

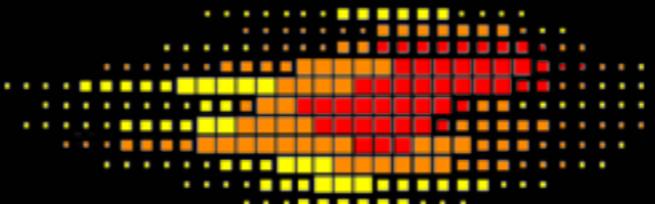


SINAPAD

ANTÔNIO TADEU GOMES

LNCC

ASSESSING THE BEHAVIOR OF HPC USERS AND SYSTEMS: THE CASE OF THE SANTOS DUMONT SUPERCOMPUTER



WSCAD 2018

9 CENTERS



LNCC

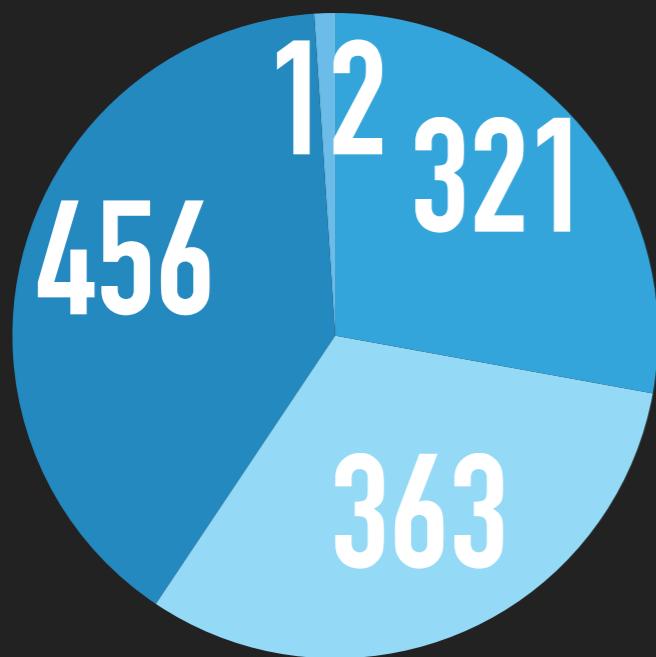


LNCC

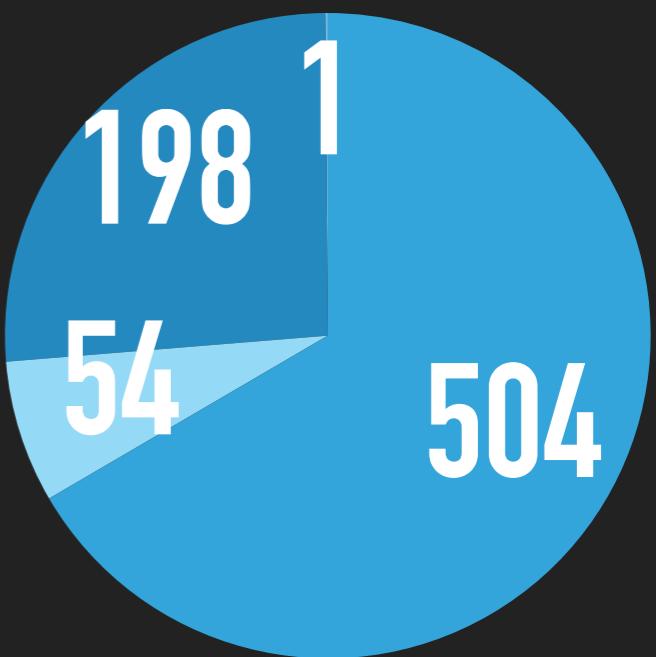


CONFIGURATION

- ▶ ~1.1 PFlops computing capability
- ▶ 756 nodes with various configurations: CPUs, GPGPUs, MICs, SHMEM
- ▶ ~1.7 PBytes Lustre storage; Infiniband interconnection
- ▶ Linux OS; Slurm resource manager



- B710 CPU
- B715 CPU+MIC
- B715 CPU+GPGPU
- Mesca2



3 OPEN CALLS

**(PROJECTS FROM 1ST CALL ENDING THIS YEAR;
FROM 3RD CALL BEGINNING THIS YEAR)**

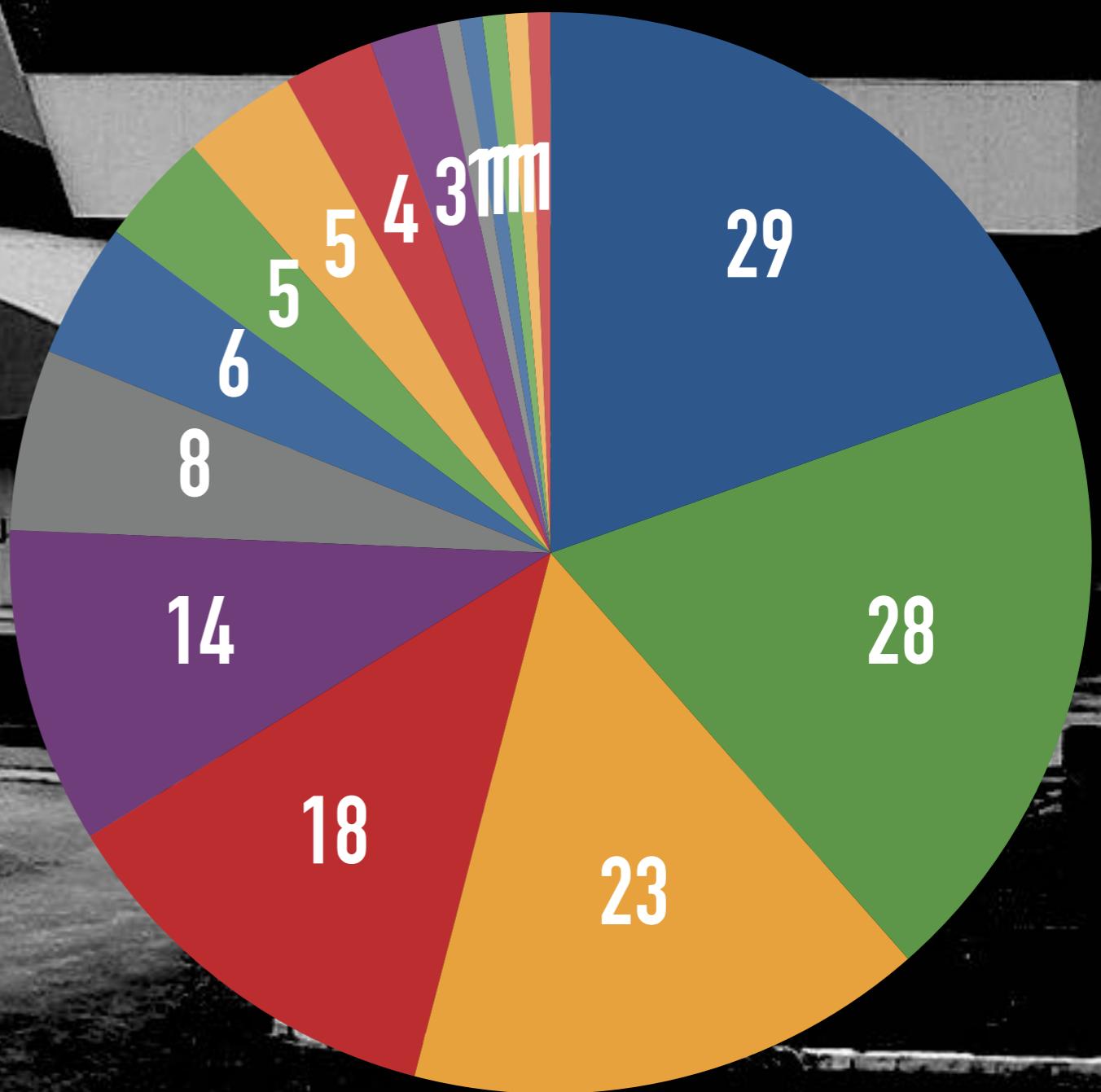
100+ PROJECTS IMPLEMENTED (PEER-REVIEWED)

