



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

Presentation of the CRESCO annual report: Research activities and results 2018 Accounting 2019

Portici, February 2020

Giuseppe Santomauro – DTE-ICT-HPC – Portici



Contents

The 2018 Report

Accounting 2019

2018: some users and research groups

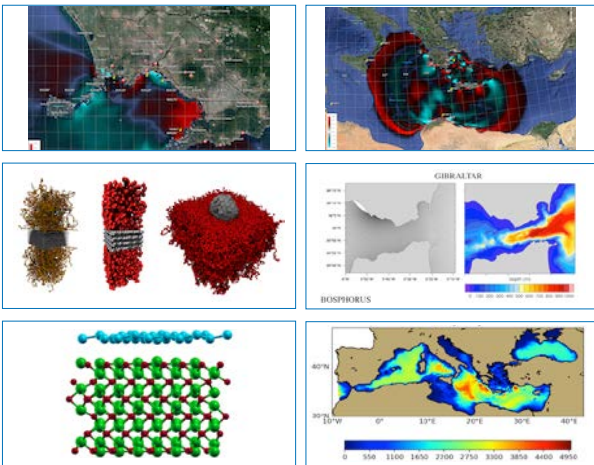
**CRESCO Report 2018:
statistics**

CRESCO usage: trends in recent years

Cresco report 2018 overview



High Performance Computing on CRESCO infrastructure: research activities and results 2018



December 2019

Number of papers: 44

Total number of authors: 152

Number of pages: 240

Document format: PDF

PDF size (print version): 34 MB

PDF size (web version): 7 MB

<https://www.enea.it/it/seguici/pubblicazioni/edizioni-enea/2019/cresco-results-2018>

Contributions provided by a selection of users of the CRESCO infrastructure

Scientific Editor: Giuseppe Santomauro, ENEA, DTE-ICT-HPC, Portici

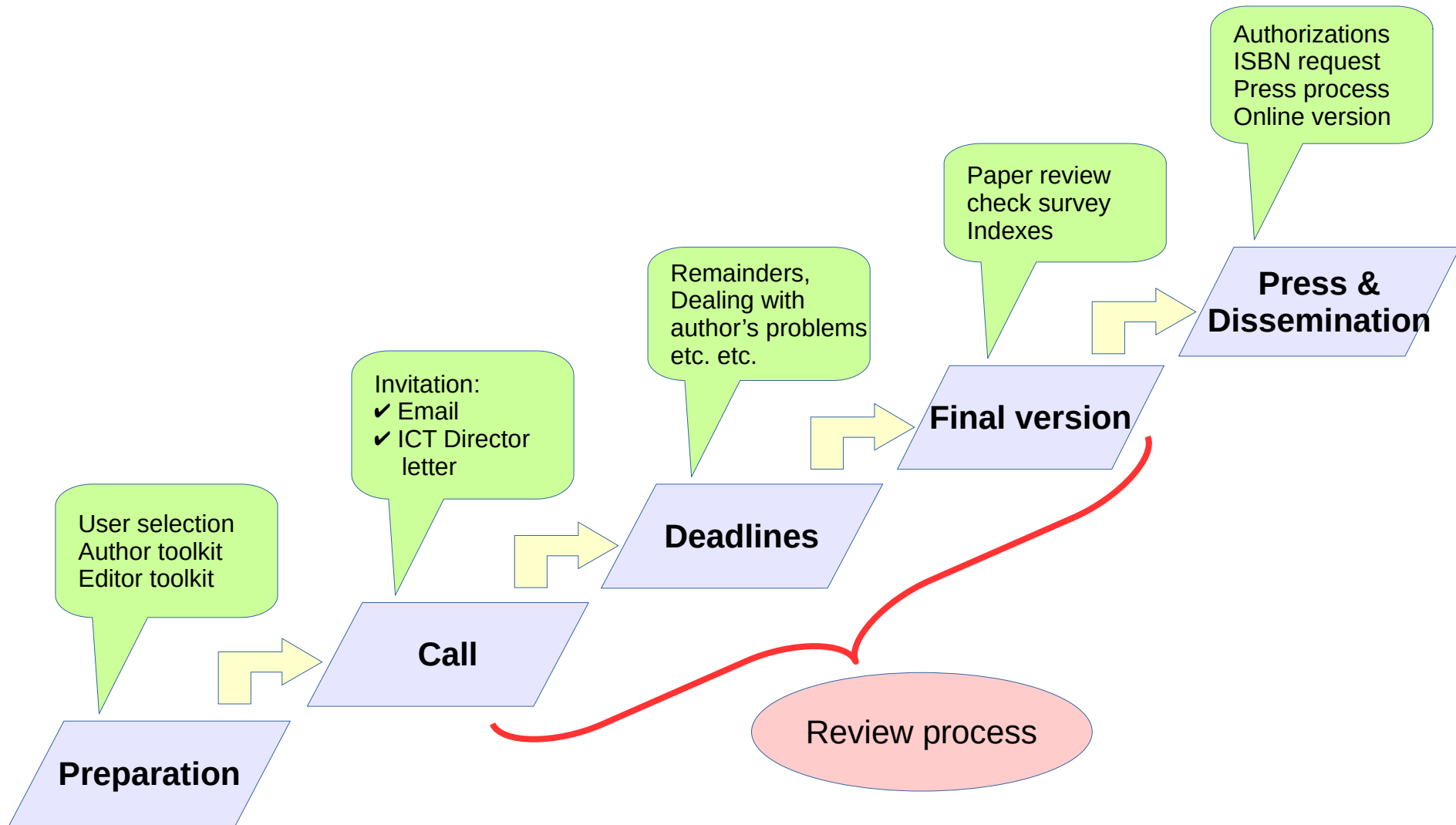
Acknowledgements: We wish to thank Gianclaudio Ferro for providing the Reporter system (<http://hdl.handle.net/10840/5791>) to collect contributions and to build the Volume

**Cover: Amedeo Trolese, ENEA, DTE-ICT-PRA, CR Frascati
ISBN: 978-88-8286-390-6**

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



Report Preparation



Report preparation history

- 2019-06:
 - 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;
 - author tool kit (reporter: <http://reporter.enea.it/>): templates;
 - some tools for the reporter system:
 - <http://reporter.enea.it/repsummary2b.php?order=date&root=206;>
 - <http://reporter.enea.it/userlist.php?order=date;>
 - [http://reporter.enea.it/findroots.php;](http://reporter.enea.it/findroots.php)
- 2019-06-12: invitation mail (~88 invited users);
- 2019-09-14: first deadline (~20 contributions only, despite the many reminders);
- 2019-[10/11]: deadline extensions, reminders, solicitations, mails, review;
- 2019-12: last contribution (Alderuccio - 19th December);
- 2019-12: authorization process for the publication by REL-PROM;
- 2019-12: final check, author index, samples for the cover (by A.Trolese);
- 2020-01: press & dissemination;
- 2020-02: presentation prepared (this presentation).

- ◆ 50 printed copies, distributed by the ICT administrative office
- ◆ Compressed PDF version online:
 - <https://www.enea.it/it/seguici/pubblicazioni/edizioni-enea/2019/cresco-results-2018>
 - https://www.cresco.enea.it/CRESCO_reports/

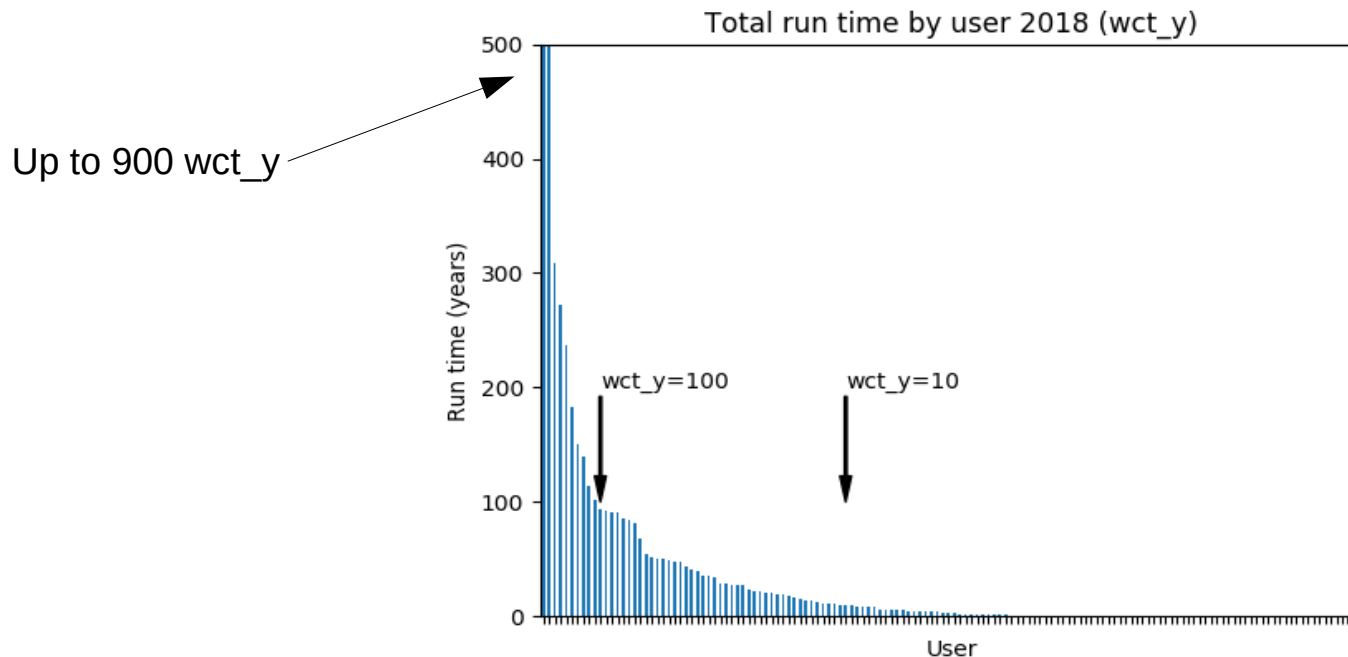
Invited Users

88/144 users invited

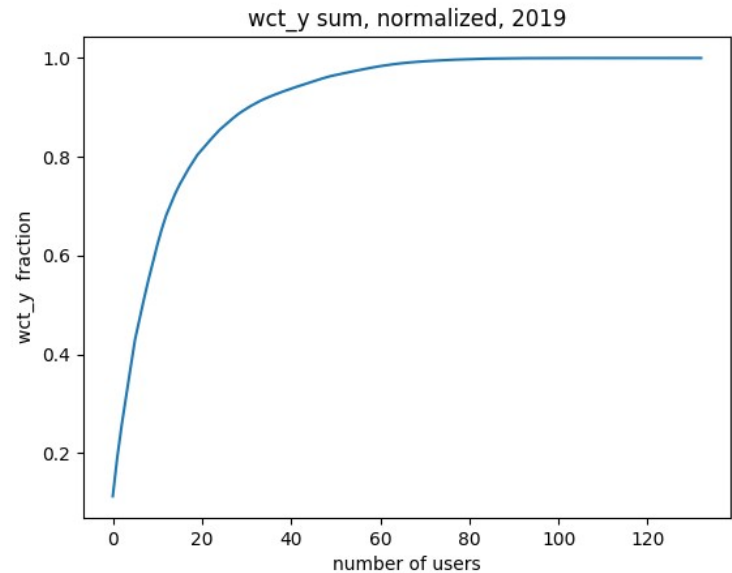
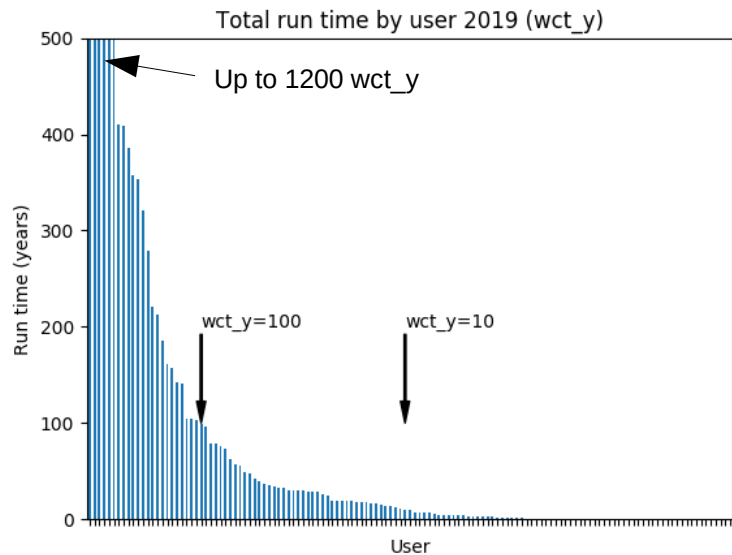
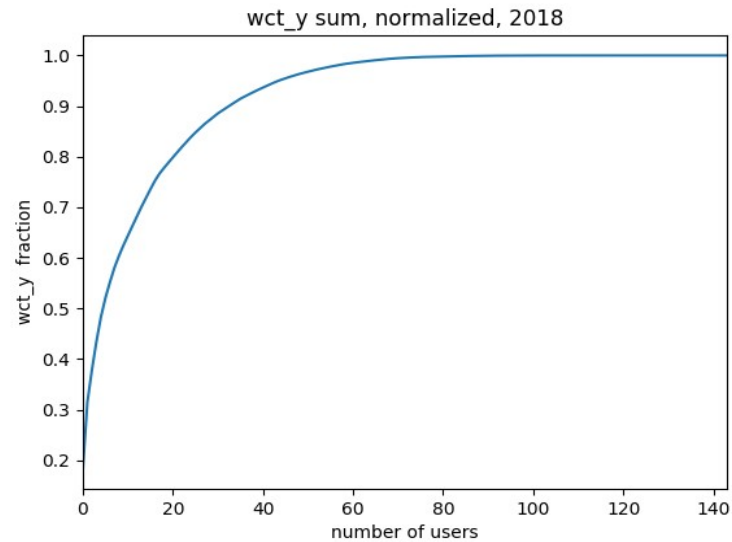
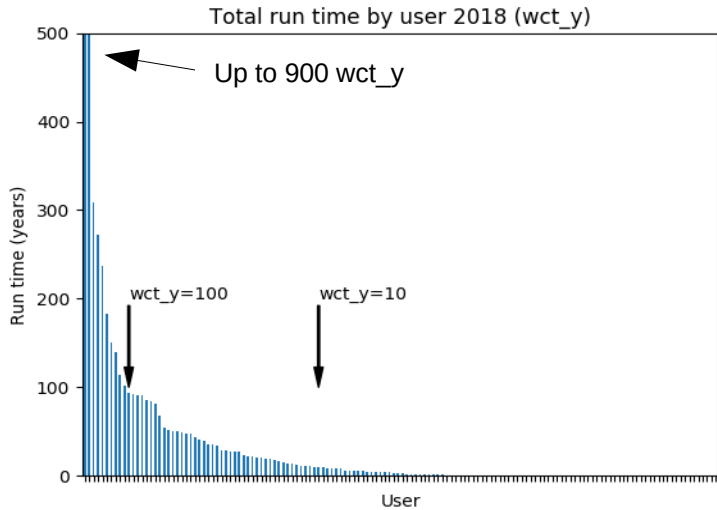
Selection criterium is:

wct_y > 1.0 || (wcty > 0.5 && njobs > 500 && av_totmem > 100000)
[in 2017/2018: wct_y > 1.0 || njobs > 100 || av_mem > 1000]

wct_y: total wall clock time (years)
njobs: number of submitted jobs
av_mem: average requested memory per core (MB)
av_nc: average number of used cores
av_totmem: av_nc*av_mem



