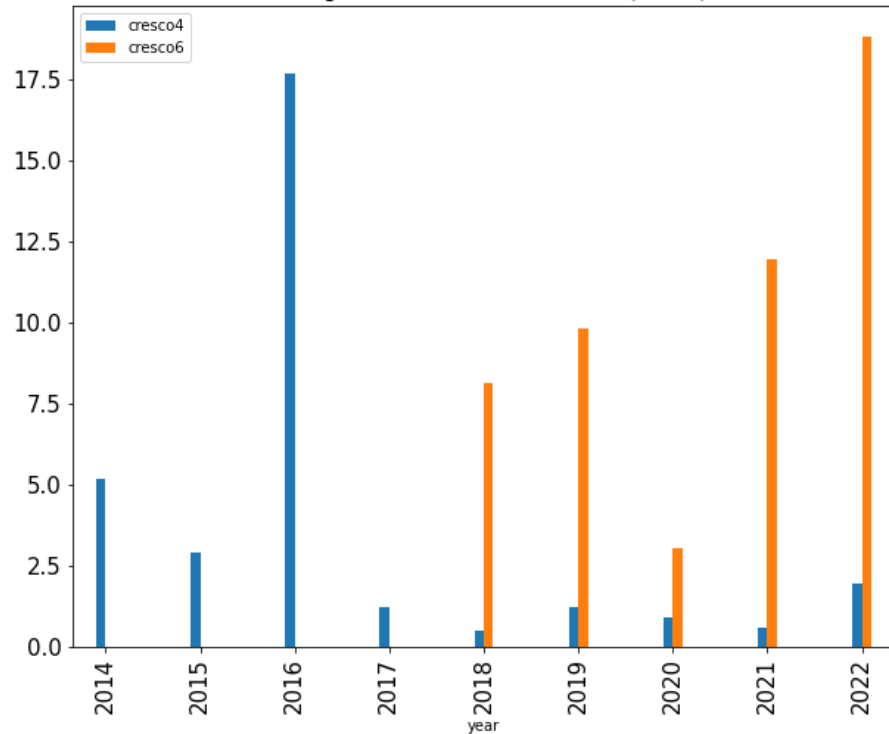
- 2021: 991 cores
- 2022: 1041 cores

Wait time (no crawler)