~550 USERS

140.000+ JOBS AND 260.000.000+ SERVICE UNITS SINCE AUG/2016

260+ TERABYTES STORED

15 AREAS

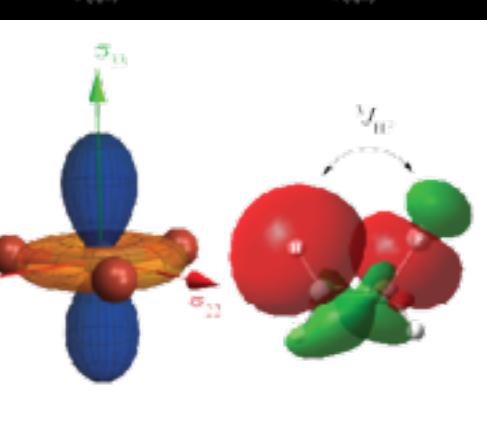
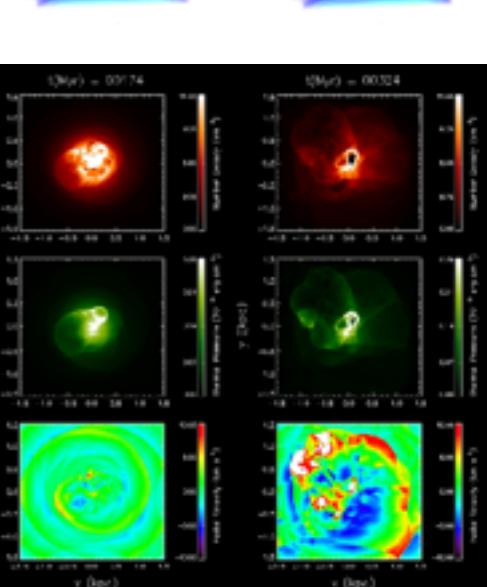
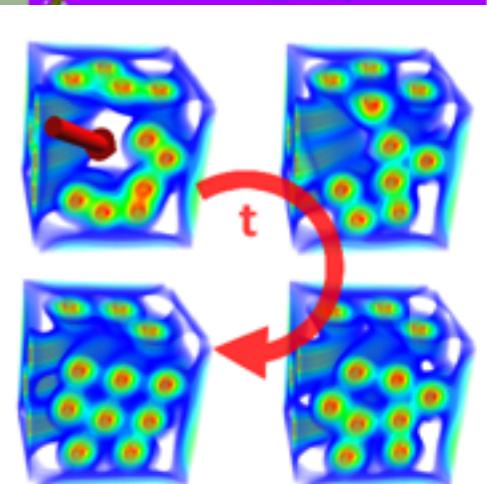
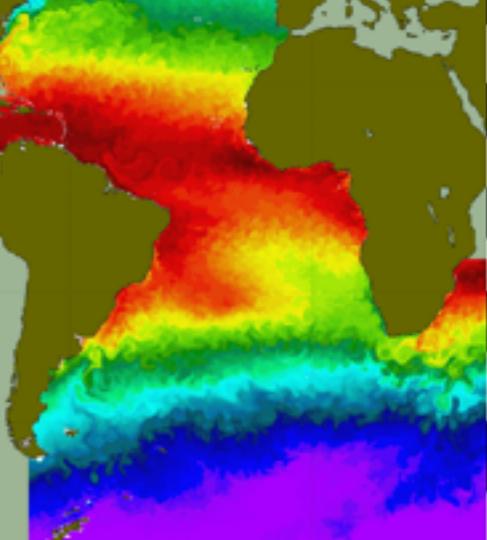
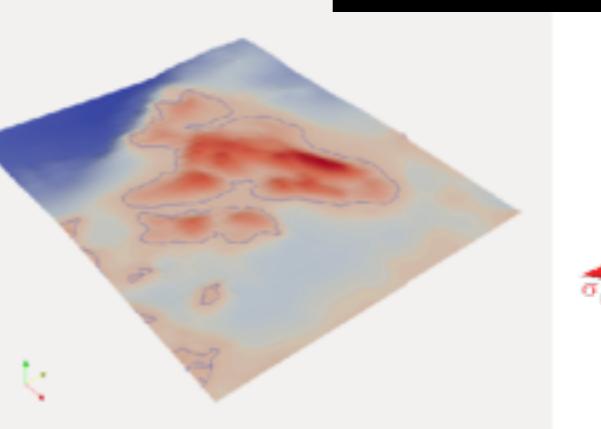
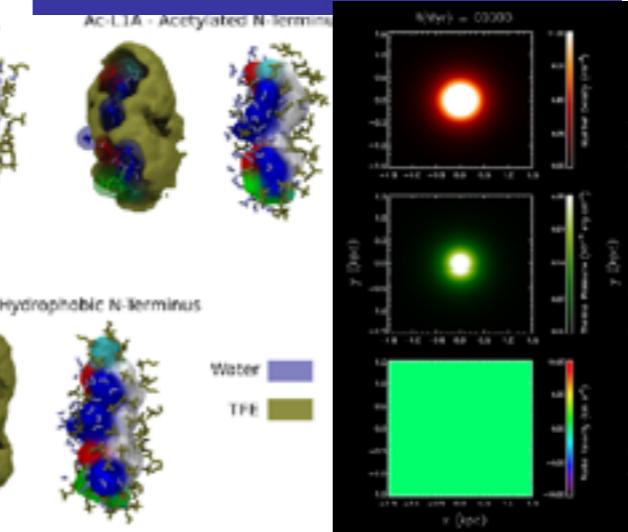
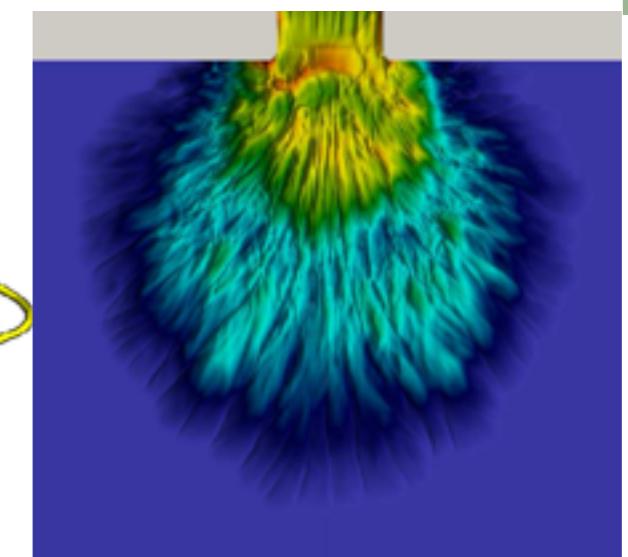
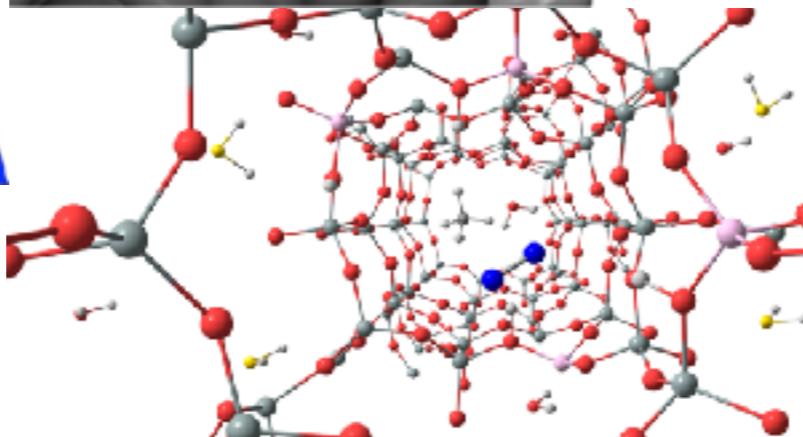
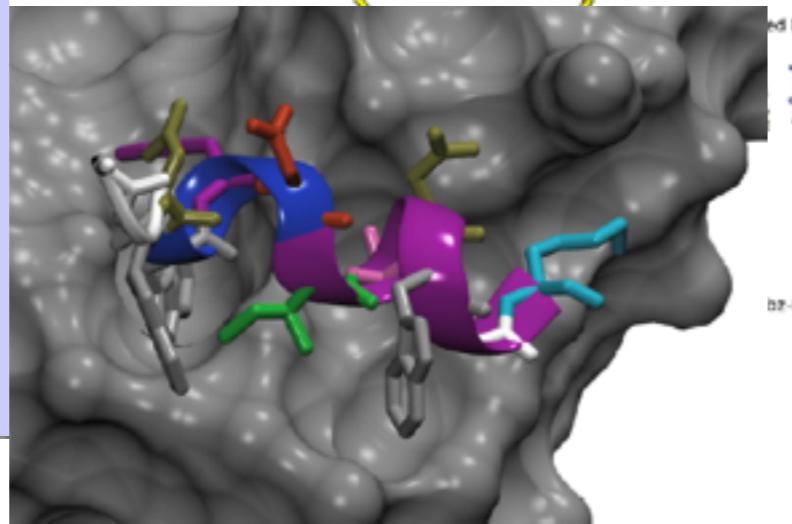
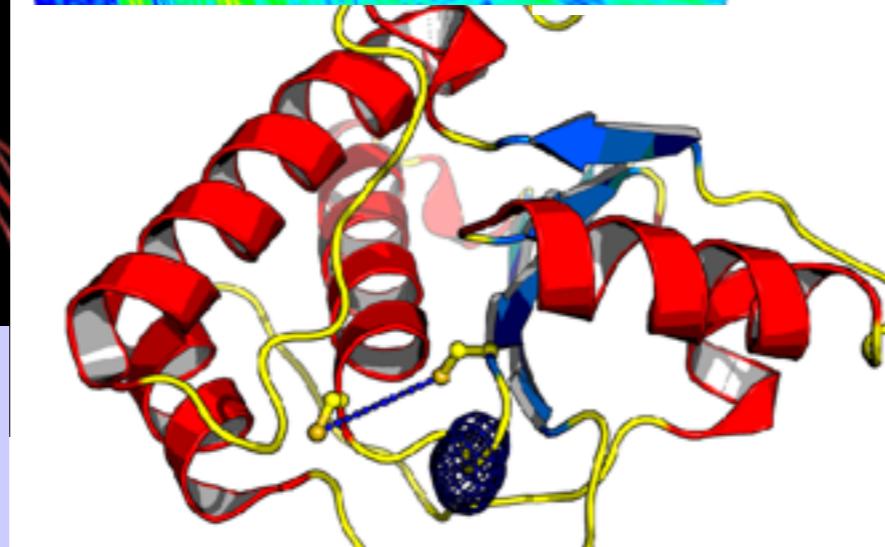
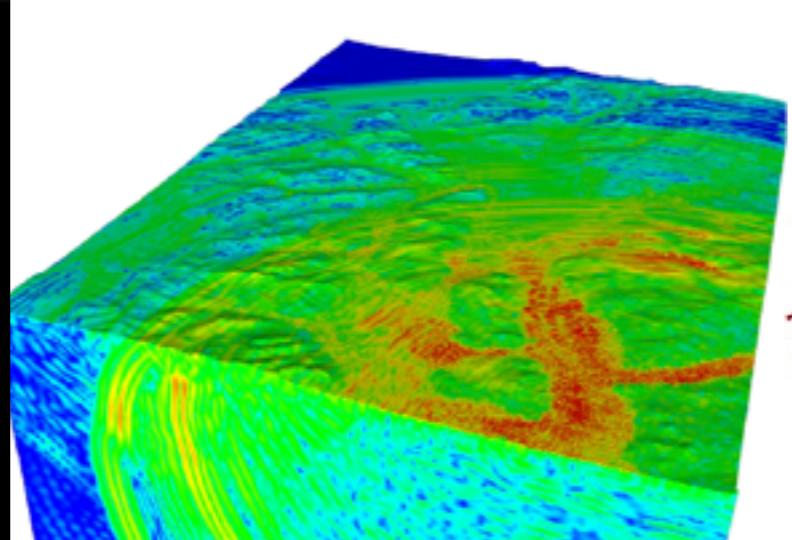
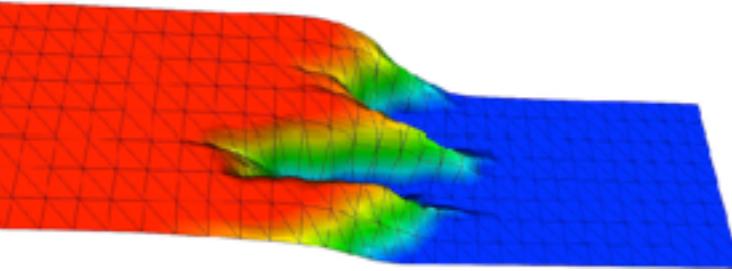
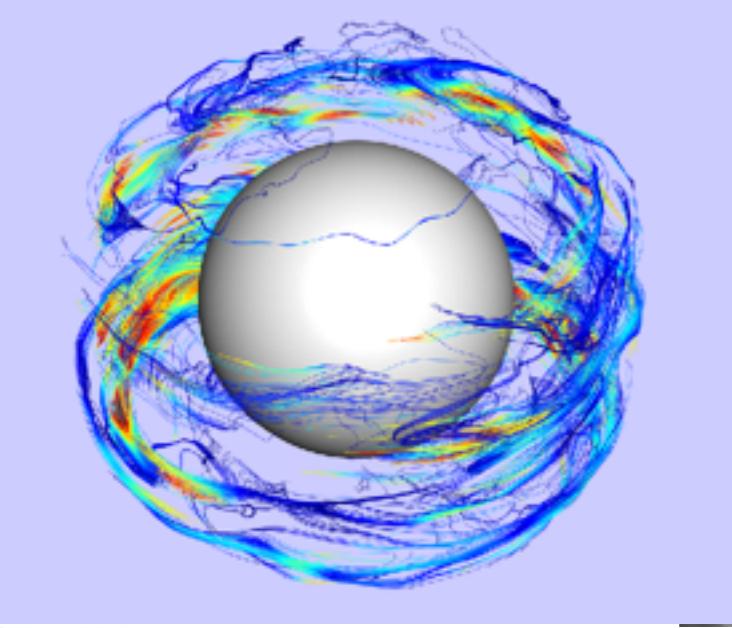