Wall clock time by user



In 2019

**~10 users are:
60-70%
of wct_y**

**~20 users are
~80%
of wct_y**

**Statistics
lead by
few power
users**

This has been reported
since the 2013
presentation
by Funel

Accounting

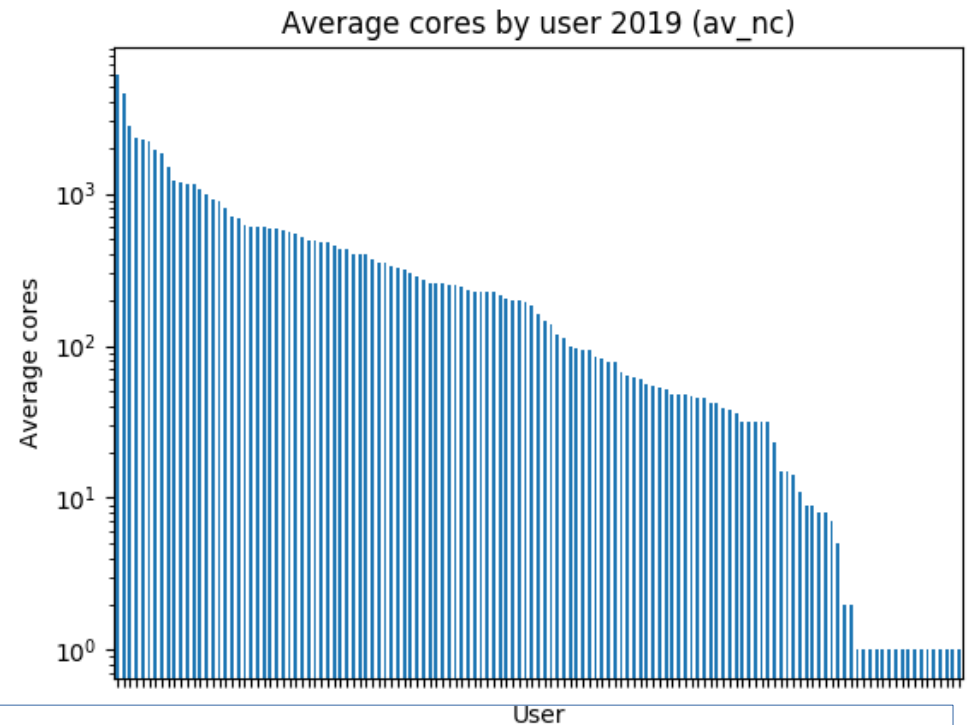
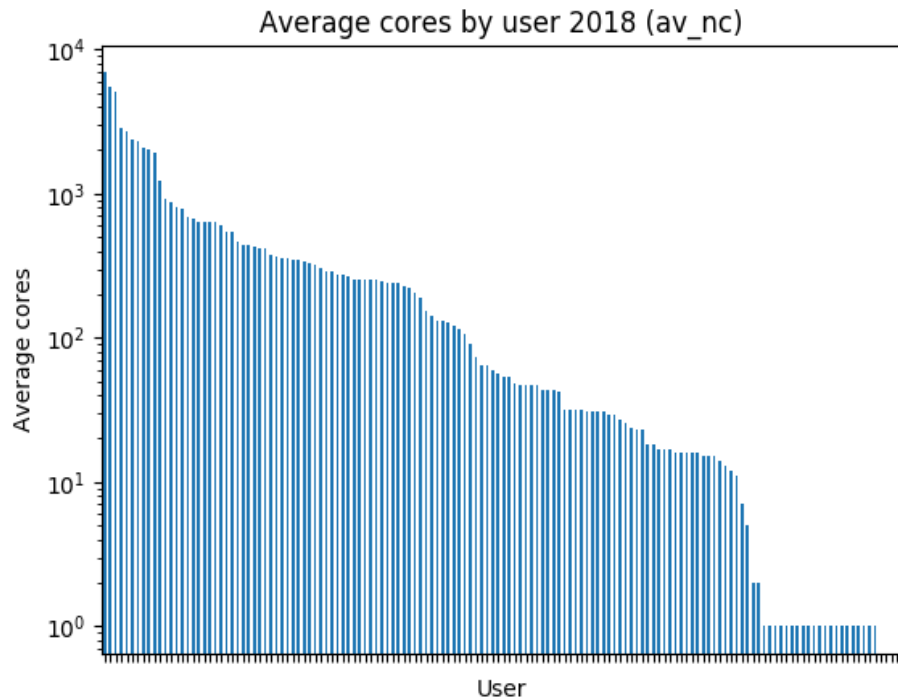
Accounting details 2018 - 2019

Cresco in 2019

Year	jobs	wct_y
2016	847184	4857
2017	571258	3895
2018	1321623	4853
2019	1675438	9992

In 2020	>2000000	>10000	?
---------	----------	--------	---

Average number of cores by user 2018-2019



Half users use more than 100 cores

Some users with more than 1000 cores in 2018-2019

CRESCO6 has ~20000 cores.

Will there be users who will use more than 10000 cores in 2020?

No! There is a limit on LSF: up to 6144 cores (unless system queue for admin).

The 2019 CRESCO Users

Users 133

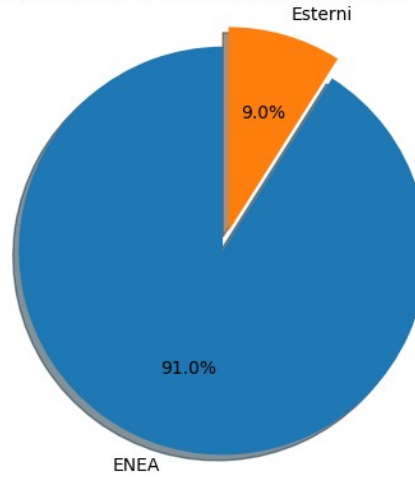
ENEA	97
DTE	34
FSN	38
SSPT	15
other	10

External	36
UniNa	10
UniRoma1	5
UniRoma2	3
CNR	2
UniFi	2
UniCal	1
UniSa	1
UniCam	1
UniBo	1
UniPg	1
UniRc	1
CRA	1
LTCalcoli	1
AriaNet	1
UNIRCJMadrid	2
UniZhejiang	1
UniBelgrade	1
AVIO	1

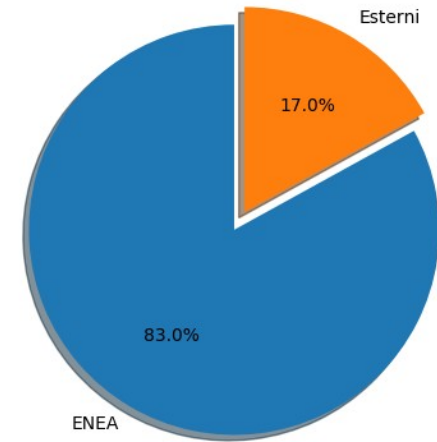
ENEA and External usage 2018-2019

2018

Number of jobs 2018: ENEA and External Users

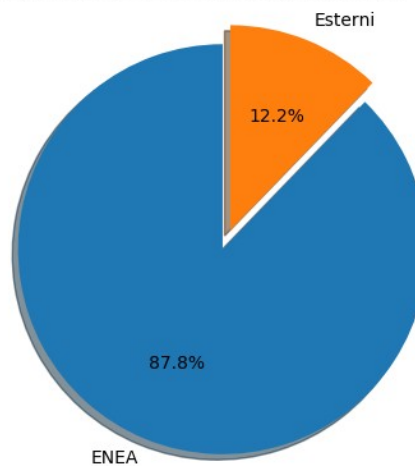


Total run time 2018: ENEA and External Users

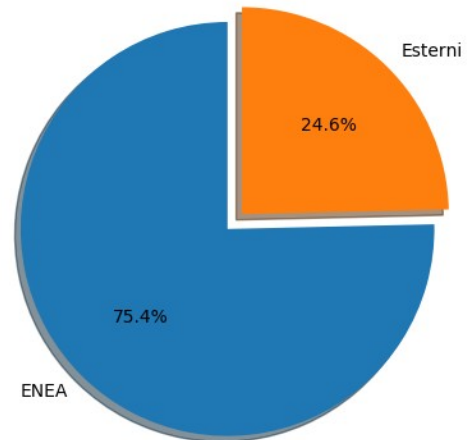


2019

Number of jobs 2019: ENEA and External Users

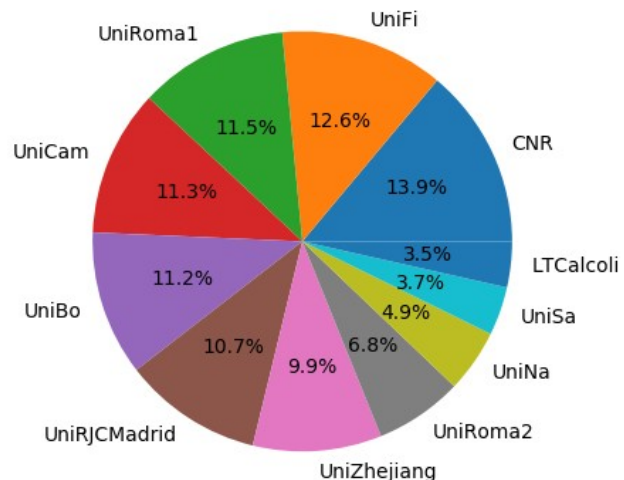


Total run time 2019: ENEA and External Users

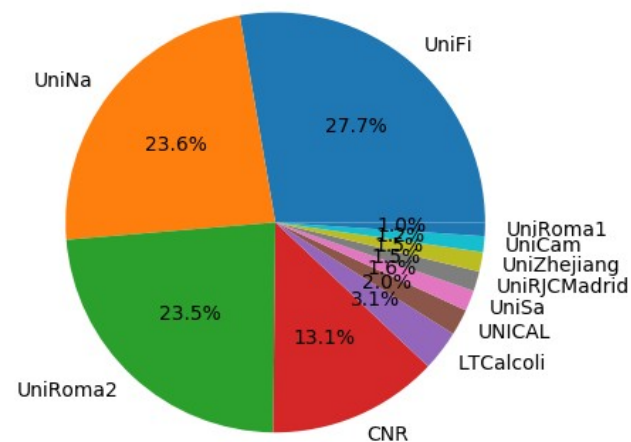


Usage by external institute – wct_y 2018-2019

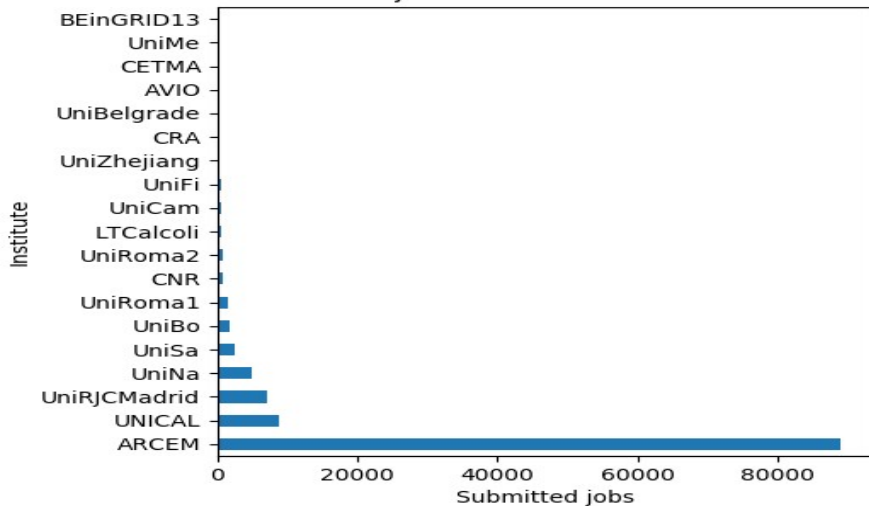
Total run time 2018 for external institutes (wct_y>10)



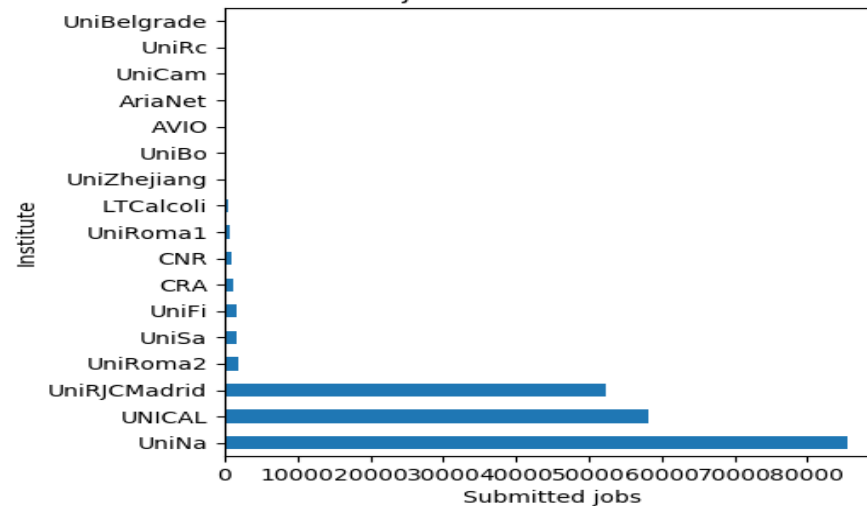
Total run time 2019 for external institutes (wct_y>10)



Submitted jobs 2018 for external institutes



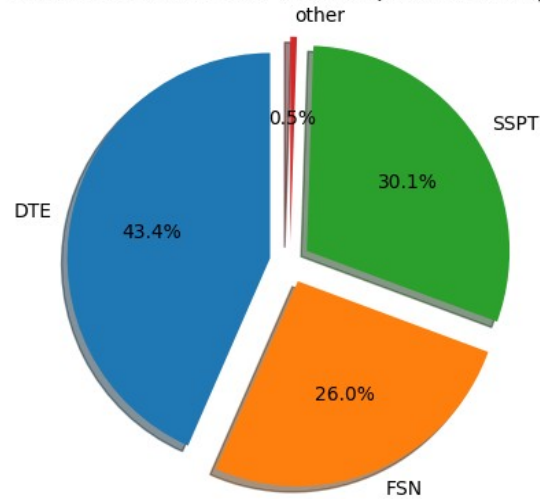
Submitted jobs 2019 for external institutes



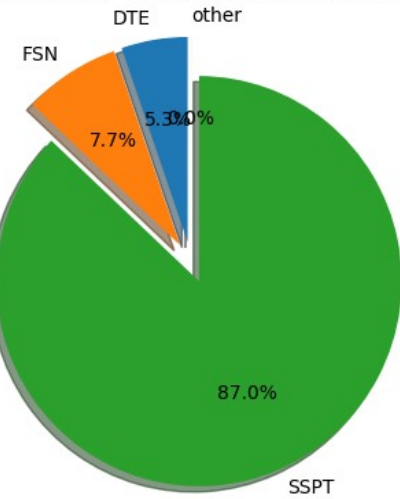
Usage by Enea department 2018-2019

2018

Total run time 2018 for ENEA department (wct_y)

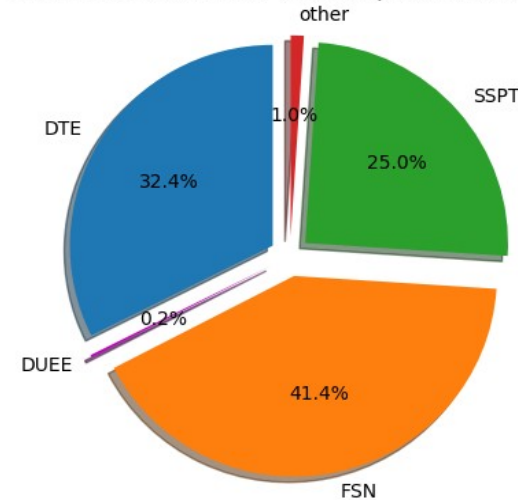


Jobs 2018 for ENEA department (njobs)

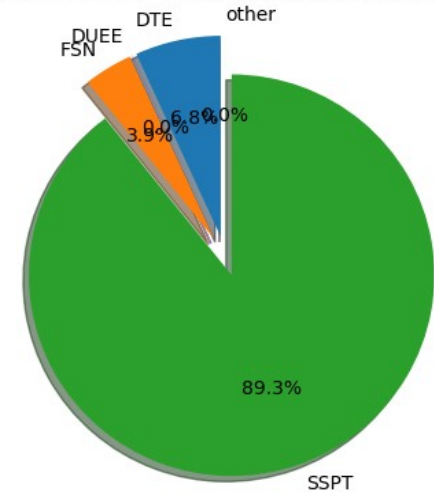


2019

Total run time 2019 for ENEA department (wct_y)