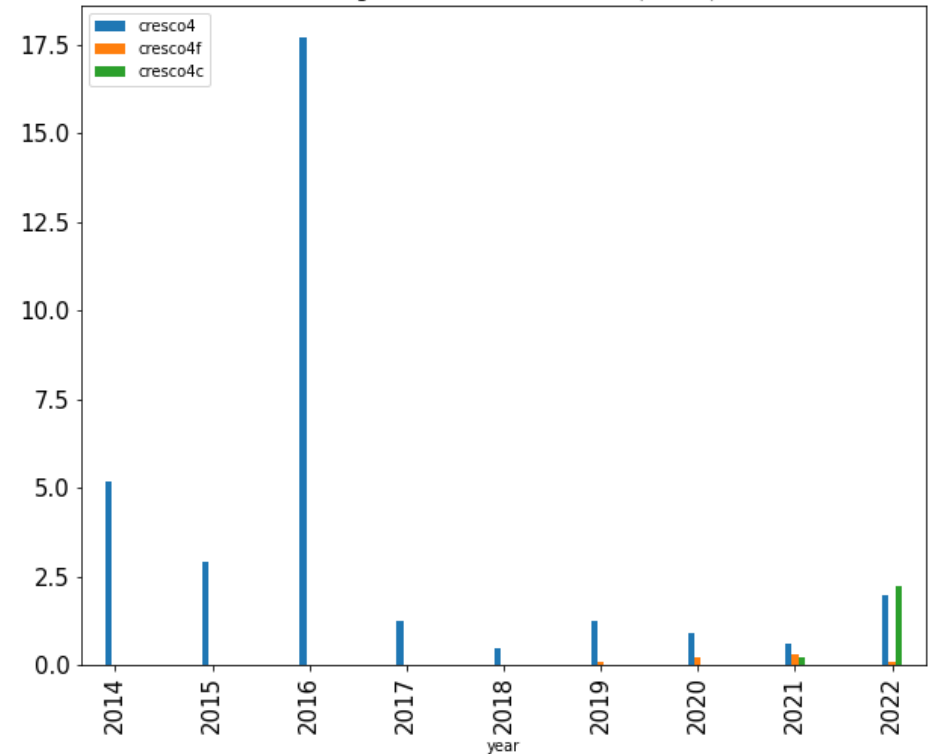


Wait time on Portici and cresco4 clusters

Average wait time Portici-cluster (hours)