● Chemistry
● Computer Science
● Material sciences
● Biodiversity

● Physics
● Geosciences
● Maths
● Linguistics

● Engineering
● Astronomy
● Climate & Weather
● Pharmacy

● Biology
● Health
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SHARE REPORT

Chromagnetic nanoparticles and gels

Jhyson Yeom^{1,2}, Wellington S. Santos¹, Mahsik Chekli^{1,2,4}, Minjeong Cha^{1,3}, André F. de Moura^{1,2}, Nicholas A. Kotov^{1,2,3,5*}

* See all authors and affiliations

Science, 19 Jan 2018;
 Vol. 358, Issue 6372, pp. 309-314
 DOI: 10.1126/science.aas7172

Article Figures & Data Info & Metrics eLetters PDF

You are currently viewing the abstract.

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Boosting chiral nanoparticle responses

Optical nanomaterials that combine chirality and magnetism are useful for magnetooptics and as chiral catalysts. Although chiral inorganic nanostructures can exhibit high circular dichroism, modulating this optical activity has usually required irreversible chemical changes. Yeom et al. synthesized paramagnetic cobalt oxide (Co_3O_4) nanoparticles with L- and D-cysteine surface ligands. These ligands created chiral distortions of the crystal lattices, and



ARTICLE

DOI: 10.1038/s41467-018-04859-5 OPEN

Rational Zika vaccine design via the modulation of antigen membrane anchors in chimpanzee adenoviral vectors

César López-Camacho¹, Peter Abbink², Rafael A. Larecca³, Wanessa Dejnirattisai³, Michael Boyd², Alex Badamchi-Zadeh², Zoë R. Wallace⁴, Jennifer Doig⁵, Ricardo Sanchez Velazquez⁶, Roberto Dias Lins Neto⁶, Danilo F. Coelho⁶, Young Chan Kim¹, Claire L. Donald⁶, Ania Owsianka⁵, Giuditta De Lorenzo⁵, Alain Kohl⁶, Sarah C. Gilbert⁷, Lucy Dorrell⁴, Juthathip Mongkolsapaya^{3,8}, Arvind H. Patel⁵, Gavin R. Screaton⁹, Dan H. Barouch⁷, Adrian V.S. Hill⁶ & Arturo Reyes-Sandoval¹

Zika virus (ZIKV) emerged on a global scale and no licensed vaccine ensures long-lasting anti-ZIKV immunity. Here we report the design and comparative evaluation of four replication-deficient chimpanzee adenoviral (ChAdOx1) ZIKV vaccine candidates comprising the addition or deletion of precursor membrane (prM) and envelope, with or without its transmembrane domain (TM). A single, non-adjacent vaccination of ChAdOx1 ZIKV

Ano	Produção bibliográfica								Produção técnica e de inovação					
	APP	AAP	LC	TAC	DMA	DMD	TDA	TDD	OPB	PP	PDT	PAT	PCSR	OPT
2017	58	8	1	67	7	6	7	10	23	9	1	1	9	40
2016	19	0	0	12	4	2	4	1	0	12	0	0	0	15
2015	0	0	0	0	0	0	5	0	0	5	0	0	0	0
2014	0	0	0	0	0	0	8	0	0	1	0	0	0	0
2013	0	0	0	0	0	0	0	0	0	1	0	0	0	0

Legenda:

Produção bibliográfica

- APP Artigos completos publicados em periódicos
- AAP Artigos aceitos para publicação
- LC Livros e capítulos
- TAC Trabalhos publicados em anais de congressos
- DMA Dissertações de mestrado em andamento
- DMD Dissertações de mestrado defendidas
- TDA Teses de doutorado em andamento
- TDD Teses de doutorado defendidas
- OPB Outras produções bibliográficas