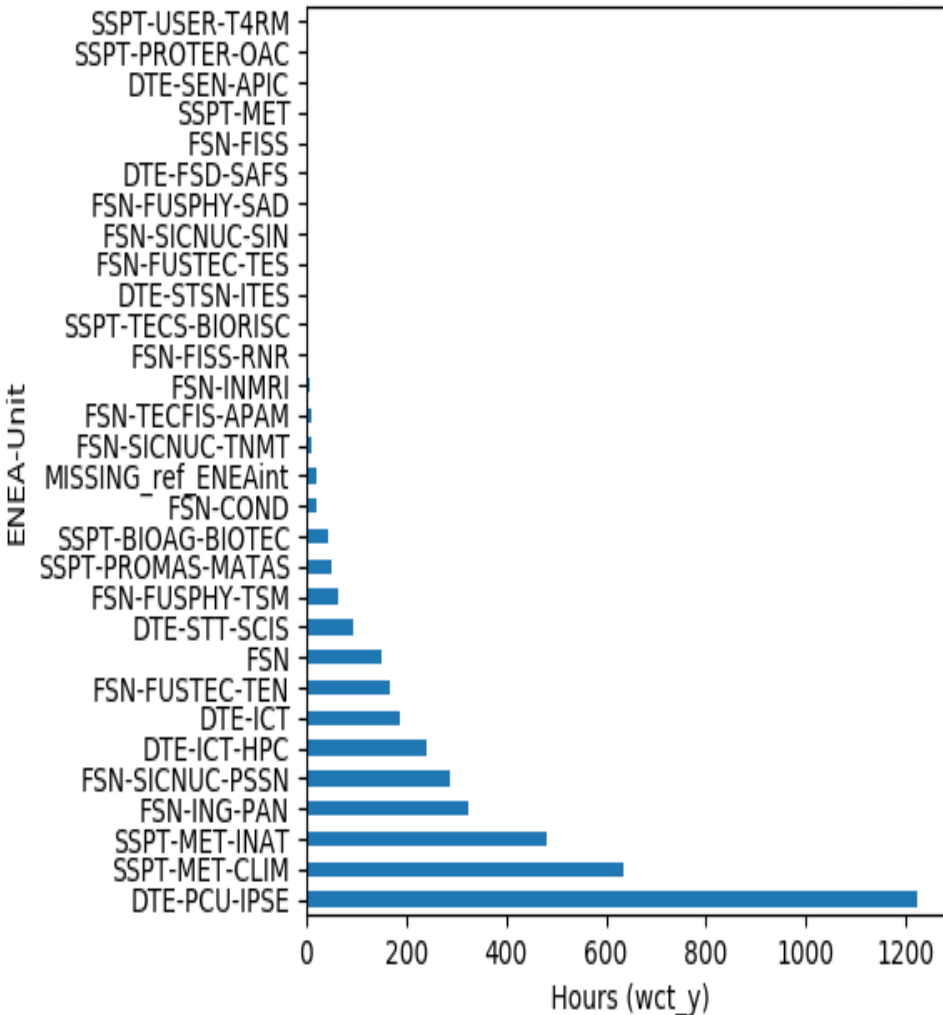


Jobs 2019 for ENEA department (njobs)



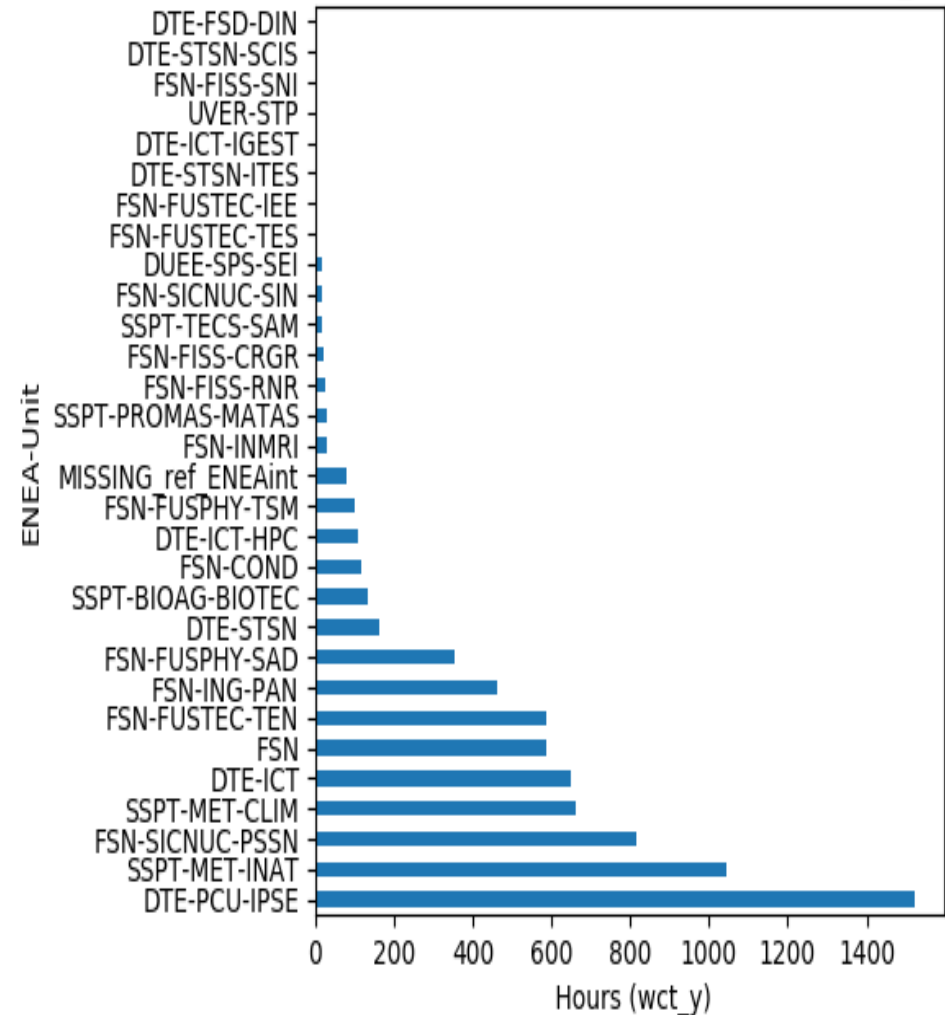
ENE A usage 2018-2019

Total run time 2018 for ENEA division (wct_y)



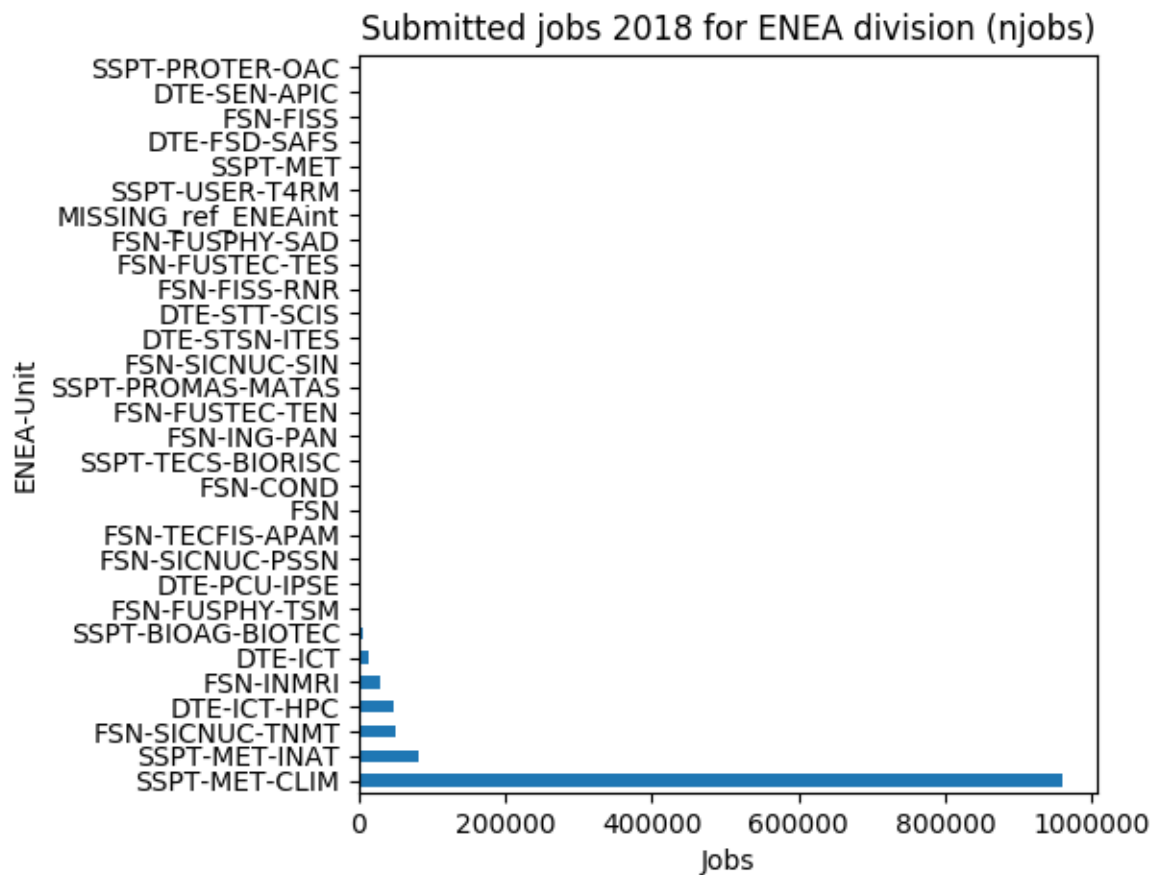
(DTE-PCU-IPSE :Giacomazzi, Picchia et al, combustion studies)

Total run time 2019 for ENEA division (wct_y)



(DTE-PCU-IPSE :Giacomazzi, Picchia et al, combustion studies)

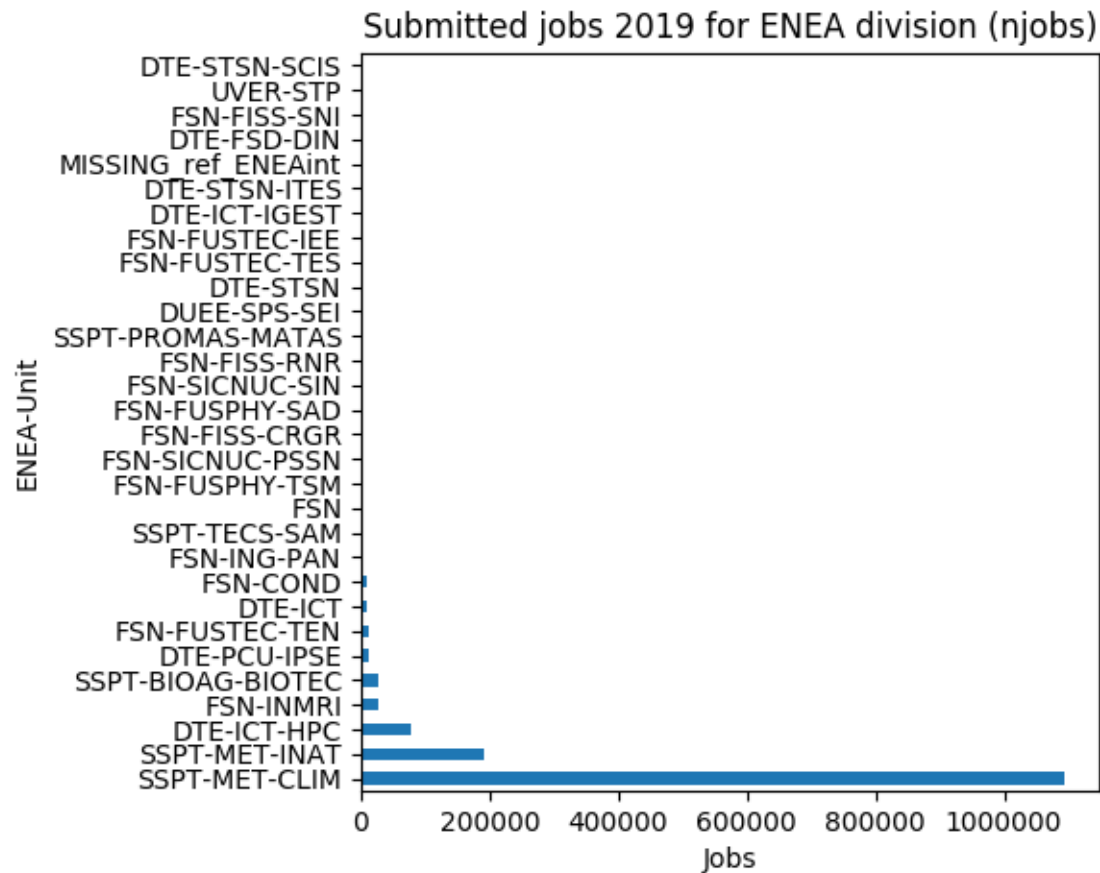
Usage by ENEA division - jobs 2018



Many jobs for climate and pollutants transport models

DIV	njobs
SSPT-MET-CLIM	959438
SSPT-MET-INAT	80145
FSN-SICNUC-TNMT	49882
DTE-ICT-HPC	46703
FSN-INMRI	29625
DTE-ICT	13311
SSPT-BIOAG-BIOTEC	5038
FSN-FUSPHY-TSM	3251
DTE-PCU-IPSE	2988
FSN-SICNUC-PSSN	2125
FSN-TECFIS-APAM	1866
FSN	1723
FSN-COND	1633
SSPT-TECS-BIORISC	1493
FSN-ING-PAN	1140
FSN-FUSTEC-TEN	780
SSPT-PROMAS-MATAS	377
FSN-SICNUC-SIN	342
DTE-STSN-ITES	200
DTE-STT-SCIS	189
FSN-FISS-RNR	133
FSN-FUSTEC-TES	133
FSN-FUSPHY-SAD	131
MISSING_ref_ENEAint	60
SSPT-USER-T4RM	28
SSPT-MET	19
DTE-FSD-SAFS	19
FSN-FISS	9
DTE-SEN-APIC	2
SSPT-PROTER-OAC	2

Usage by ENEA division - jobs 2019



Many jobs for climate and pollutants transport models

DIV	njobs
SSPT-MET	1283738
DTE-ICT	236251
DTE-???	50801
FSN-INMRI	27205
SSPT-BIOAG	26816
DTE-PCU	12599
FSN-FUSTEC	11732
FSN-COND	7499
FSN-ING	3709
FSN-FUSPHY	2916
SSPT-TECS	2805
FSN	2293
SSPT-PROMAS	2108
FSN-SICNUC	2019
FSN-FISS	1342
SSPT-PVS	880
DUEE-SPS	293
DTE-STSN	283
SSPT-PROTER	108
FSN-???	32
DTE-FSD	6
UVER-STP	3

2018 Power Users

2018: Some users and research groups

Power users 2018

Users with the highest wct_y

Top12 users generated ~2/3 of total wct_y

#	user	wct_y
1	eugenio	892,2810
2	sannino2	633,6330
3	pconsole	308,3020
4	dcecere	272,7690
5	pergreff	236,4900
6	adani	182,7600
7	meineri	151,0140
8	palombi	139,0630
9	anavf	113,3430
10	disidoro	102,0970
11	grena	93,9278
12	mancinig	92,3208
13	gcoletta	91,4852
14	briganti	91,4240
15	gutierre	85,1983

Tot: ~4850 wct_y

Users with many jobs:

Top15 users submitted 96% of total njobs

#	user	njobs
1	sannino2	959409
2	rizzi	89010
3	lomeo	49882
4	palombi	33302
5	pimpinel	29625
6	disidoro	27315
7	forair	21150
8	briganti	18332
9	tagarell	8720
10	adani	8148
11	ferriani	7701
12	gutierre	5315
13	leporea	4112
14	buonocor	3794
15	pizzirus	3414

Tot: ~1300000 jobs

Some research groups (environment)

Environment SSPT-MET-INAT (MINNI air transport model)

user	wct_y	njobs
adani	182,76	8148
disidoro	102,10	27315
briganti	91,42	18332
forecast	50,97	2007
forair	47,40	21150
villanim	5,17	79
cappelle	0,54	3051
frusso	0,16	37
petralia	0,03	4
vitali	0,01	22
Tot	480,56	80145