Average wait time on cresco4 (hours)



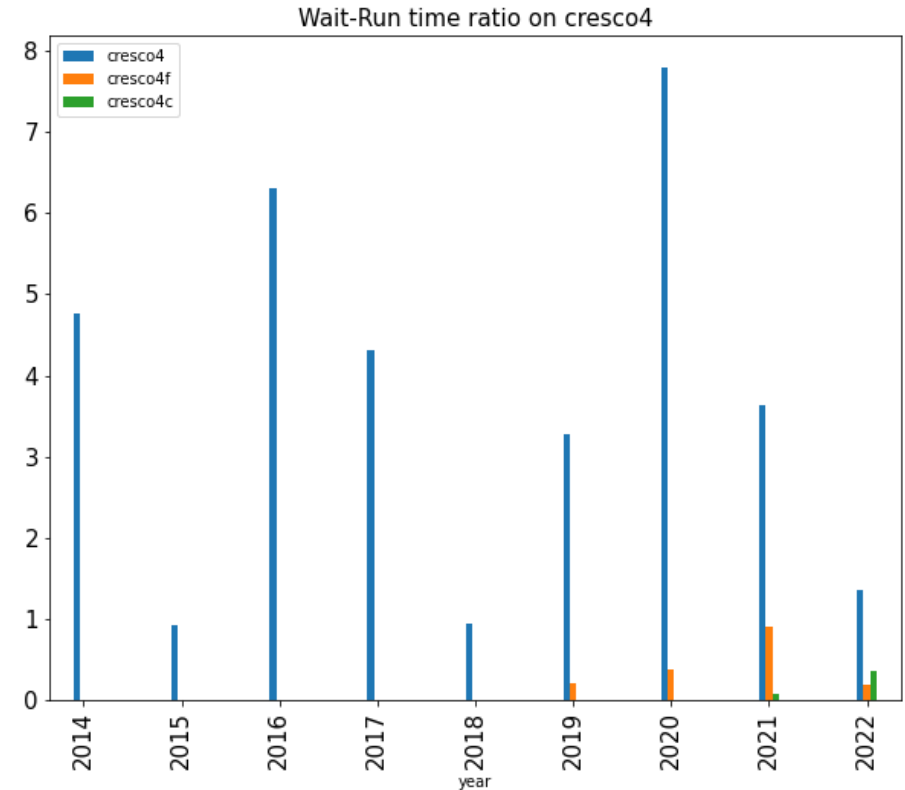
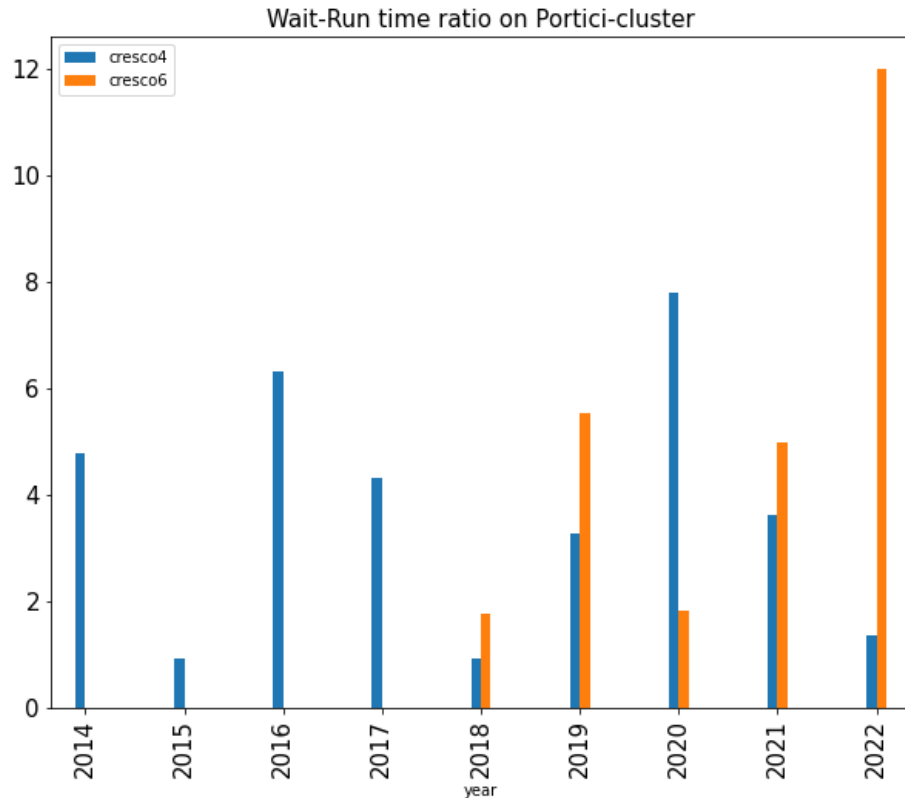
CRESCO6 wait time