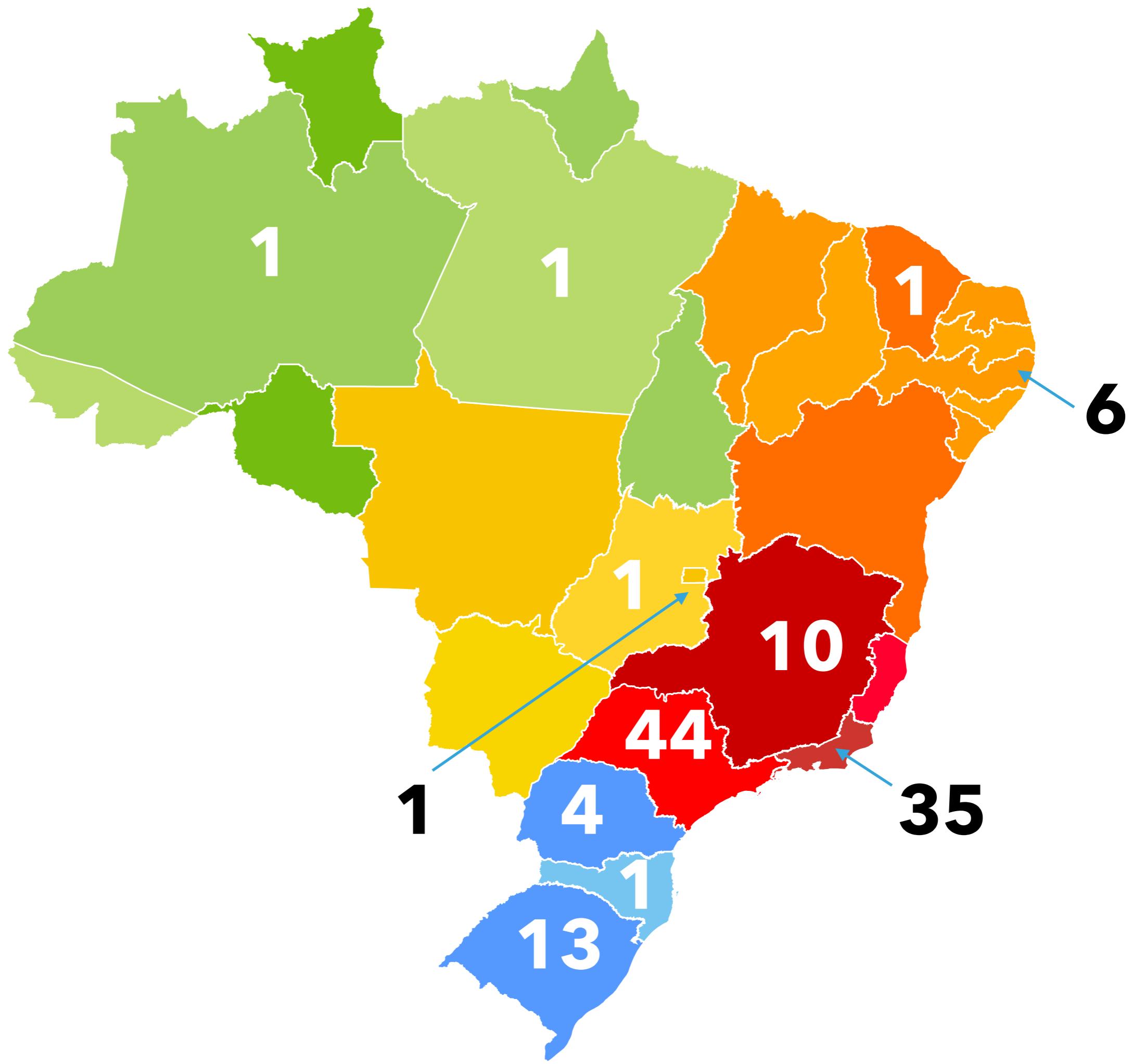
Projetos

- PP Projetos de pesquisa financiados
- PDT Projeto de desenvolvimento tecnológico

Produção técnica e de inovação

- PAT Patentes
- PCSR Programas de computador sem registro
- OPT Outras produções técnicas

+100 PROJECTS IN SDUMONT





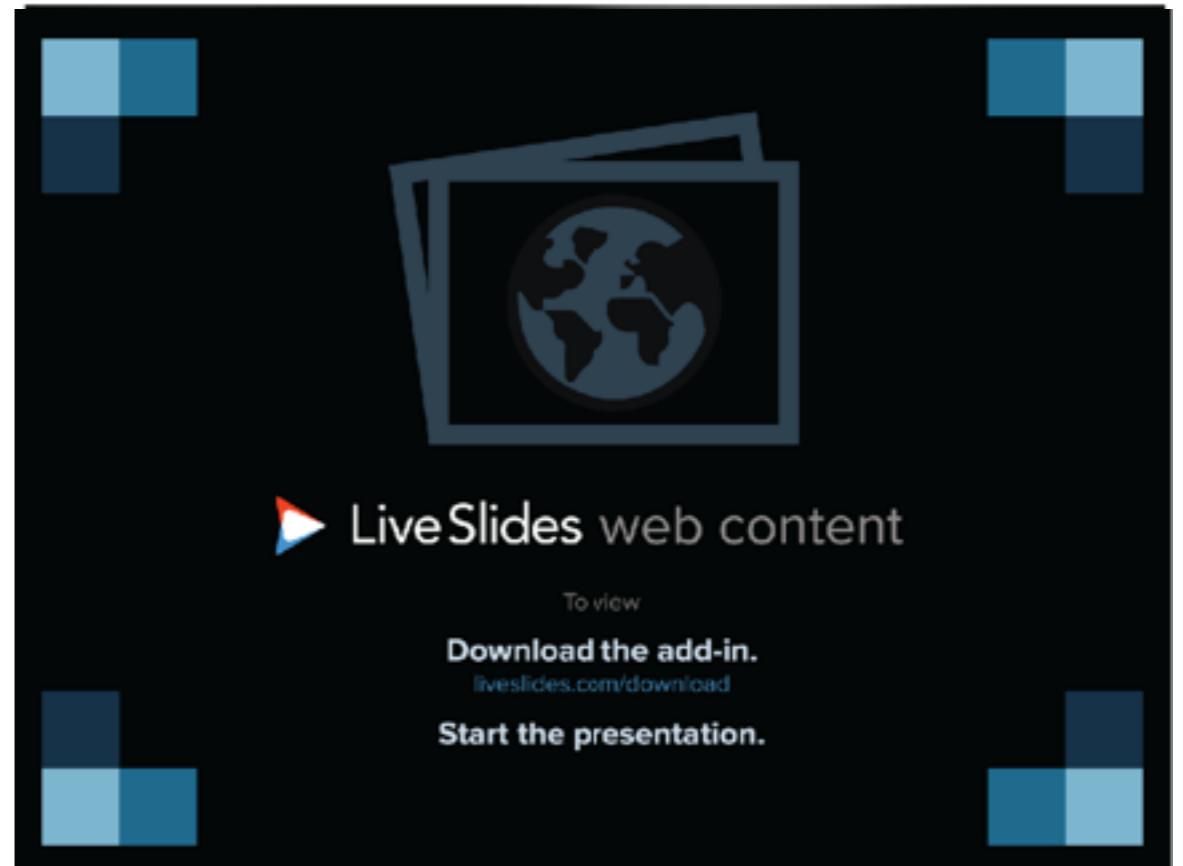
IS THIS CAPACITY
USED
EFFICIENTLY?

USERS/DEVELOPERS READINESS FOR SUPERCOMPUTING

- ▶ (./configure && make) and go for it!
- ▶ Not just a matter of **coding or not coding**:
"Yeah, my gromacs 3.0.4 compiled!"
- ▶ **New methods** (mathematical and computational) to the rescue?
"Hmmm, not sure it will work..."
 - ▶ Don't blame them
 - ▶ At LNCC/SDumont a **parallelization and optimization** group does exist
 - ▶ Problem of **scale...**

USERS READINESS FOR TIME-SHARING SYSTEMS

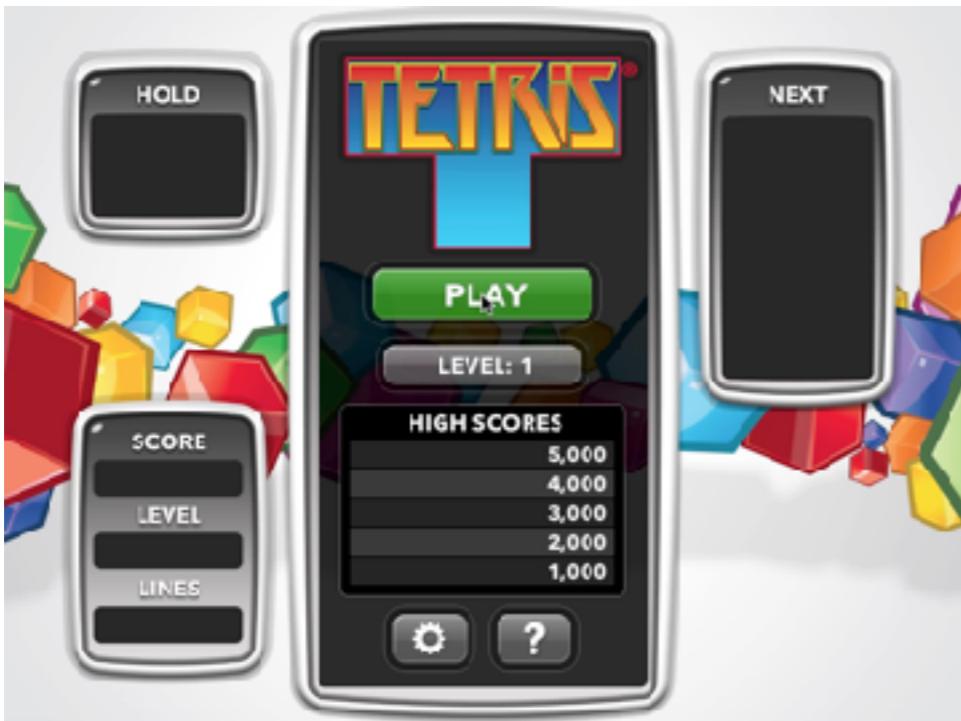
- ▶ "1963 Timesharing: A Solution to Computer Bottlenecks"



<https://youtu.be/Q07PhW5sCEk>

USERS READINESS FOR TIME-SHARING SYSTEMS

- ▶ "1963 Timesharing: A Solution to Computer Bottlenecks"
- ▶ Today it's more like a Tetris game



<https://youtu.be/Q07PhW5sCEk>

- ▶ Concept of job geometry

THE USERS' AND JOBS' BEHAVIOR

- ▶ Analysis using Slurm accounting facility
- ▶ "Exclusive mode", Default time estimation = max W.C.T.