Climate studies and modeling SSPT-MET-CLIM (ENEA-Casaccia)

user	wct_y	njobs
sannino2	633,63	959409
struglia	0,91	21
lombardi	4e-05	8
Tot	633,64	959438

Some research groups (fusion)

Magnetohydrodynamics FSN-FUSPHY-TSM (Fusion - Frascati)

user	wct_y	njobs
wangt (china)	81,32	332
sergio	27,82	1358
vlad	27,31	199
casolari (pisa)	5,11	131
fogaccia	3,97	202
cardinal	0,06	1357
fusco	5e-04	4
innocent	5e-07	2
Tot	145,60	3585

ITER-DEMO, MC: mcnp (Neutronics) FSN-FUSTEC-TEN (Fusion – Frascati)

user	wct_y	njobs
moro	34,86	119
morof	47,26	54
luisr	43,23	204
acolange	28,88	568
gmariano	27,73	374
villari	11,73	153
villari2	10,12	53
flammini	7,96	153
snoce	6,34	23
park	4,62	18
fonnesu	0,00	5
calamida	0,00	3
Tot	222,73	1727

Some research group (combustion)

Combustion processes (CFD) DTE-PCU-IPSE (Casaccia)

user	wct_y	njobs
eugenio	892,281	2182
dcecere	272,769	457
dinando	51,672	275
calchett	5,624	54
nunzio	0,003	20
Tot	1222,350	2988

Some research group (neutronics)

Montecarlisti ENEA/FSN-ING-PAN (BOlogna)

user	wct_y	njobs
pconsole	308,30	1044
kb	49,63	983
kwb	0,16	192
Tot	358,09	2219

MCNPX (for a neutron generator) ENEA - UniRoma1

user	wct_y	njobs
lepore	9,34	401
gandolfo	21,40	368
Tot	30,74	769

Some research group (molecular dynamics)

Salerno University

user	wct_y	njobs
credendi	19,53	1792
denicola	10,99	594
zhao	0,08	59
Tot	30,60	2445

Camerino University

user	wct_y	njobs
mancinig	92,32	391
mancini	0,04	45
Tot	92,36	436

Naples University

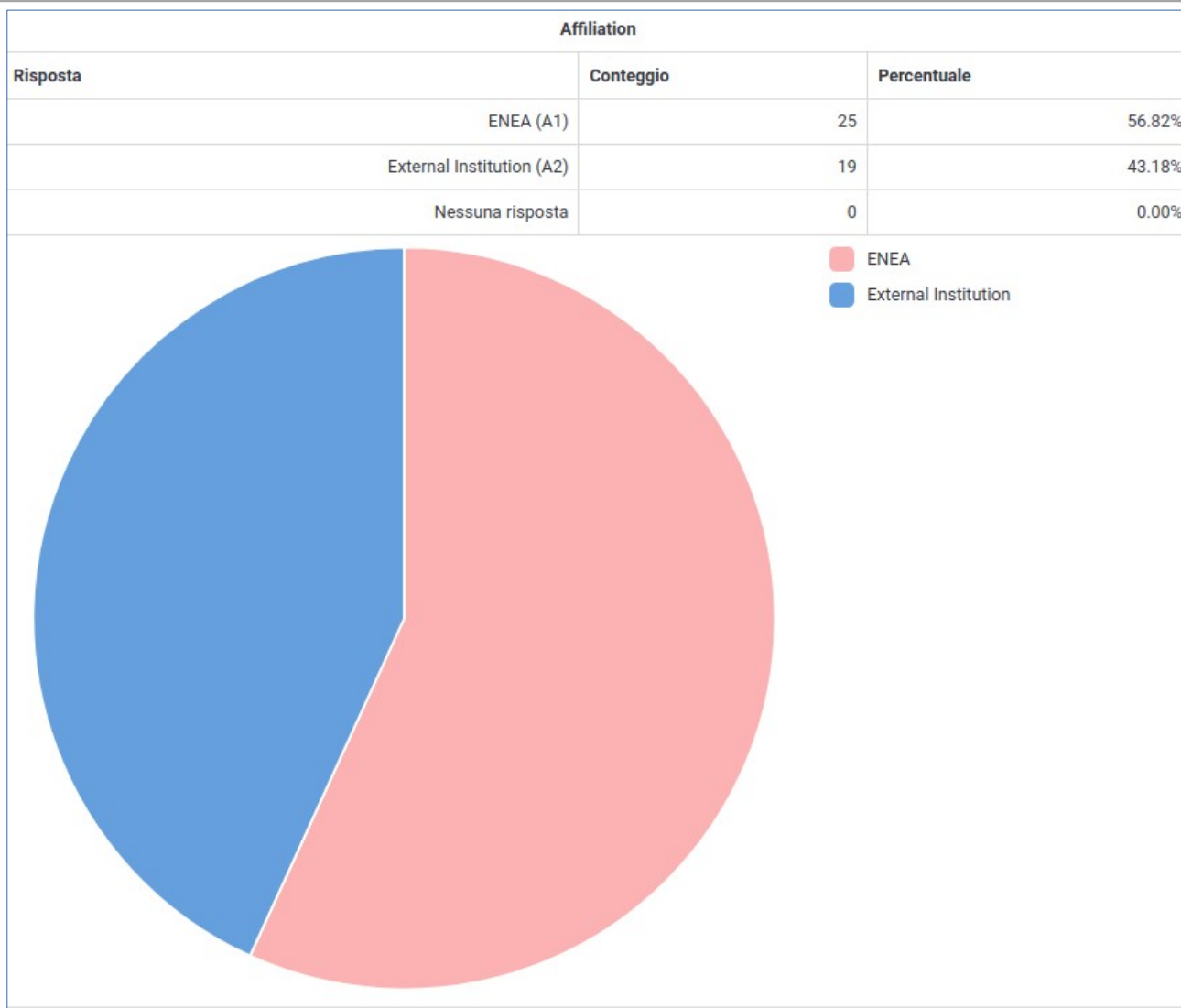
user	wct_y	njobs
mconte	5,80	154
cannunz	1,98	53
sbianco	1,85	343
fiorillo	0,22	98
aesposit	0,00	16
amchiar	0,00	6
Tot	9,85	670

2018 report statistics

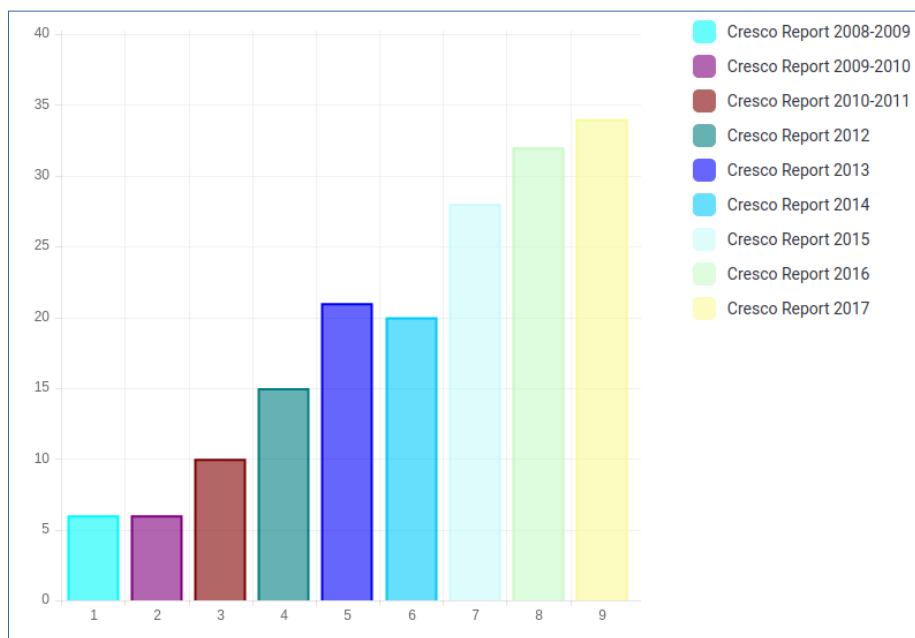
Contributed papers: statistics

- ◆ Invited users: 88/144
wcty > 1.0 || (wcty > 0.5 && njobs > 500 && av_totmem > 100000)
previously (wcty > 1.0 || njobs > 100 || avmem > 1000.0)
- ◆ Survey responses: 45 (-1 deleted, +9 incomplete)
- ◆ Papers: 44 (152 authors, 3.42 author/paper)
- ◆ Missing authors with wct_y > 50 : 4 (1 deleted user on warc, on top22)
- ◆ Missing authors with wct_y > 20 : 6 (1 changed work, on top40)
- ◆ 2018: we had 44 papers (G.Santomauro editor)
- ◆ 2017: we had 38 papers (M.Galli editor)
- ◆ 2016: we had 45 papers (M.Gusso editor)
- ◆ 2015: we had 46 papers (G.Ponti editor)
- ◆ 2014: we had 28 papers (F.Ambrosino editor)
- ◆ 2013: we had 36 papers (A.Funel editor)
- ◆ 2012: we had 31 papers (F.Palombi, D.Piccinelli)

ENEA and external Users



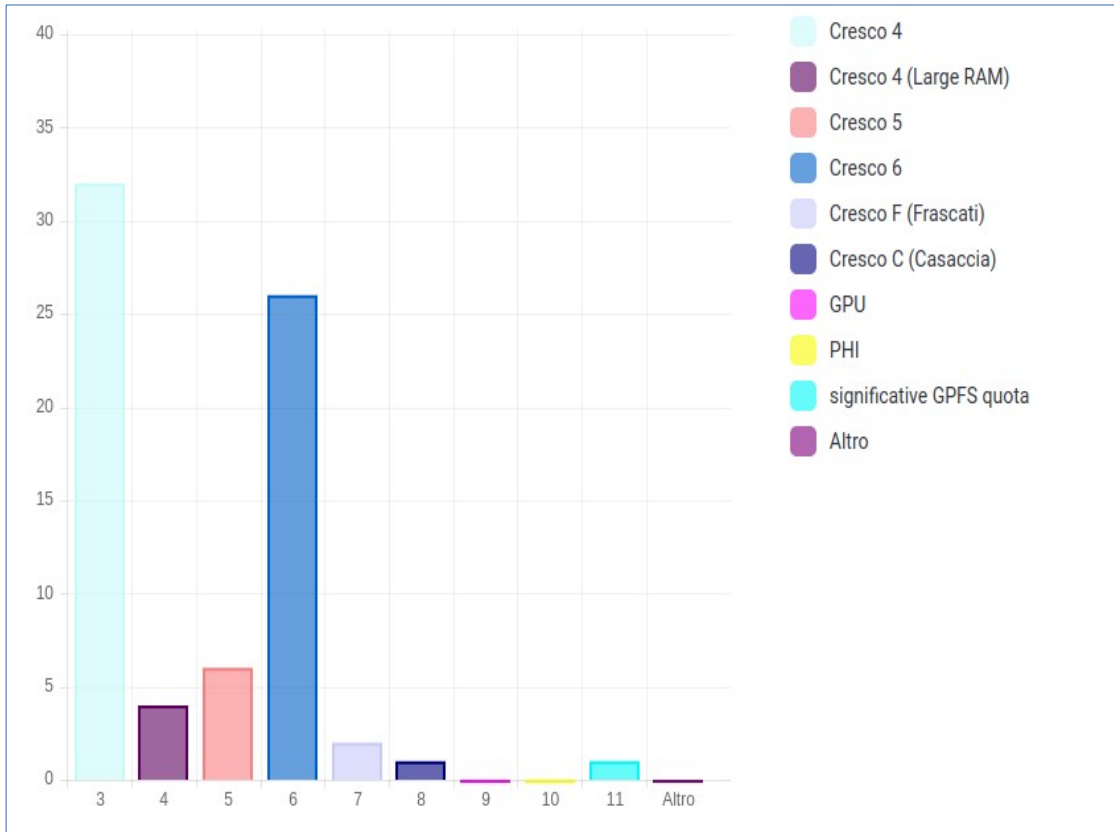
Contribution to a previous CRESCO Report



	Conteggio	Percentuale
Cresco Report 2008-2009 (1)	6	14.63%
Cresco Report 2009-2010 (2)	6	14.63%
Cresco Report 2010-2011 (3)	10	24.39%
Cresco Report 2012 (4)	15	36.59%
Cresco Report 2013 (5)	21	51.22%
Cresco Report 2014 (6)	20	48.78%
Cresco Report 2015 (7)	28	68.29%
Cresco Report 2016 (8)	32	78.05%
Cresco Report 2017 (9)	34	82.93%

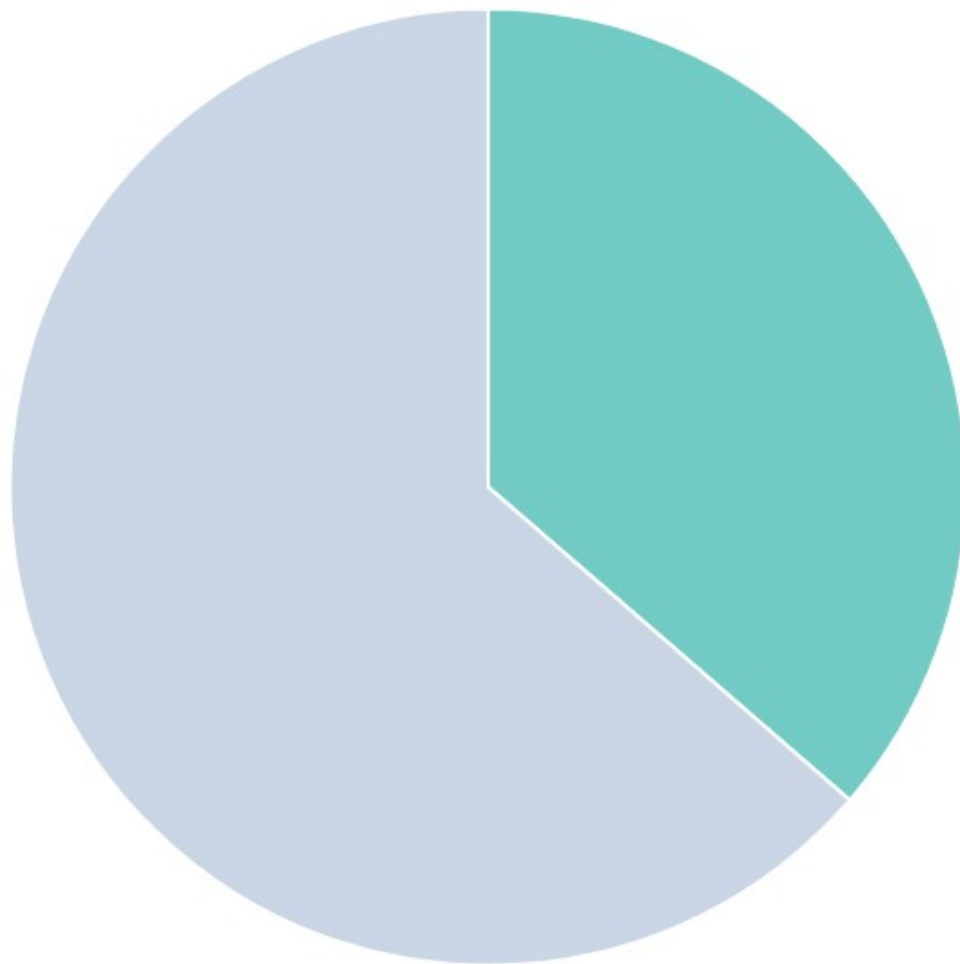
No contribution to previous reports: 6 (13%)

Clusters



Hardware			
	Conteggio	Percentuale	
Cresco 4 (3)	32	72.73%	
Cresco 4 (Large RAM) (4)	4	9.09%	
Cresco 5 (5)	6	13.64%	
Cresco 6 (6)	26	59.09%	
Cresco F (Frascati) (7)	2	4.55%	
Cresco C (Casaccia) (8)	1	2.27%	
GPU (9)	0	0.00%	
PHI (10)	0	0.00%	
significative GPFS quota (11)	1	2.27%	