- 2021: ~12 hours
- 2022: ~19 hours

Wait/Run time



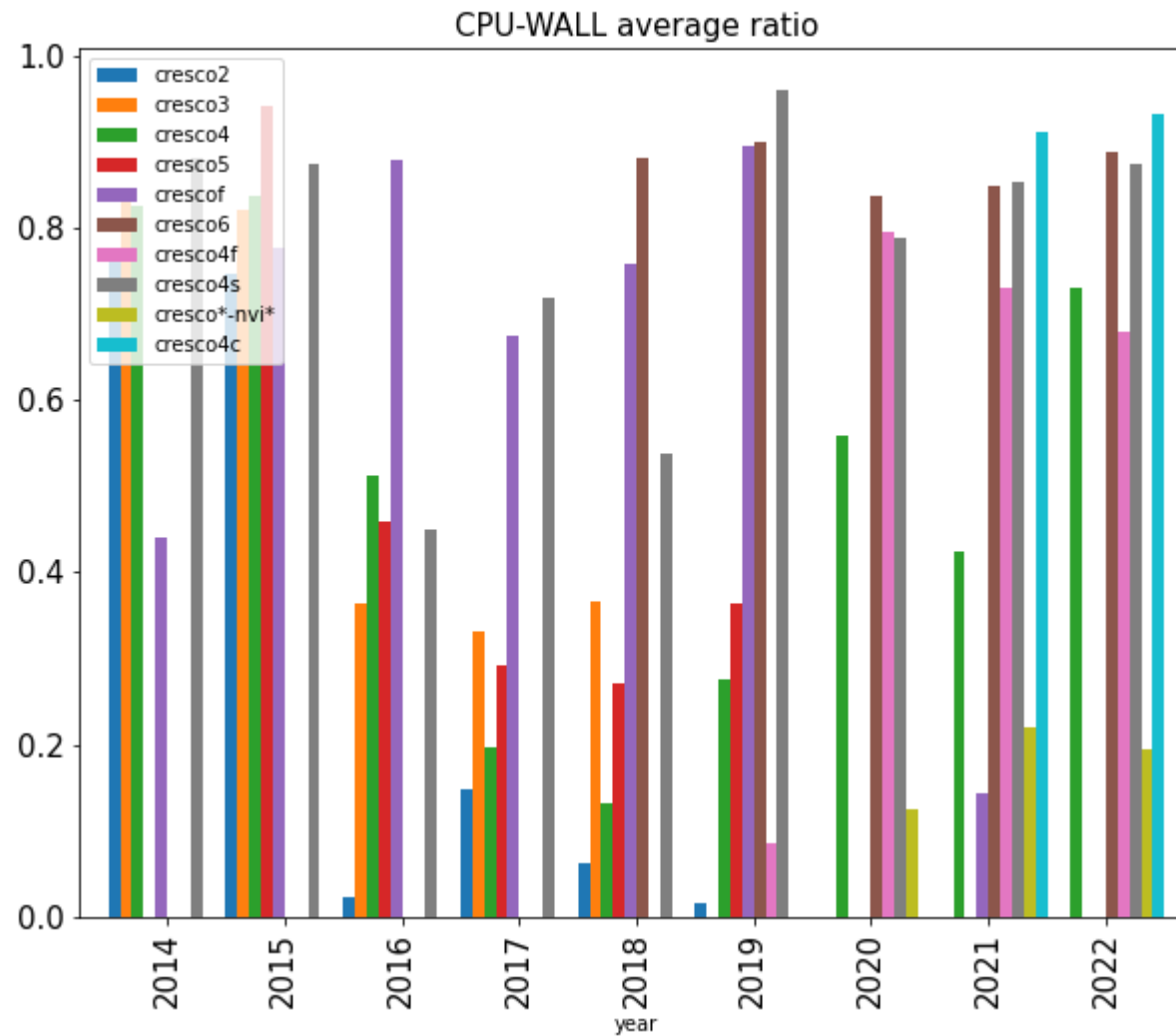
Wait/Run time on Portici and cresco4 clusters