Partition	Max W.C.T. (hours)	Max # cores	Max # executing jobs per user	Max # enqueued jobs per user
cpu	48	1200	4	24
nvidia	48	1200	4	24
phi	48	1200	4	24
mesca2	48	240	1	6
cpu_dev	2	480	1	1
nvidia_dev	2	480	1	1
phi_dev	2	480	1	1
cpu_scal	18	3072	1	8
nvidia_scal	18	3072	1	8
cpu_long	744	240	1	1
nvidia_long	744	240	1	1

THE JOBS' BEHAVIOR

- ▶ Overall statistics from Aug/2016 to May/2018
- ▶ Job status

Status	Total number of jobs	% of total
COMPLETED	77147	53,55 %
FAILED	30847	21,41 %
CANCELLED	25197	17,49 %
TIMED-OUT	10809	7,50 %
NODE FAILURE	53	0,04 %

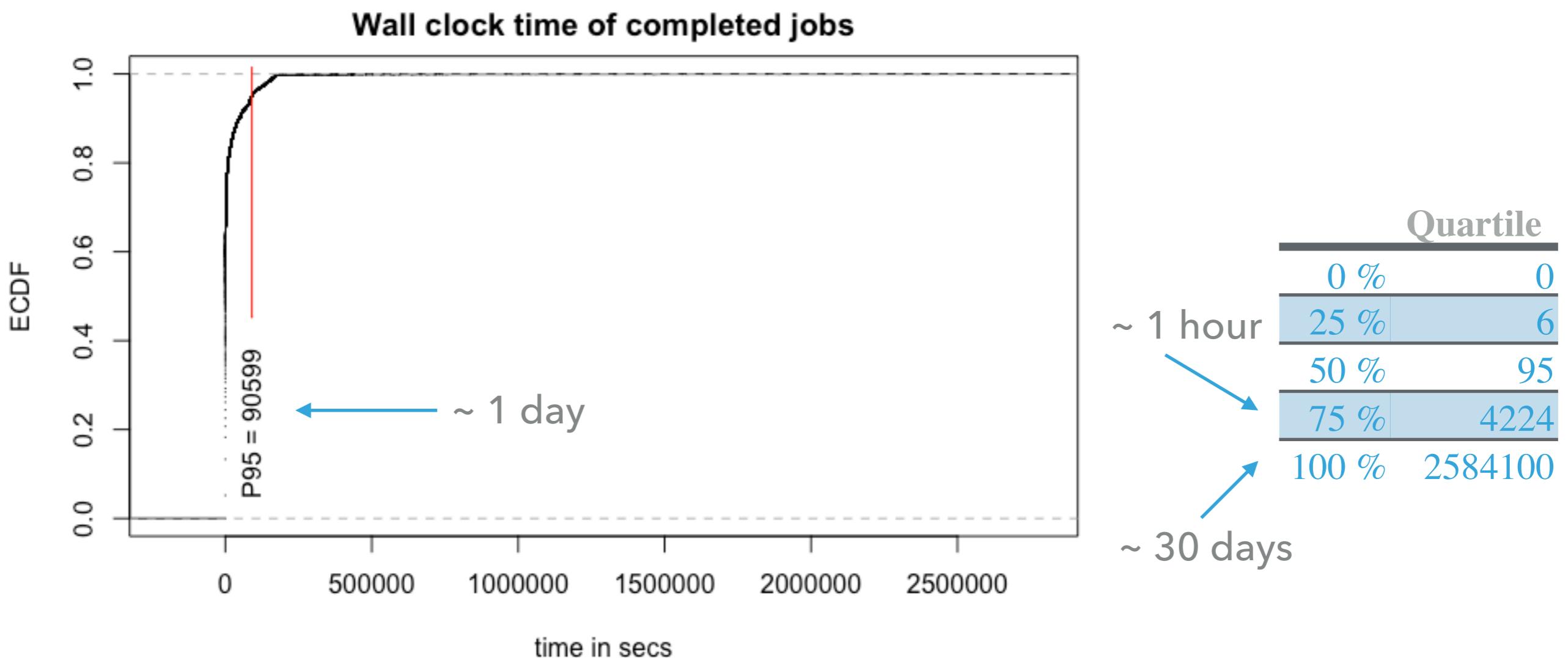
THE JOBS' BEHAVIOR (CONTINUED)

- ▶ Overall statistics from Aug/2016 to May/2018
- ▶ Percentage of completed jobs in each partition

Partition name	Total number of jobs	% of total
cpu	34856	49,89 %
cpu_dev	21858	31,29 %
nvidia	9049	12,95 %
nvidia_dev	2115	3,03 %
mesca2	776	1,11 %
cpu_long	608	0,87 %
cpu_scal	467	0,67 %
nvidia_long	68	0,10 %
nvidia_scal	68	0,10 %

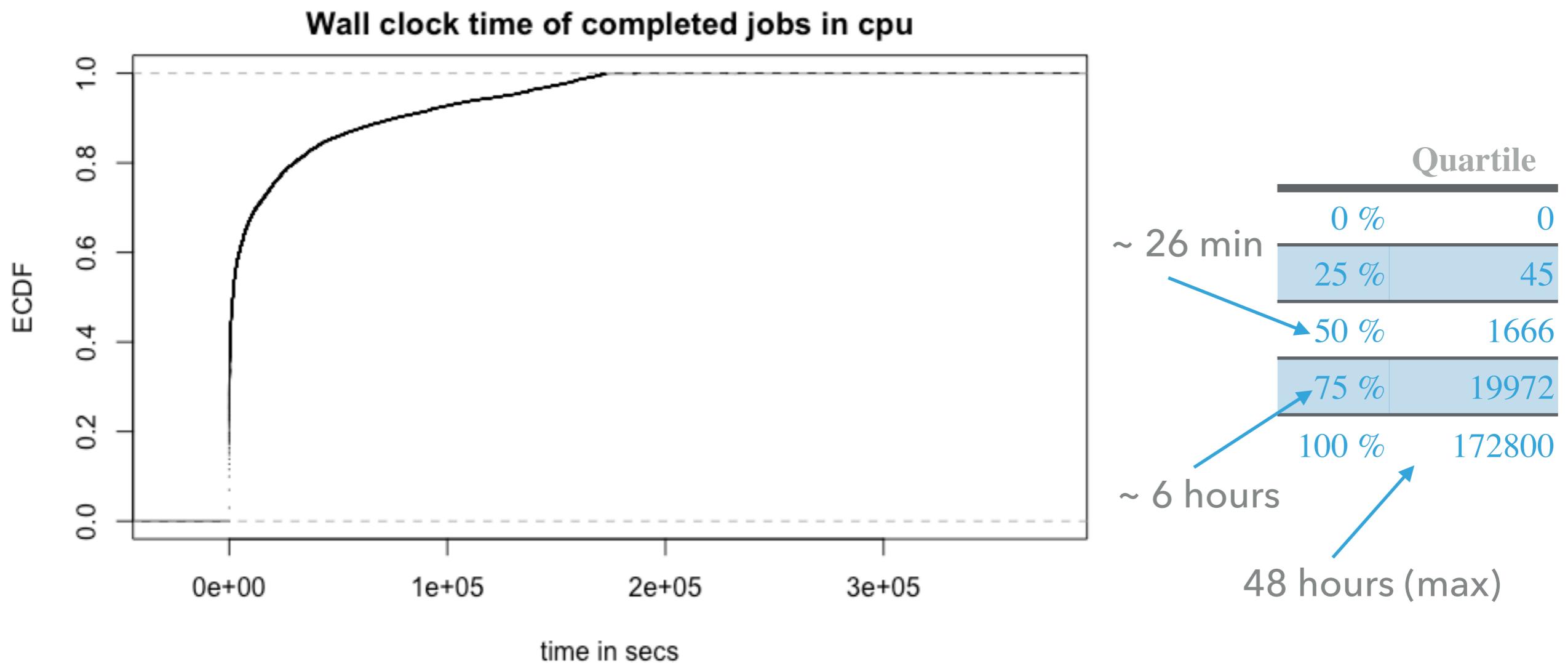
THE JOBS' BEHAVIOR (CONTINUED)