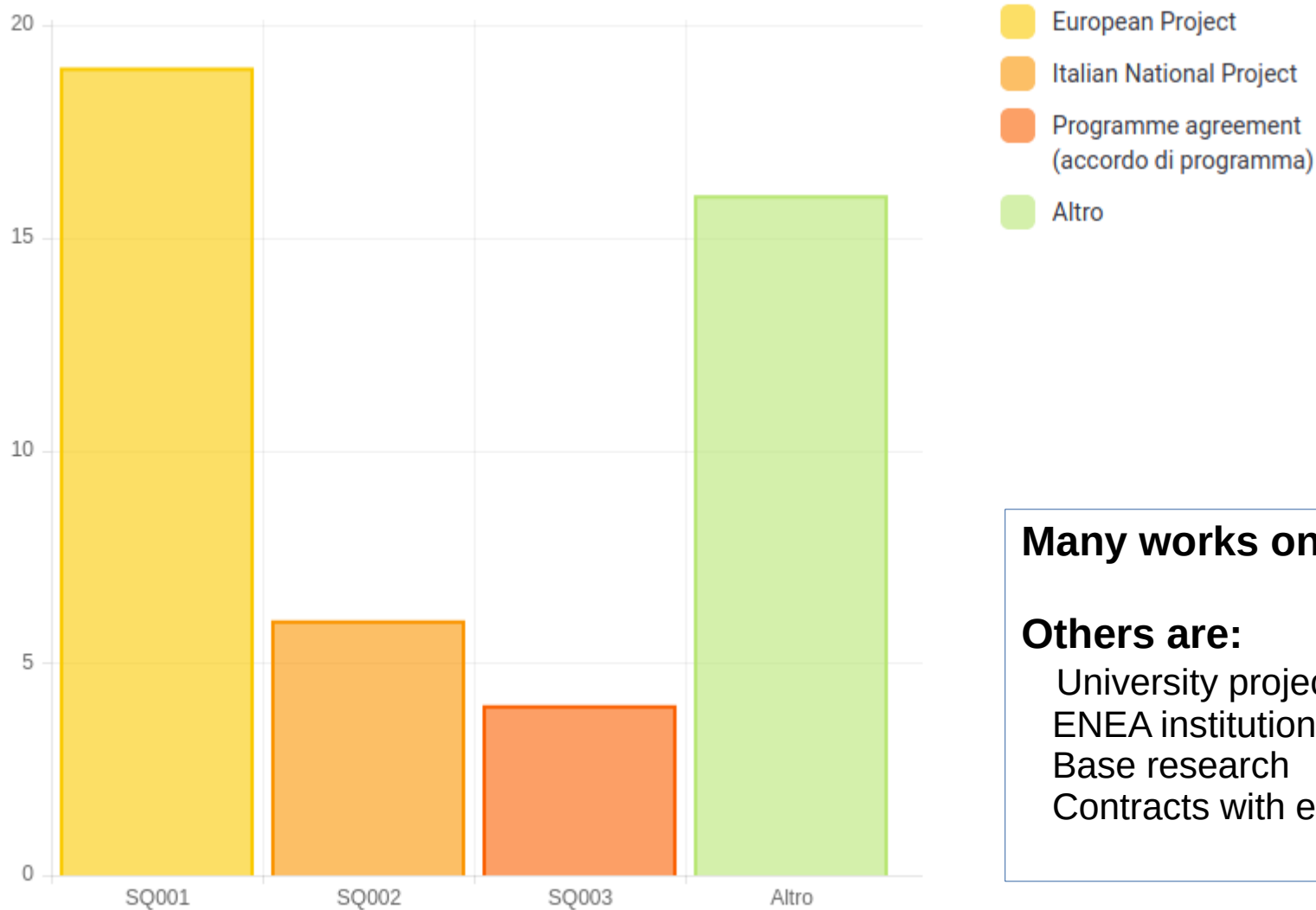
Template Type



- LaTeX
- MS Word document

	Conteggio	Percentuale
LaTeX (1)	16	36.36%
MS Word document (2)	28	63.64%
Nessuna risposta	0	0.00%

Context of the Activity

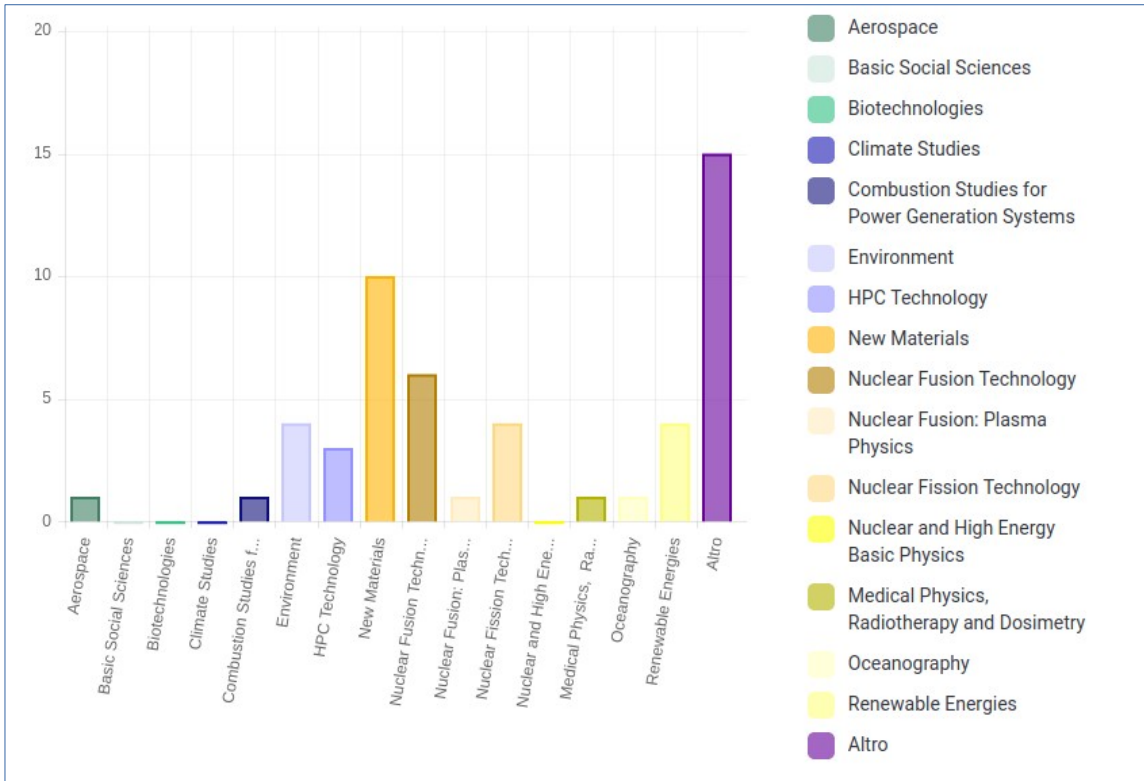


Many works on EU projects

Others are:

- University projects
- ENEA institutional activities
- Base research
- Contracts with external entities

Research Domains

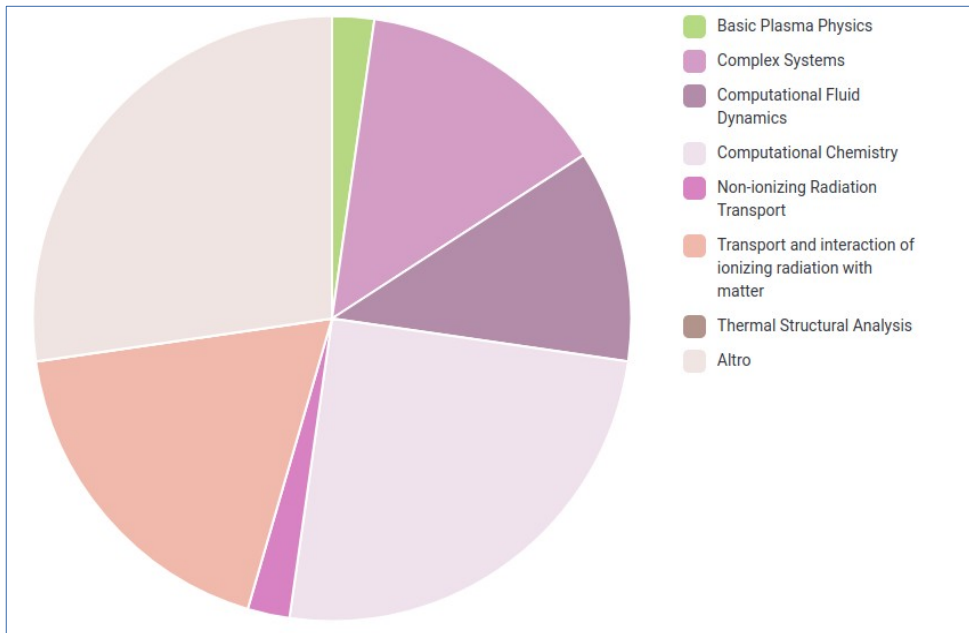


Aerospace (SQ001)	1	2.27%
Basic Social Sciences (SQ004)	0	0.00%
Biotechnologies (SQ003)	0	0.00%
Climate Studies (SQ002)	0	0.00%
Combustion Studies for Power Generation Systems (SQ005)	1	2.27%
Environment (SQ006)	4	9.09%
HPC Technology (SQ007)	3	6.82%
New Materials (SQ008)	10	22.73%
Nuclear Fusion Technology (SQ009)	6	13.64%
Nuclear Fusion: Plasma Physics (SQ010)	1	2.27%
Nuclear Fission Technology (SQ011)	4	9.09%
Nuclear and High Energy Basic Physics (SQ012)	0	0.00%
Medical Physics, Radiotherapy and Dosimetry (SQ013)	1	2.27%
Oceanography (SQ014)	1	2.27%
Renewable Energies (SQ015)	4	9.09%
Altro <input type="button" value="Sfogliare"/>	15	34.09%

Other includes:

Finite differences for 3D hyperbolic systems
 Operations Research
 Hybrid MHD-gyrokinetic simulations
 Density Functional Theory
 Atmospheric modelling
 Graph theory
 BIG DATA - Text Mining

Modeling & Simulation Background



Computational Chemistry is the main actor (11 papers)

Complex Systems and Transports has also many contributions

Other fields are: neutronics, climate

Basic Plasma Physics (1)	1	2.27%
Complex Systems (2)	6	13.64%
Computational Fluid Dynamics (3)	5	11.36%
Computational Chemistry (4)	11	25.00%
Non-ionizing Radiation Transport (5)	1	2.27%
Transport and interaction of ionizing radiation with matter (6)	8	18.18%
Thermal Structural Analysis (7)	0	0.00%
Altro Sfogliare	12	27.27%

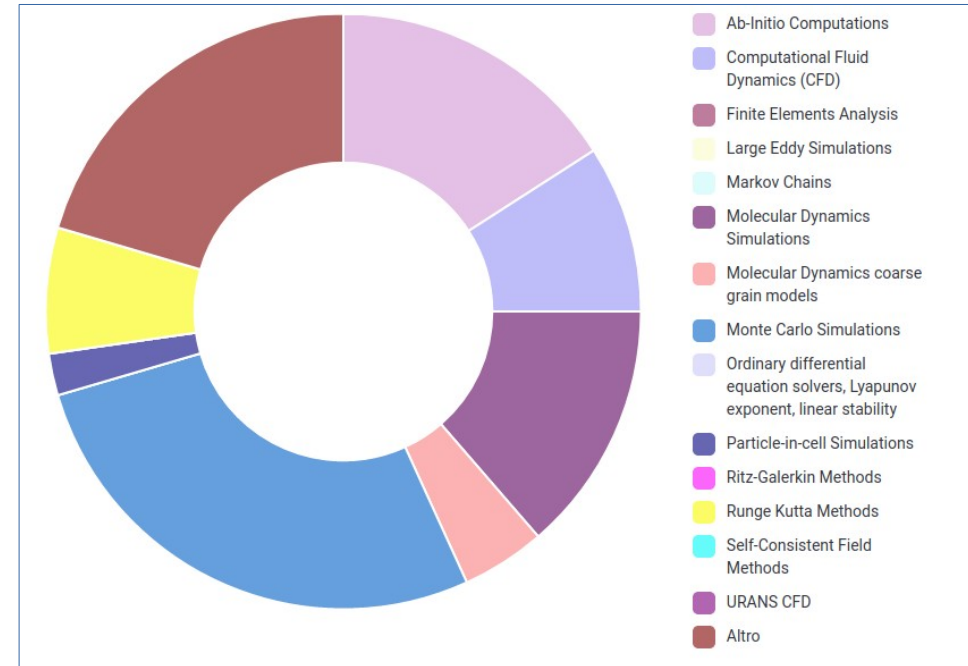
Other:

HPC infrastructure analysis
 Neutronics
 transport in mesoscopic systems
 Ecological transport
 Statistical process monitoring
 Computational Physics
 Geophysics
 Condensed Matter Physics
 Atmospheric dynamics
 Network analysis
 BIG DATA - Text Mining

Computational Methodology

Computational Methodology:

	Conteggio	Percentuale
Ab-Initio Computations (1)	7	15.91%
Computational Fluid Dynamics (CFD) (2)	4	9.09%
Finite Elements Analysis (3)	0	0.00%
Large Eddy Simulations (4)	0	0.00%
Markov Chains (5)	0	0.00%
Molecular Dynamics Simulations (6)	6	13.64%
Molecular Dynamics coarse grain models (7)	2	4.55%
Monte Carlo Simulations (8)	12	27.27%
Ordinary differential equation solvers, Lyapunov exponent, linear stability (9)	0	0.00%
Particle-in-cell Simulations (10)	1	2.27%
Ritz-Galerkin Methods (11)	0	0.00%
Runge Kutta Methods (12)	3	6.82%
Self-Consistent Field Methods (13)	0	0.00%
URANS CFD (14)	0	0.00%
Altro <input type="button" value="Sfogliare"/>	9	20.45%

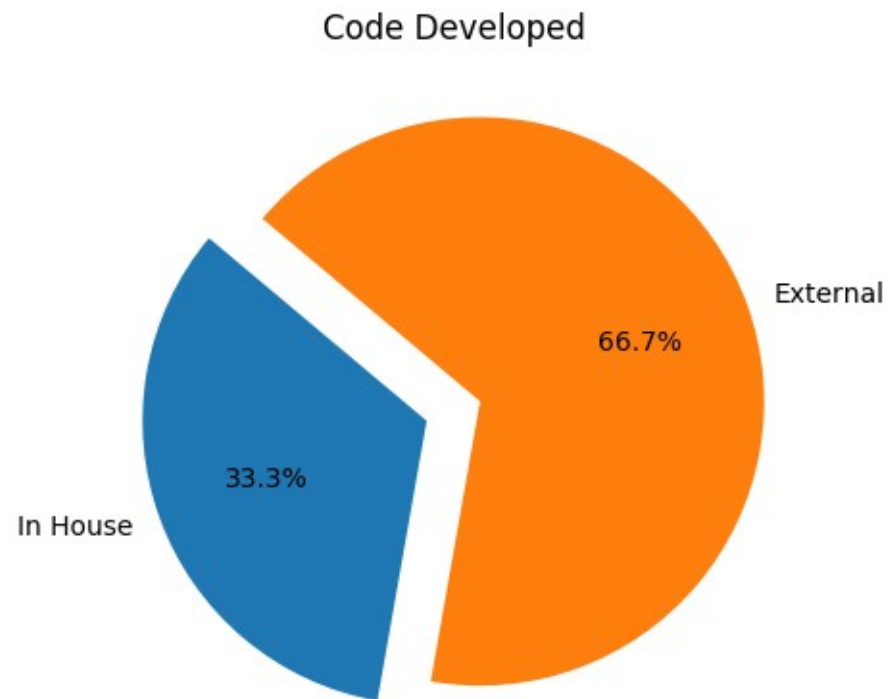


About half of the Montecarlo papers use MCNP,
Also Ab-Initio and Molecular Dynamics are important.

There is also different methodologies, difficult to classify.