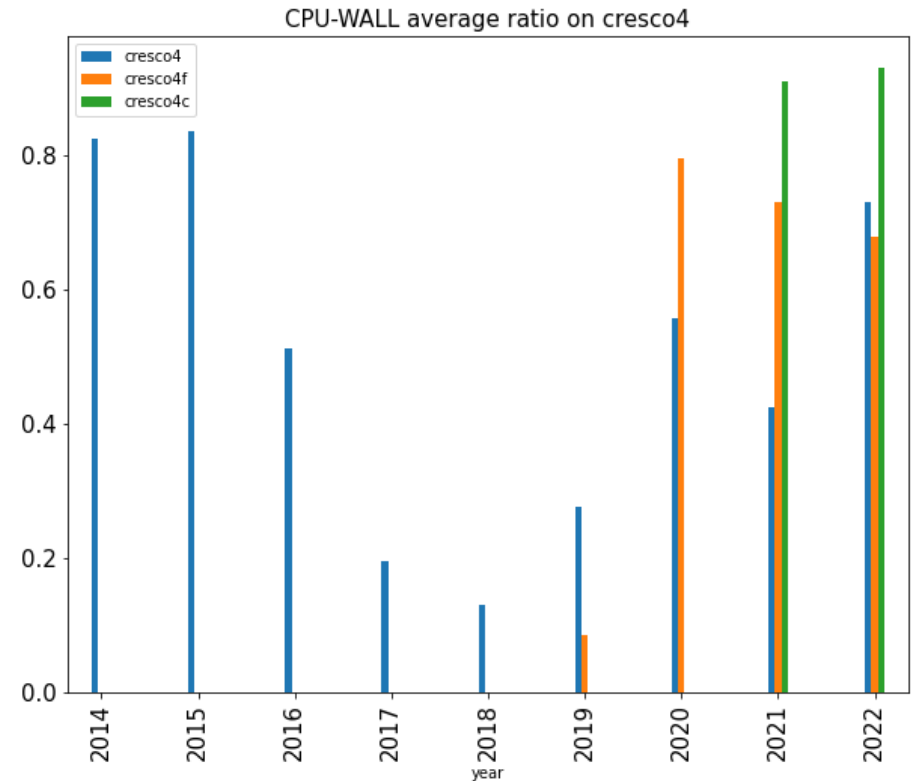
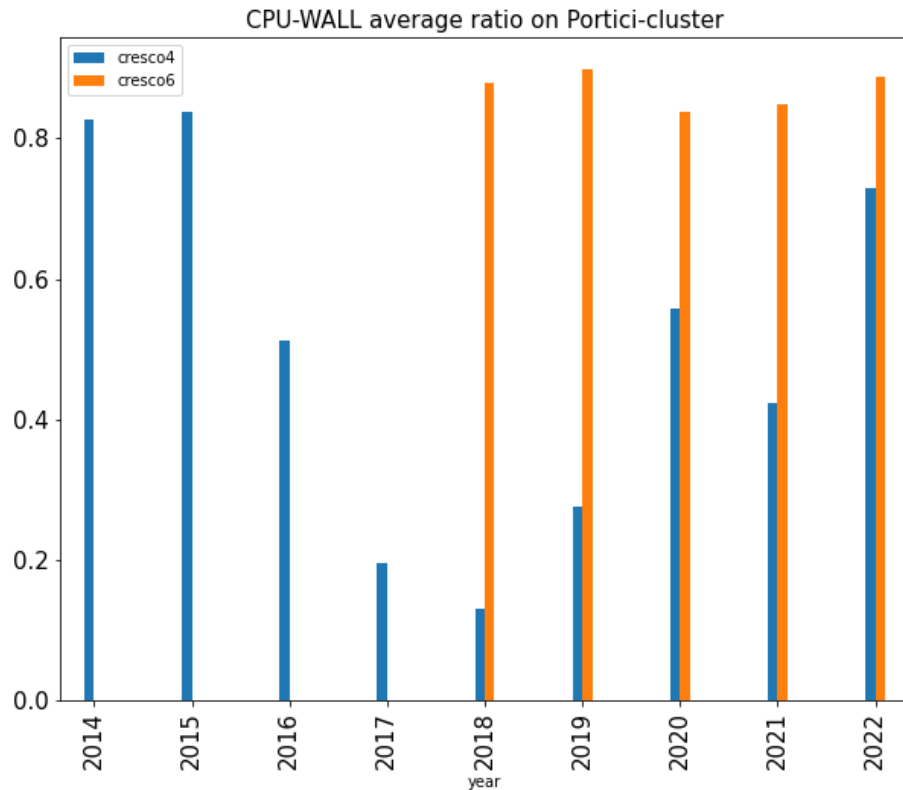
CRESCO6 wait-run time ratio in:

- 2021: ~5
- 2022: ~12

CPU time / Wall Clock time



CPU time / Wall Clock time



CRESCO6 cpu_s/wct_s in:

- 2021: ~0,85
- 2022: ~0,89

Acknowledgments

Special thanks to:

The whole CRESCO team:

always working hard to maintain the clusters alive

Giovanni Bracco:

for accounting data files

Marcello Galli (*retired*):

for the ruby/python scripts to automate large part of the work

Catia Masella:

for assistance in the use of the “Survey” system

Antonella Andreini, Paola Giaquinto:

for the printed version of the Report

S. Giusepponi, D. De Chiara, M. Gusso

for the technical support and their valuable advices

The CRESCO users:

for their contributions to the 2021 annual report

Acknowledgments from a CRESCO User to the CRESCO TEAM

Nel ringraziarvi ancora per il vostro fantastico lavoro vi saluto calorosamente.

Valerio D'Alessandro (vdales)

*Università Politecnica delle Marche, Dipartimento di
Ingegneria Industriale e Scienze Matematiche*

**ANY
QUESTIONS?**