- ▶ Wall-clock time statistics from Aug/2016 to May/2018



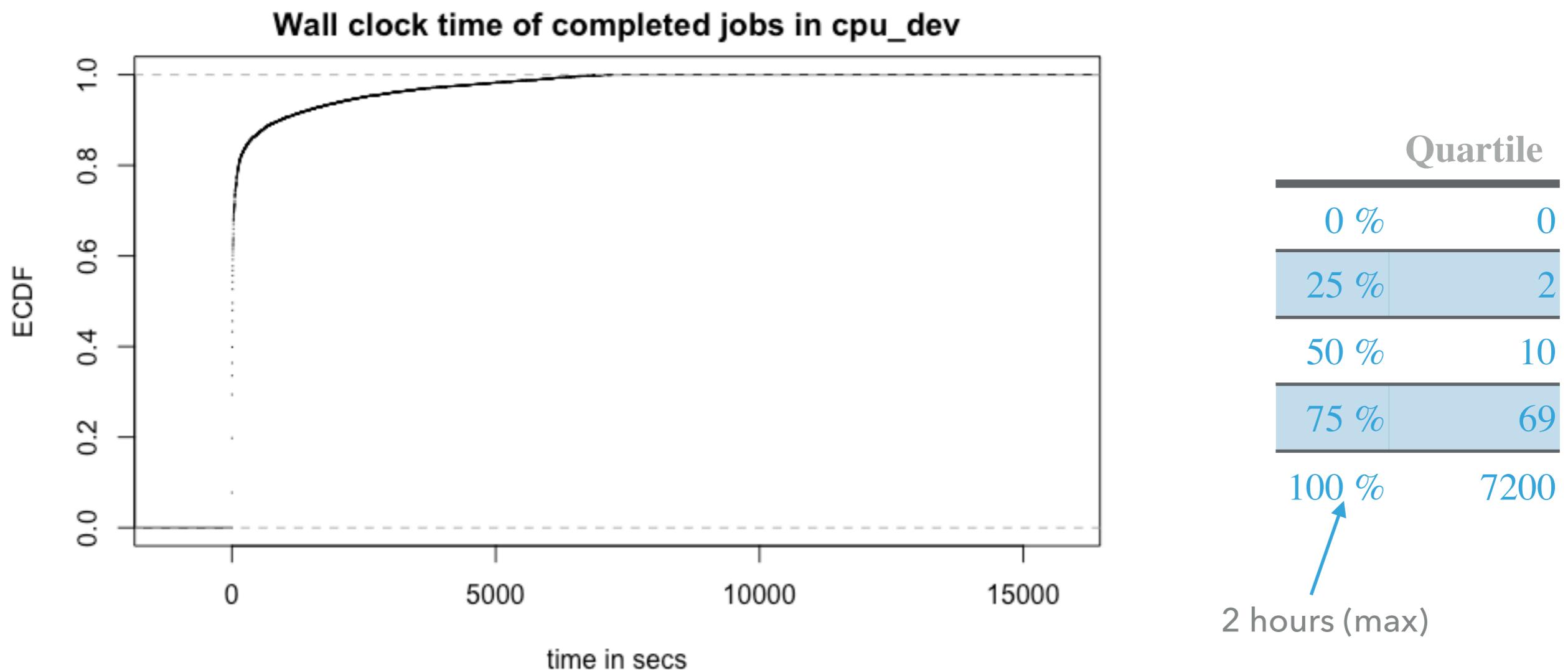
THE JOBS' BEHAVIOR (CONTINUED)

- ▶ Wall-clock time statistics from Aug/2016 to May/2018



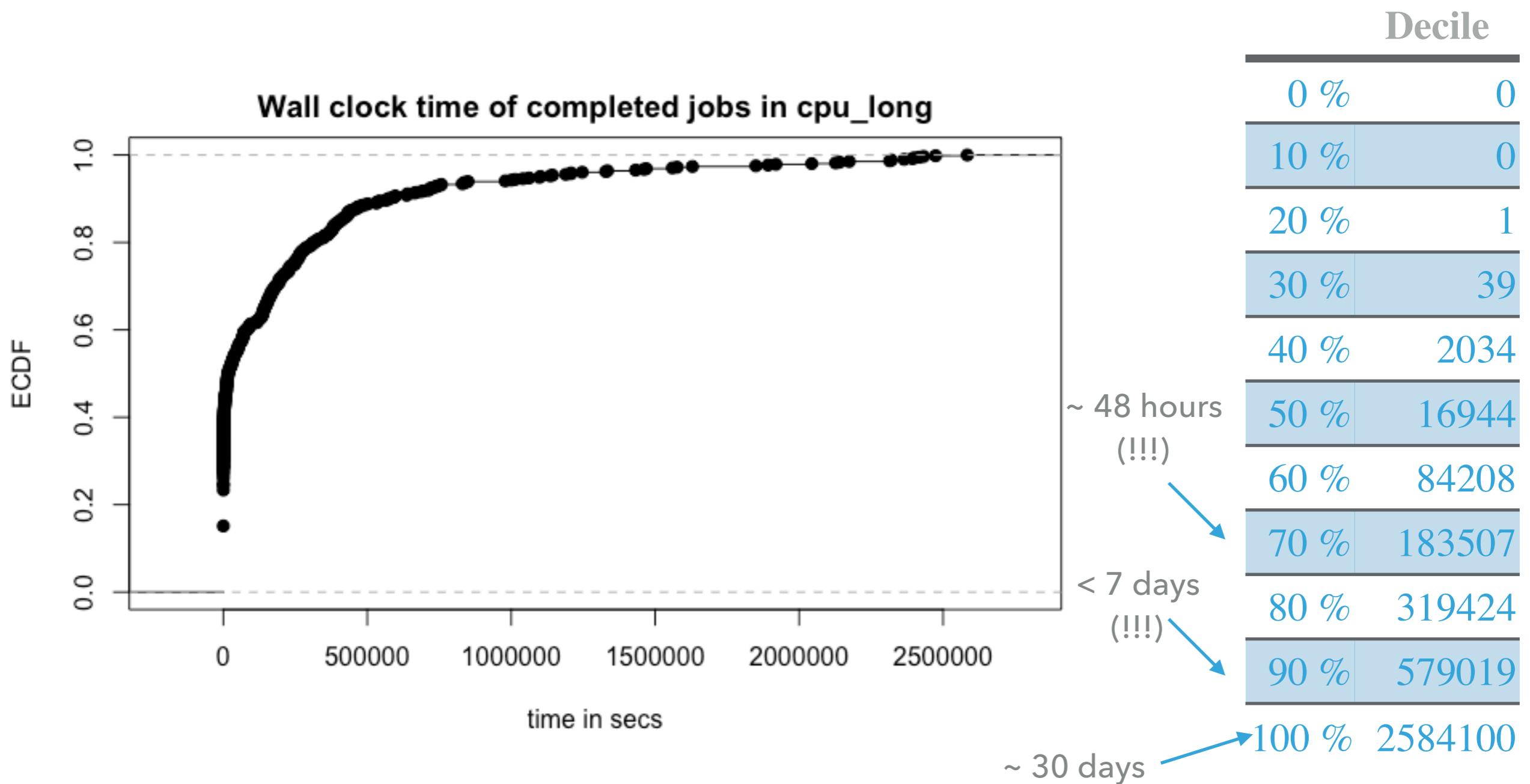
THE JOBS' BEHAVIOR (CONTINUED)

- ▶ Wall-clock time statistics from Aug/2016 to May/2018



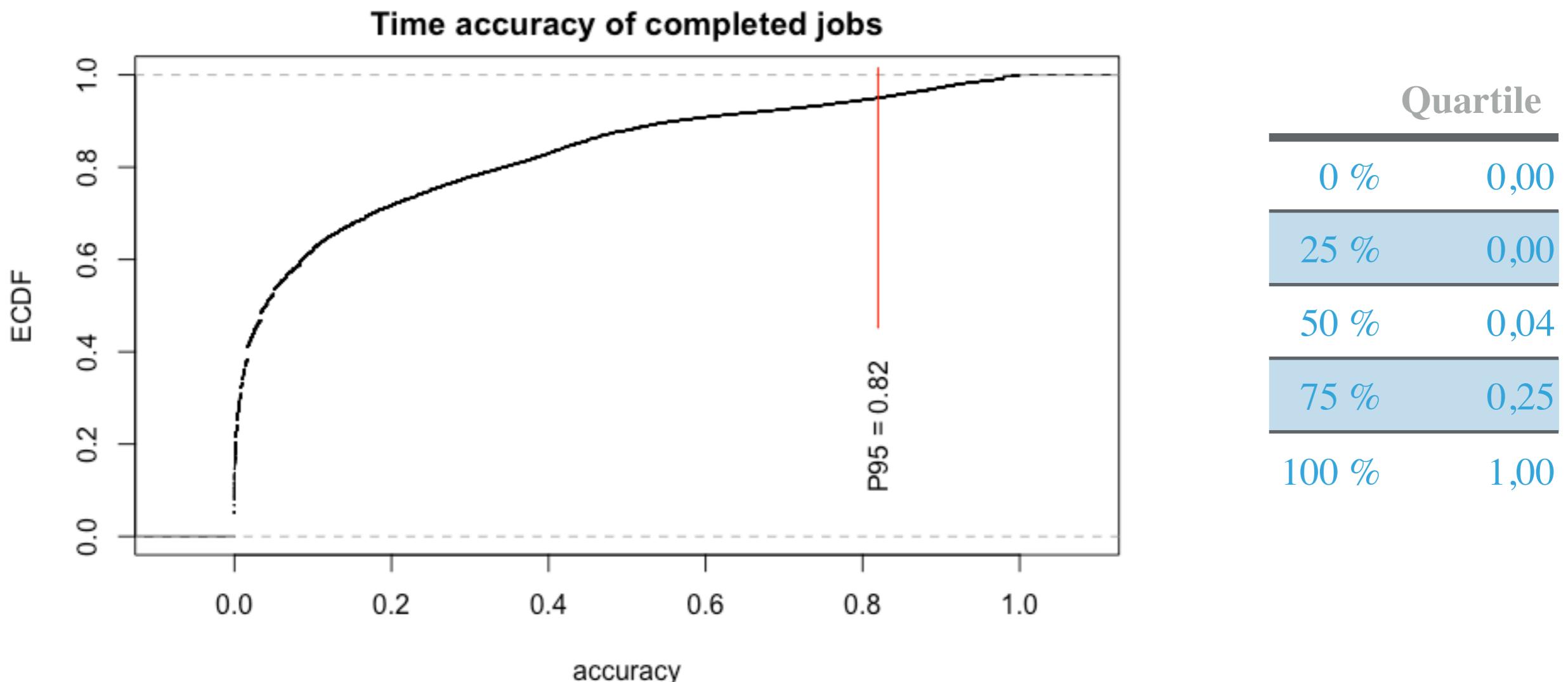
THE JOBS' BEHAVIOR (CONTINUED)