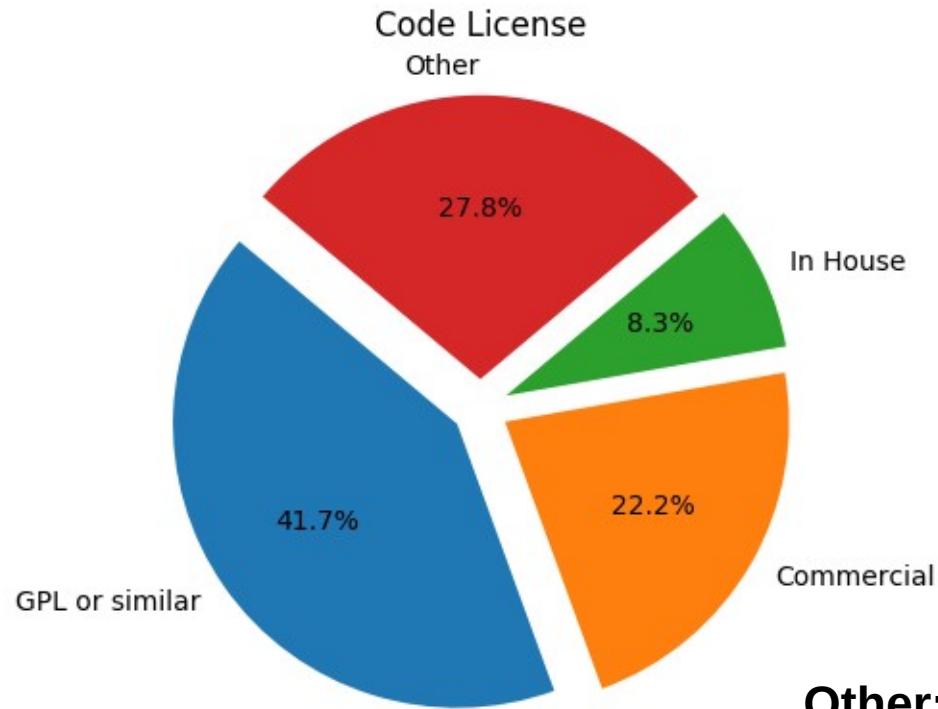
Code Development

1/3 of contributors works on software code



License type

Most of code has a free-type license, ~20% commercial software

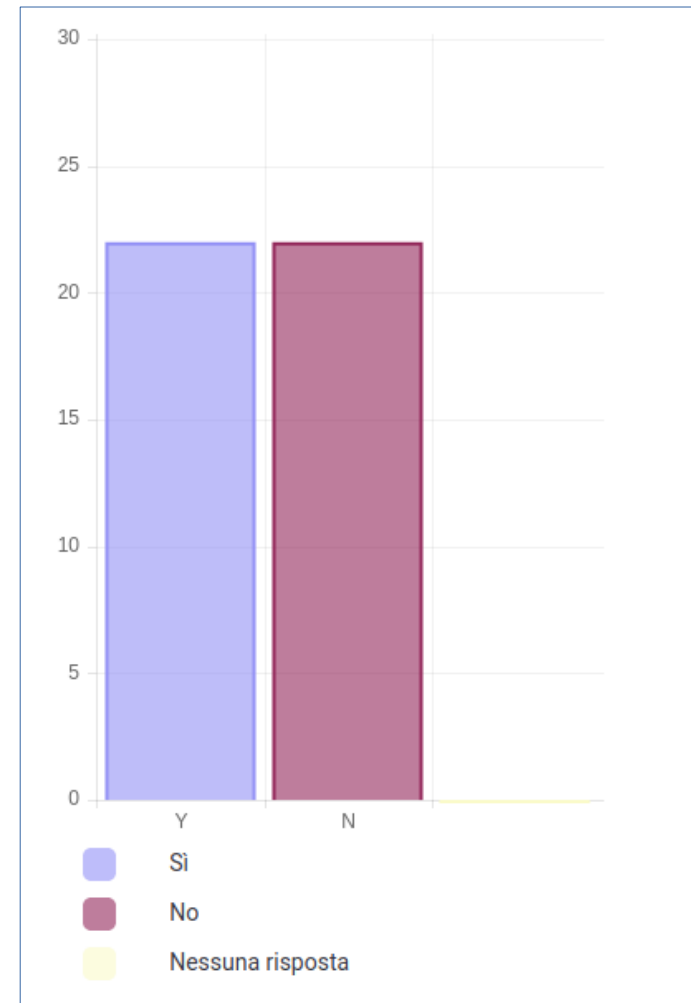


Other:

- Provided by CRESCO
- Not defined (in house code)
- Agreement with code owners

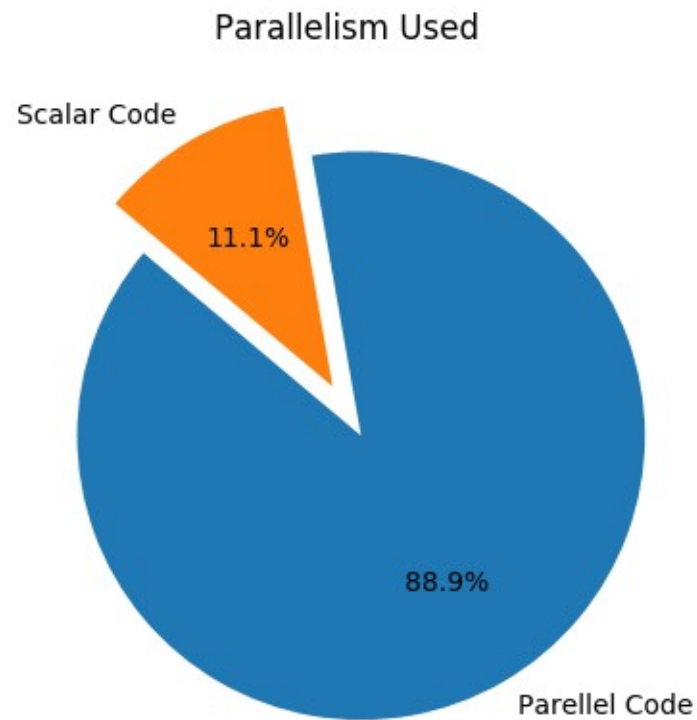
Scalability tests?

Scalability: Have you done scalability tests of the code?			
Risposta	Conteggio	Percentuale	
Si (Y)	22	50.00%	
No (N)	22	50.00%	
Nessuna risposta	0	0.00%	



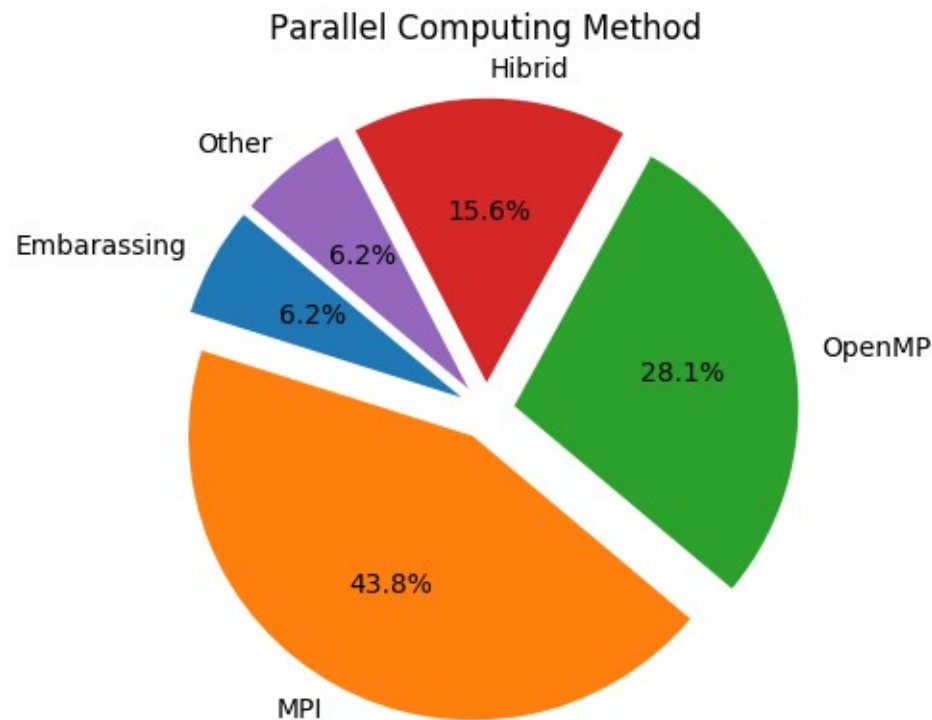
Parallelism implemented?

~ 10% of scalar code



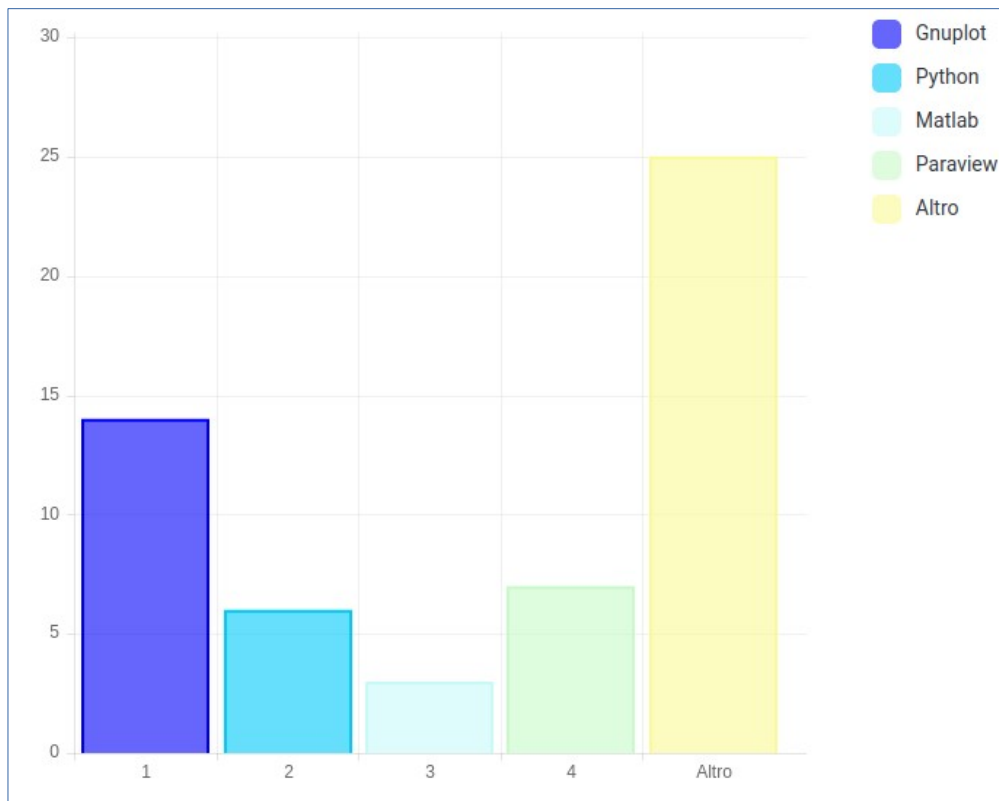
Type of parallelism implemented

Most users use MPI, but large fraction of hybrid code



Other:
MPI and MPI/OpenMPI
Job Array

Data Visualization software



About **20 different tools** are cited:

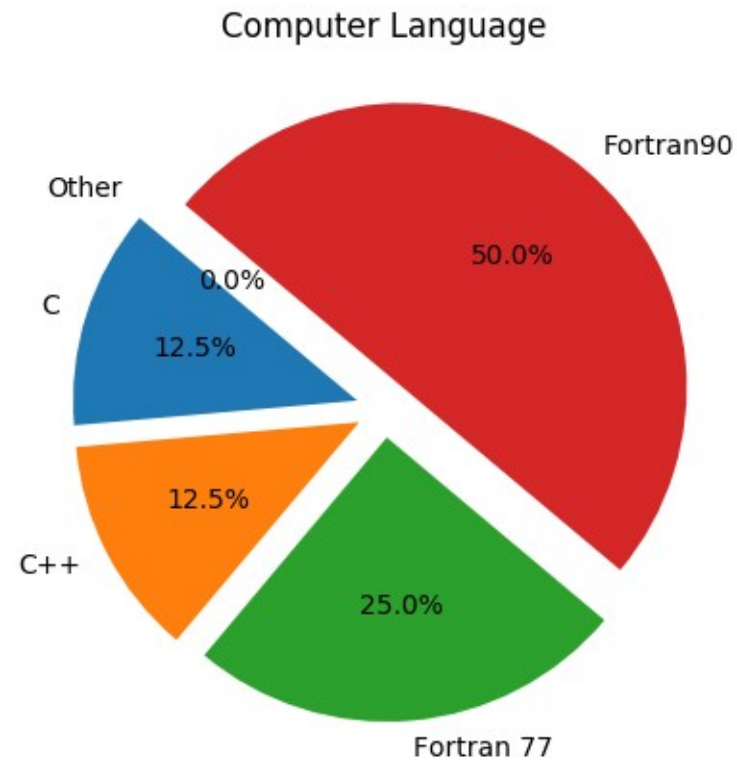
- most are free tools: **R, vmd, Grace**
- few are commercial: **idl, ansys, excel**
- some are “in house”

Answers in Other:

own local program
crystal09
N/A
VMD
IDL
Excel
vmd
Grace
excel
MCNP
MCNPX
POV-Ray
none
Tecplot360
Grace, VMD
NCL
NCL
CERN plotting libraries
vmd, xcrysden
Ansys
excel
XCrysden, xmgrace
VESTA
R
VMD, Ovito

Computer Languages

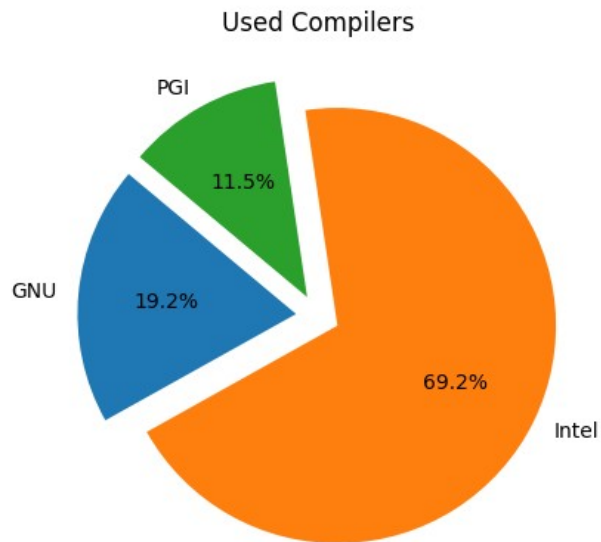
The most used language is Fortran: 75%;
followed by C and C++: 25%
1/3 of Fortran is the ancient 77 version



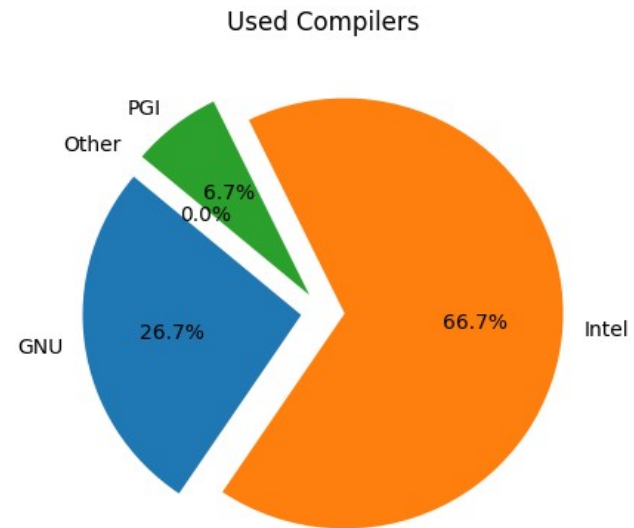
Note:
none used python, java, matlab

Compilers

Report 2017



Report 2018



The Intel compiler is the most used ~70%

Some Used Software

~40 different software cited (~20% are MonteCarlo programs)

MCNP: 8 answers - different versions are used

Other MC codes:

EGS4 (the new EGSnrc version)

Molecular Dynamics:

GROMACS : 2 answers

LAMMPS : 2 answers

Environment:

WRF (Weather Research and Forecasting)

Other:

R, TALTAC, Quantum Espresso, Ansys Fluent,...