- ▶ Wall-clock time statistics from Aug/2016 to May/2018



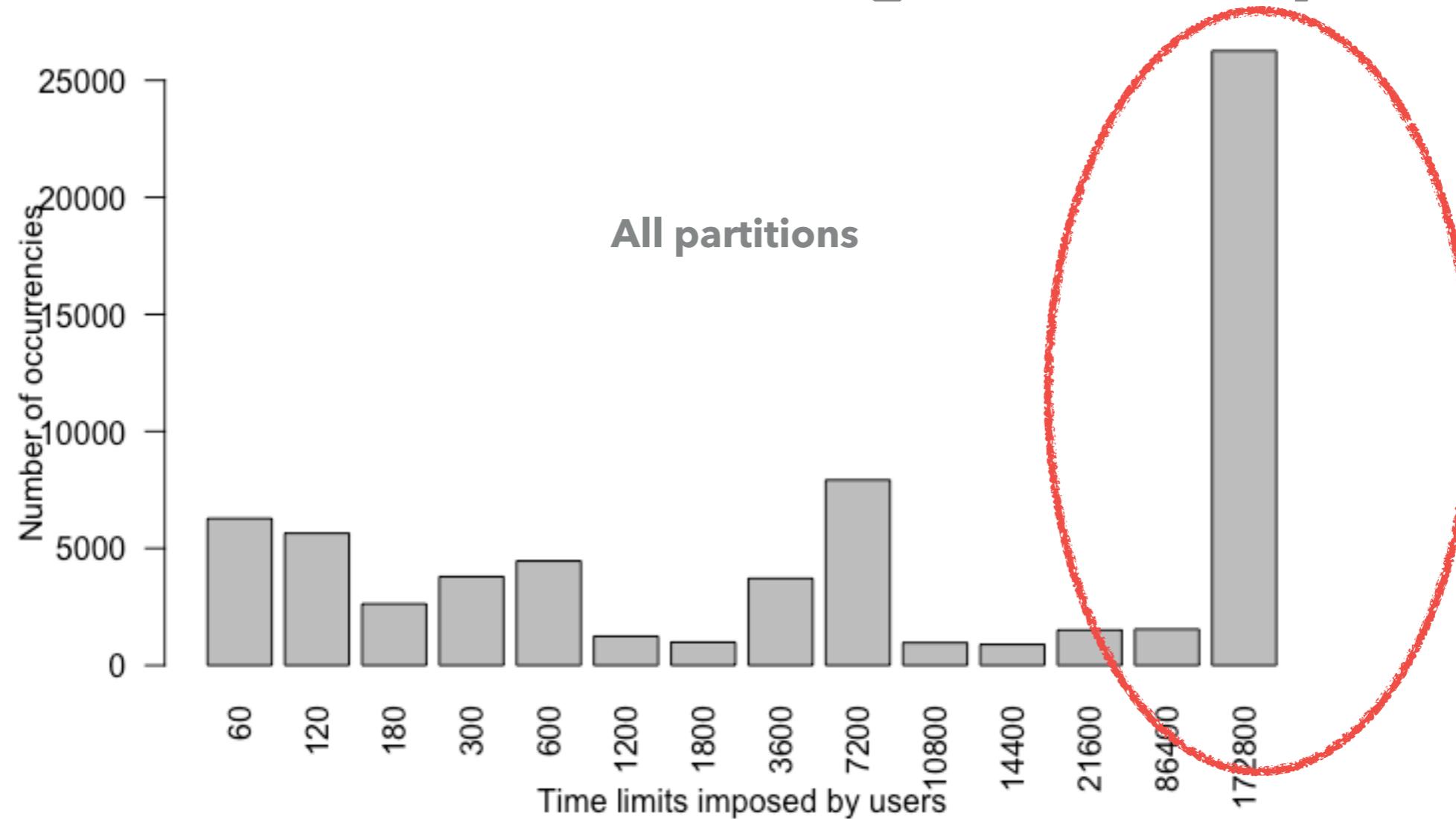
THE USERS' BEHAVIOR

- ▶ Estimated time statistics from Aug/2016 to May/2018



THE USERS' BEHAVIOR (CONTINUED)

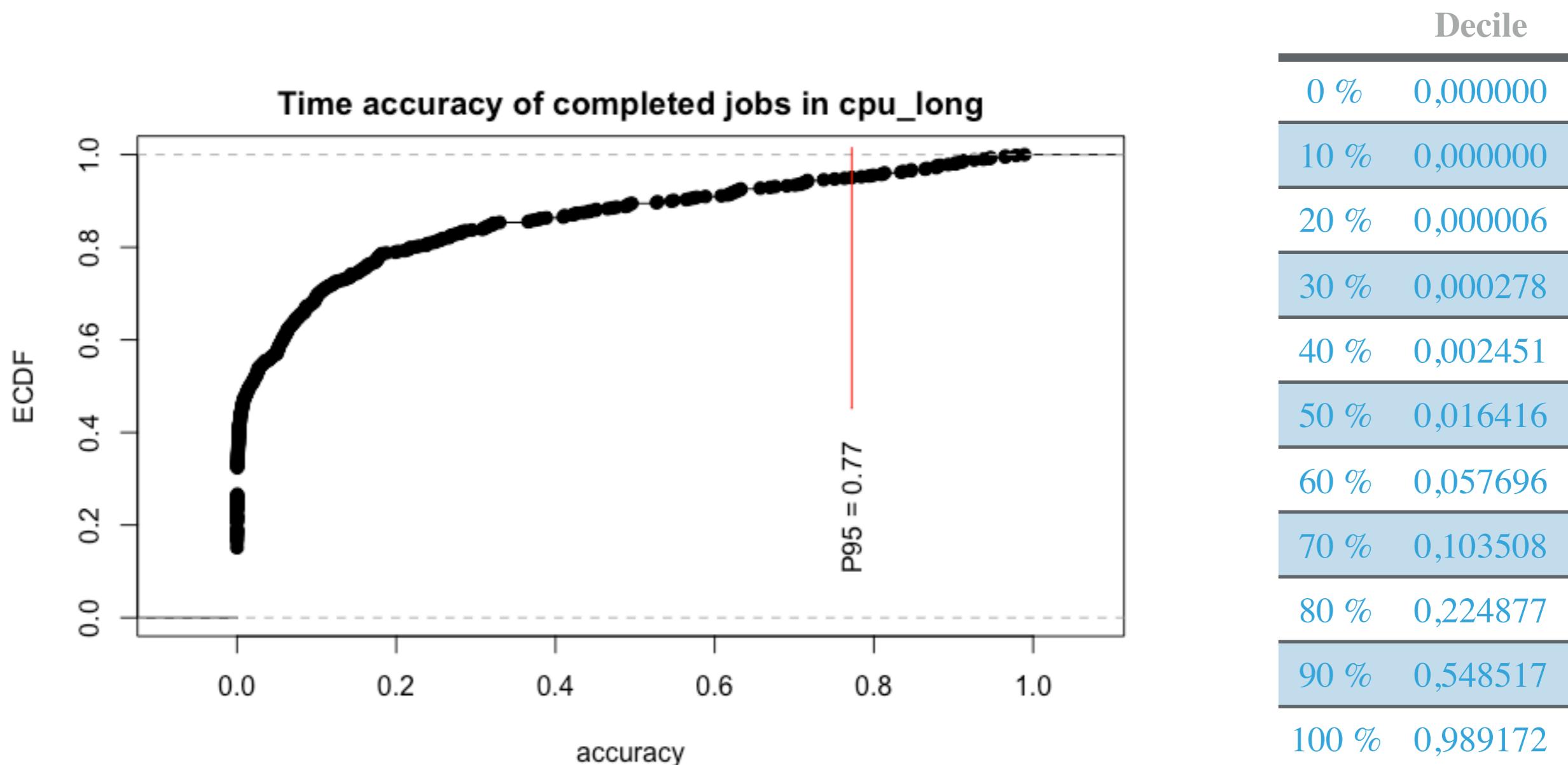
- ▶ Estimated time statistics from Aug/2016 to May/2018