Most used libraries

Linear systems:

LAPACK : 4 answers

BLAS : 4 answers

Fast Fourier Transform:

FFTW : 4 answers

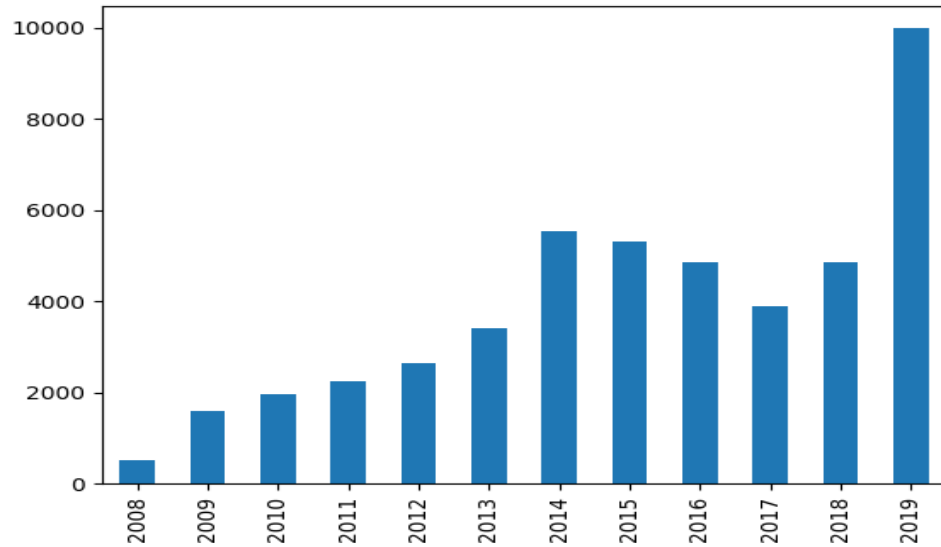
Network Common Data Form (NETCDF): 3 answers

JEFF (NEA Nuclear Data Library): 3 answers

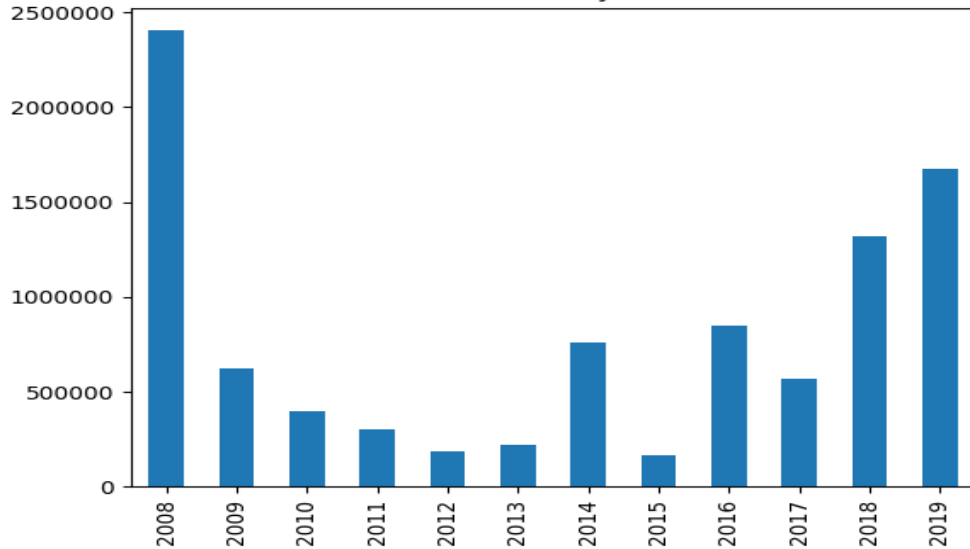
Trends 2008-2019

Cresco Usage 2008-2019

Cresco Wall Clock Time (Years)



Cresco Number of Jobs (Years)

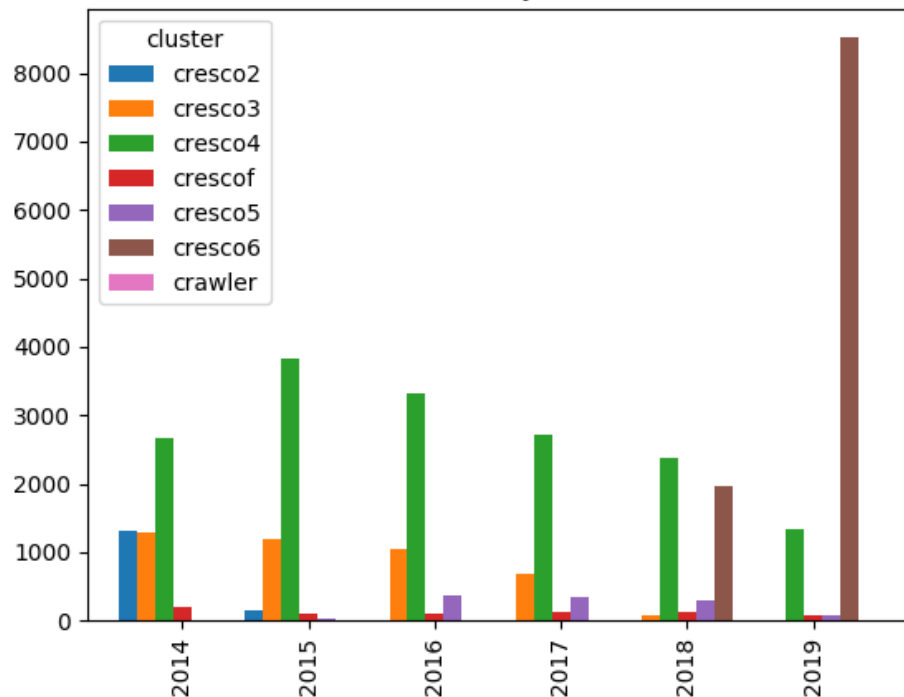


Some major events

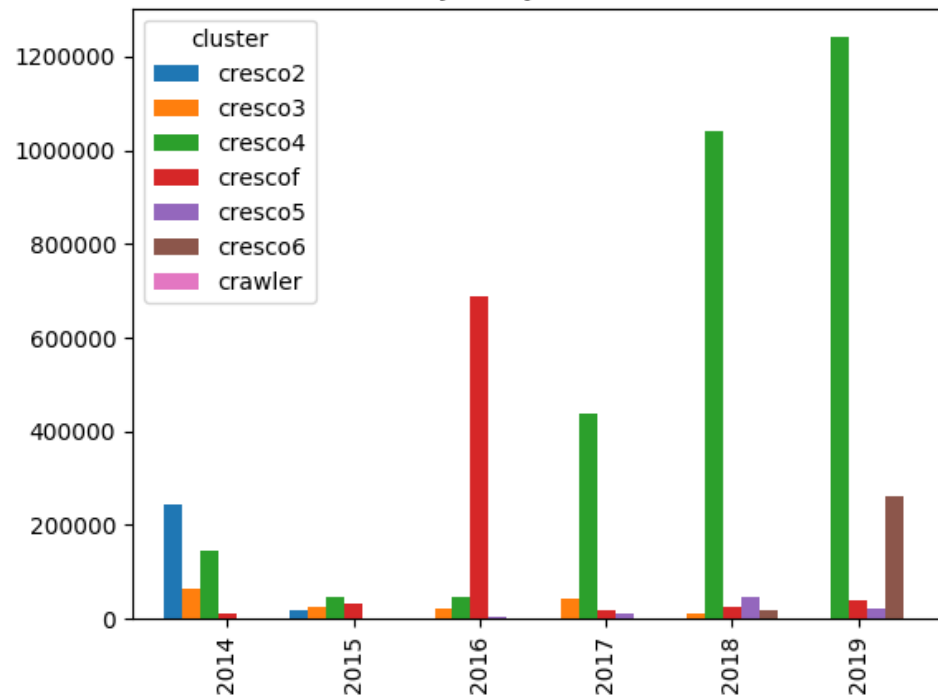
YEAR	CLUSTER	POWER
2008	CRESCO1 CRESCO2	25 TFlops
2013	CRESCO3	20 TFlops
2014	CRESCO4	100 TFlops
2015	CRESCO5	24 TFlops
2018	CRESCO6	0.7 PFlops
2019	CRESCO6+	1.4 PFlops

Usage by clusters in recent years

Total time by cluster



Jobs by cluster



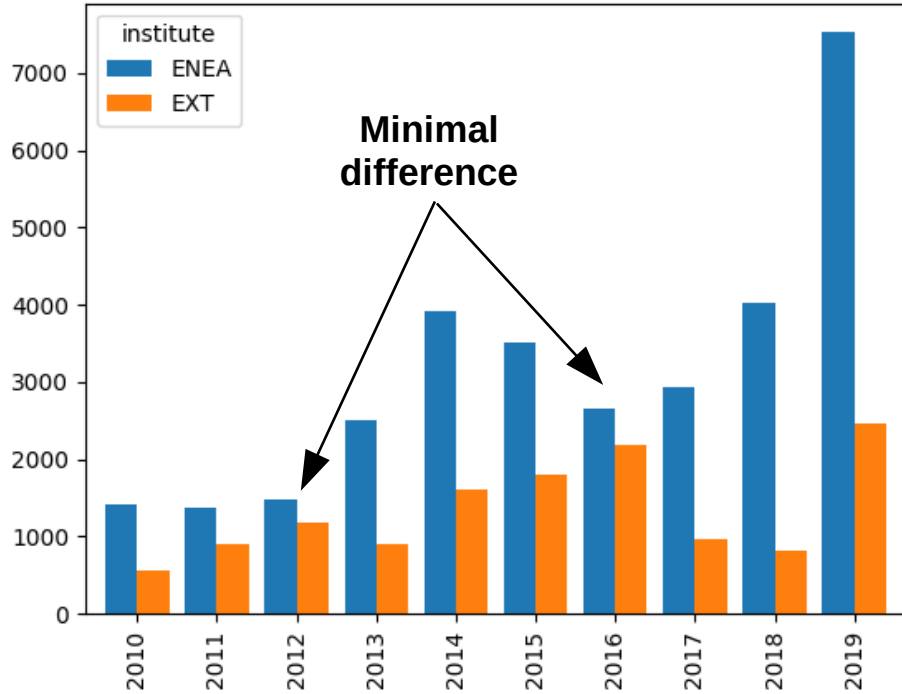
Up to 2018 CRESCO4 was the major actor:

- increase of number of jobs
- decrease of wall time

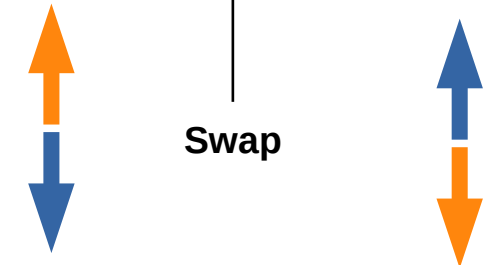
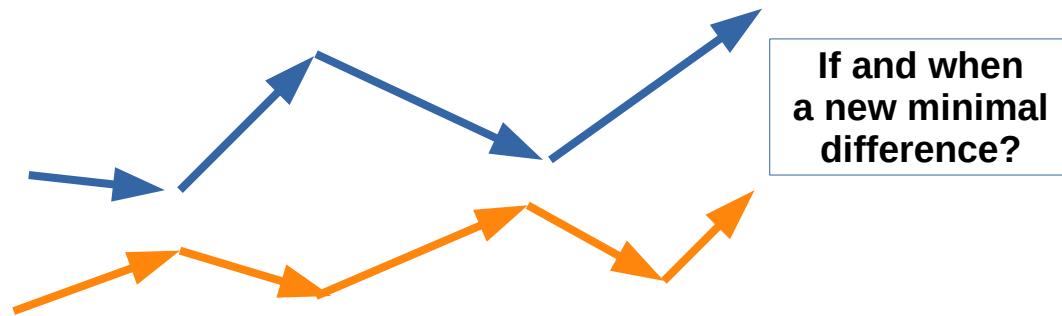
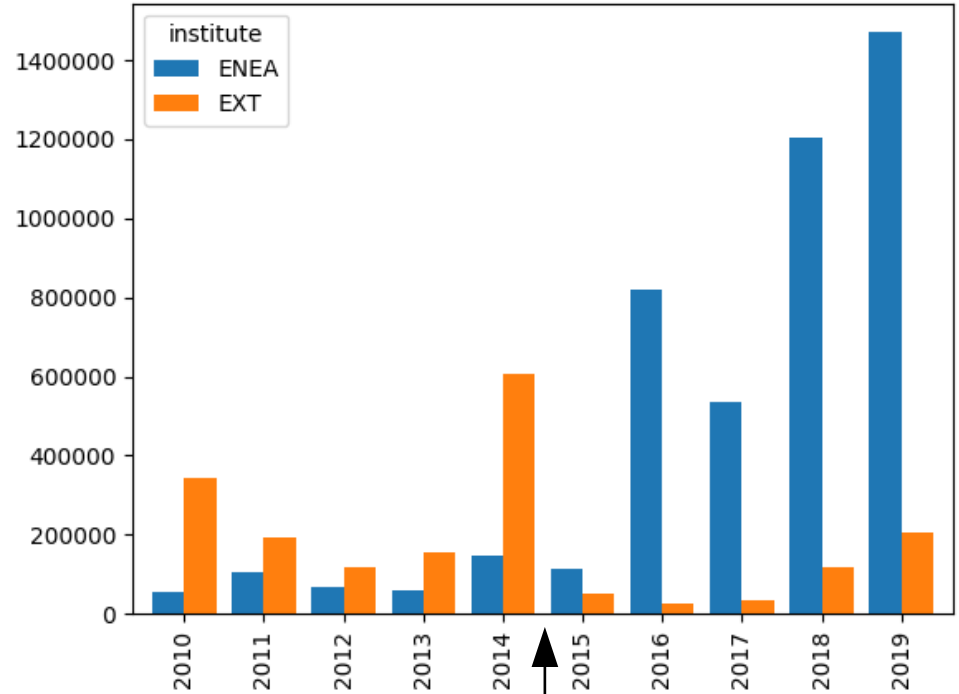
From 2018-2019: some big runs on CRESCO6

ENEA and External Users

wct_y ENEA and external users



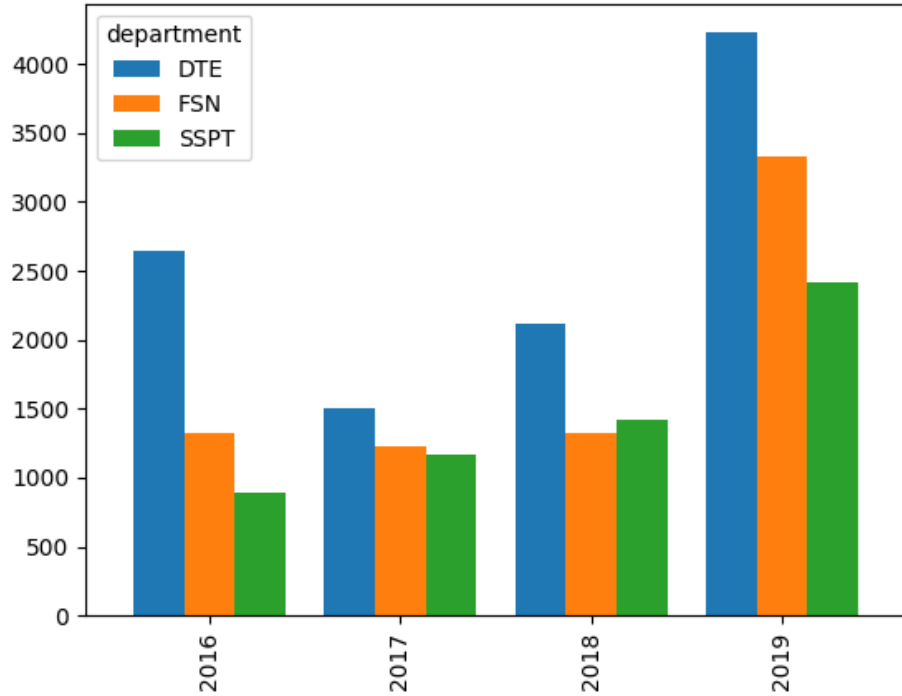
njobs ENEA and external users



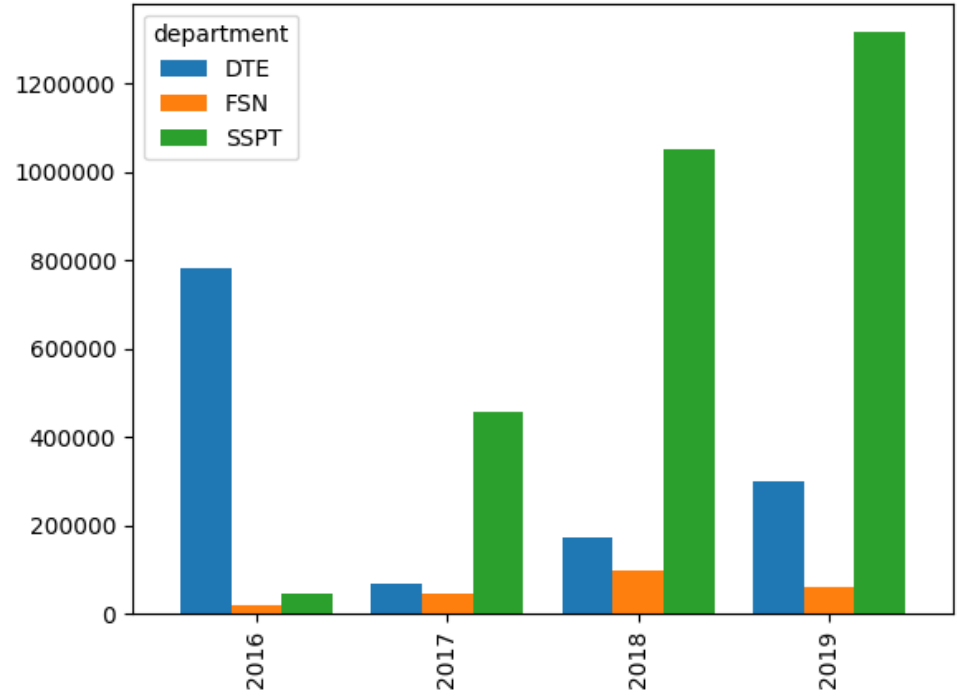
Oscillating usage by users

ENEA Department Usage

wct_y ENEA departments

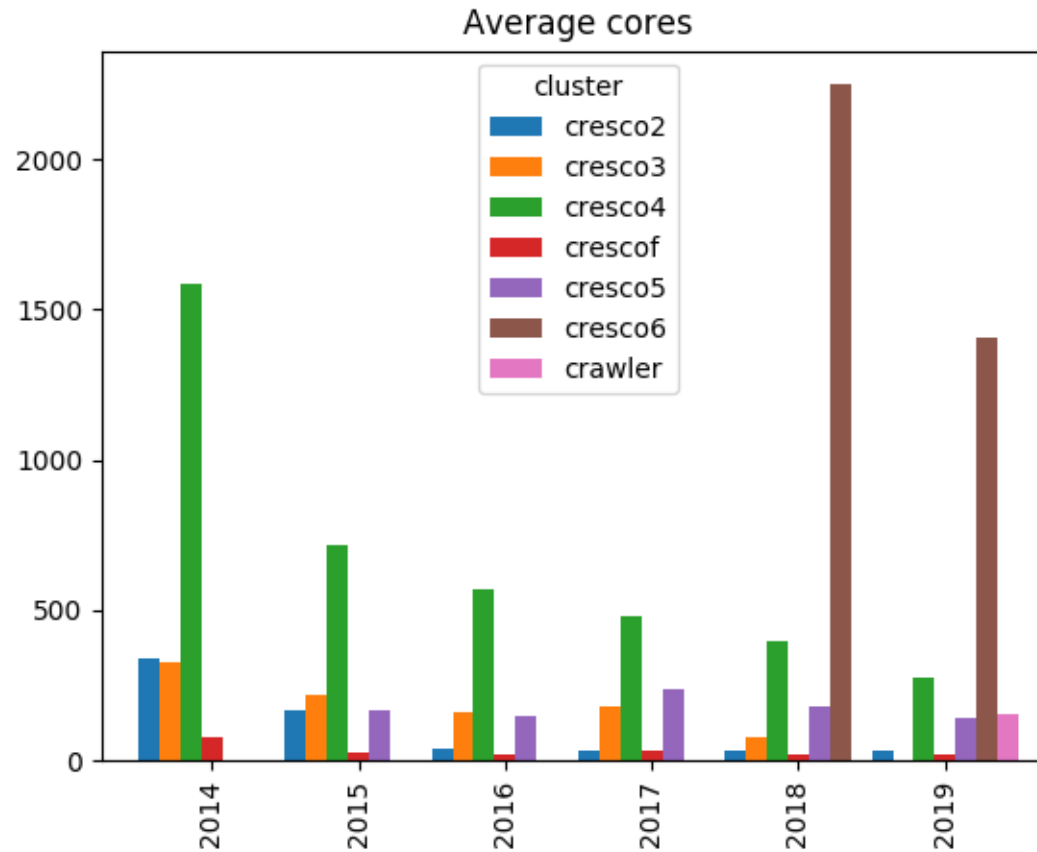


njobs ENEA departments



Increasing number of jobs by SSPT in 2016-2019

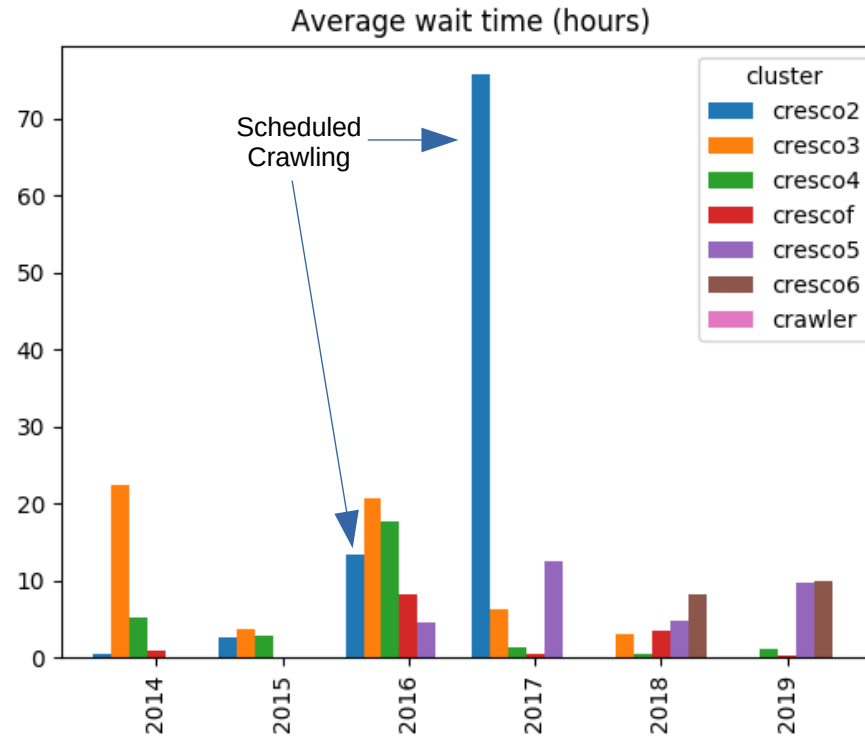
Parallelism



CRESCO4: less usage of parallelism in recent years?

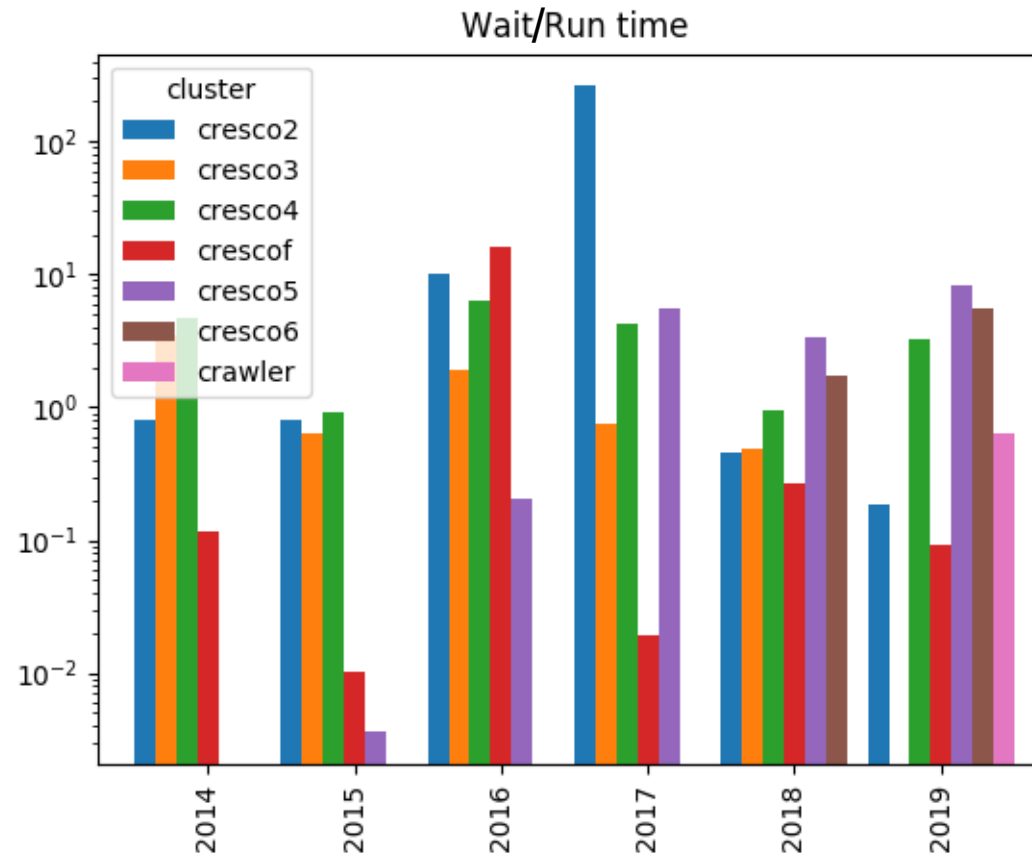
In 2018 first CRESCO6 tests used many cores

Wait time



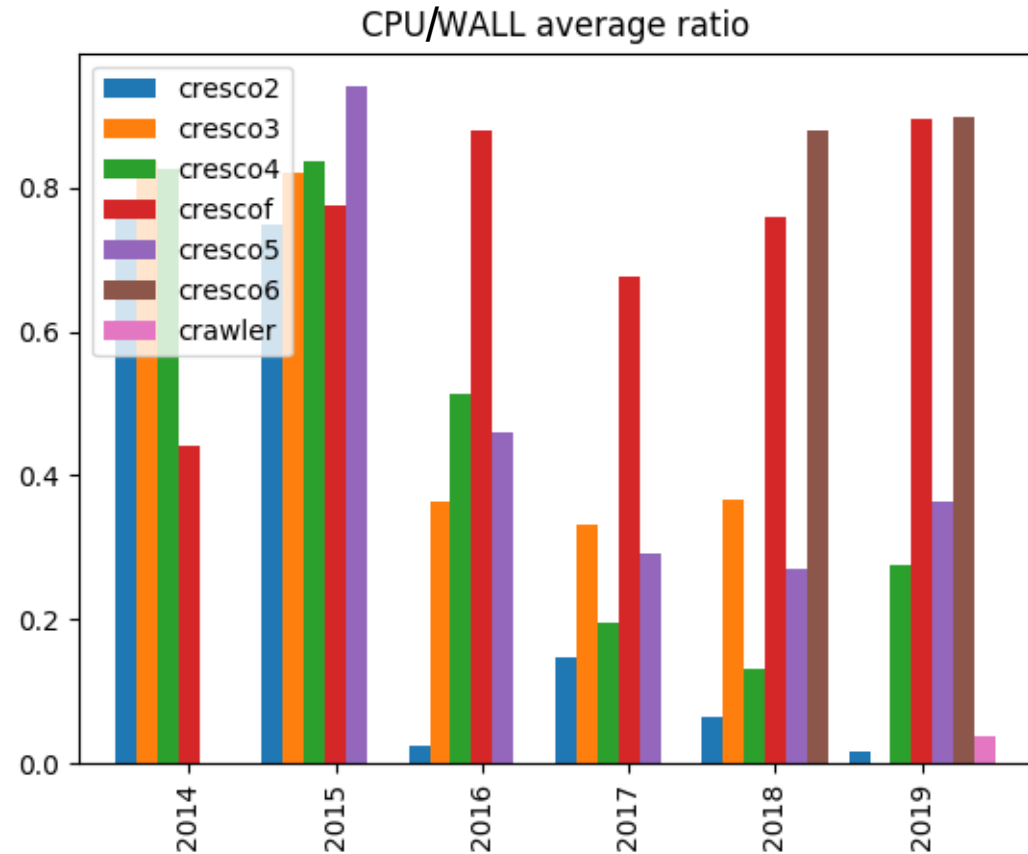
CRESCO[3-4]: decreasing in last years. Events in 2016?

Wait/Run time



More clusters then faster queues

CPU/Wall time



Constant decrease for CRESCO4

Ratio at ~90% for CRESCO6

Acknowledgments

Special tanks to:

Marcello Galli:

for assistance in the report preparation and many advices

Catia Masella:

for assistance in the use of the “Survey” system

Gianclaudio Ferro:

for assistance in the use of the “Reporter” system

Amedeo Trolese:

for the report cover design

Giuliano Ghisu, Paola Giaquinto:

for the printed version and the internet distribution of the report

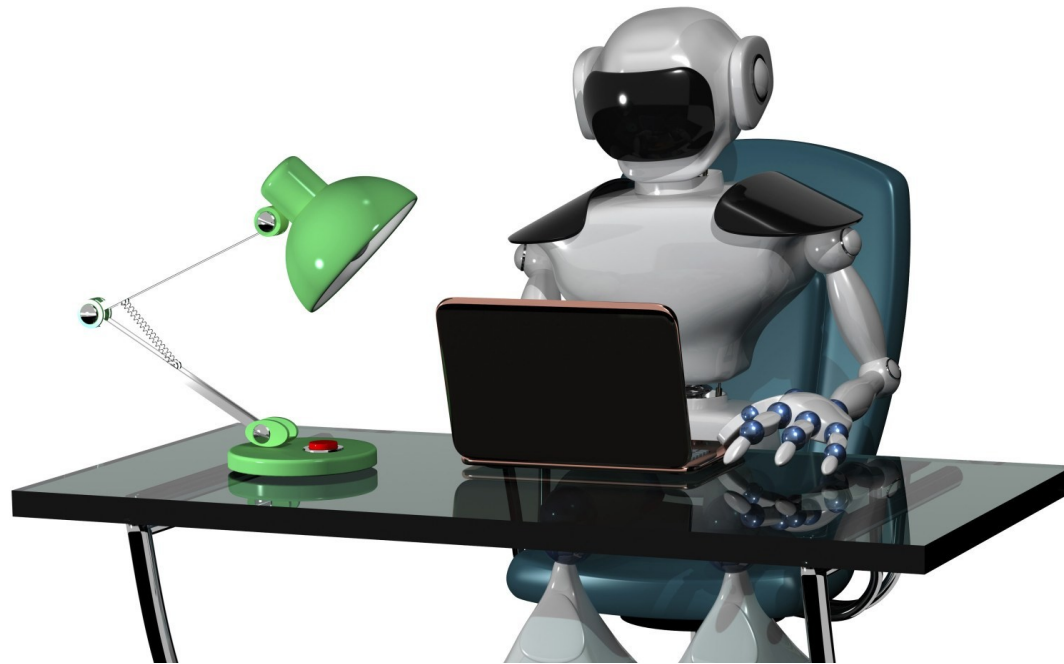
The whole CRESCO team:

always working hard to mantain the clusters alive

The CRESCO users:

for their contributions to the 2018 annual report

Any questions?



Personal comments

On Report Preparation:

- Time to begin: on March? (For 2018 Report start was on June)
- Only one template: LaTeX? (For 2018 Report only 36% of users used LaTeX)

On CRESCO usage:

- How about Big Data?