* only those with more than 500 occurrences

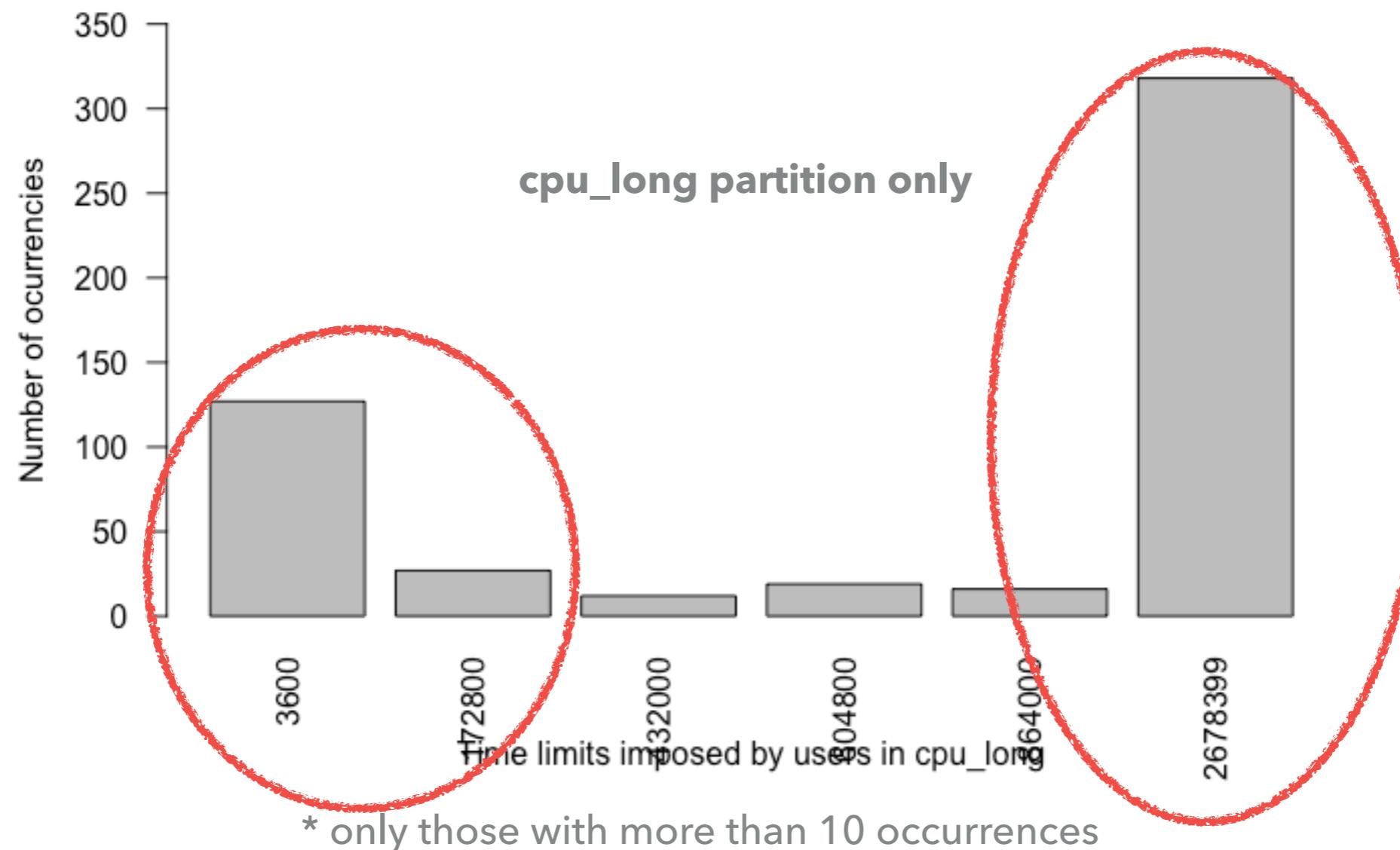
THE USERS' BEHAVIOR (CONTINUED)

- ▶ Estimated time statistics from Aug/2016 to May/2018



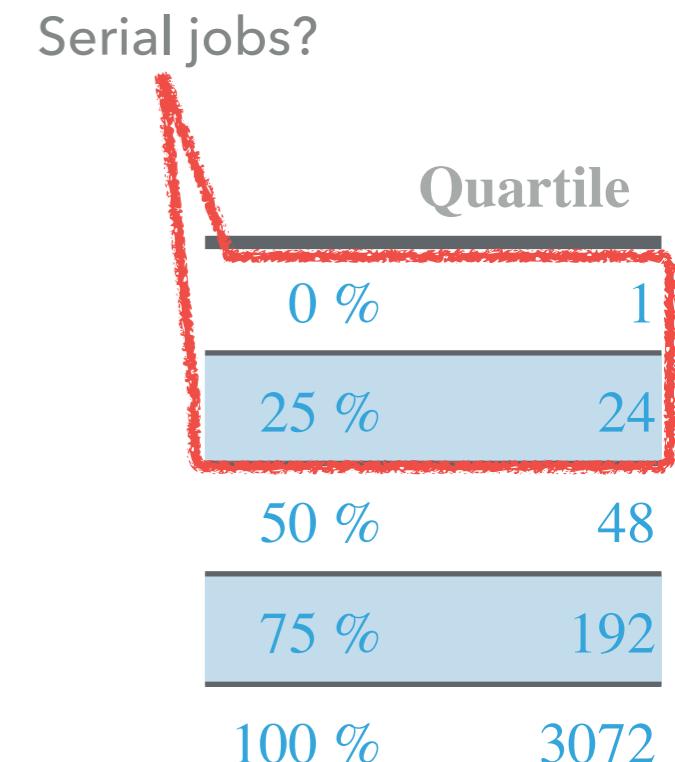
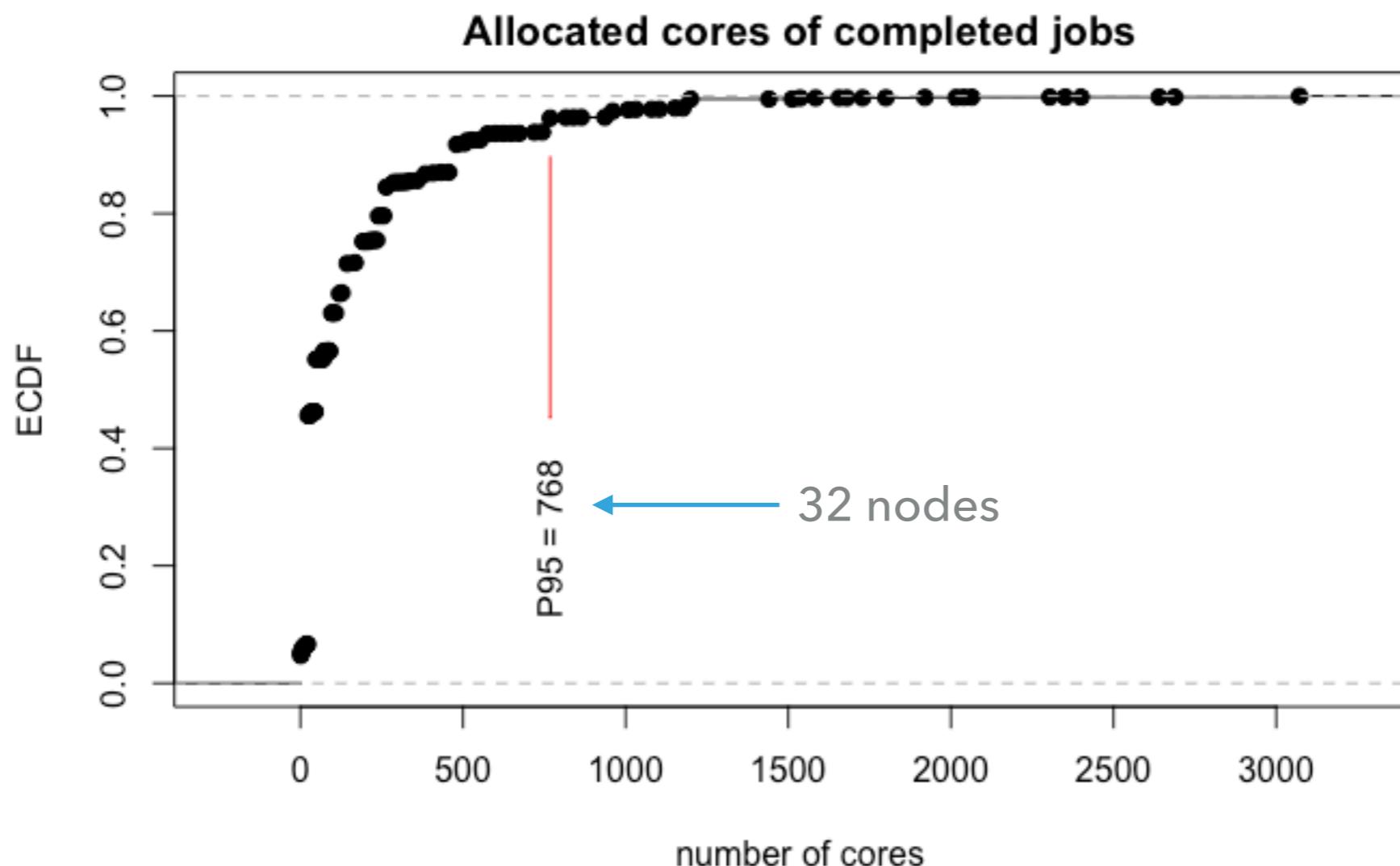
THE USERS' BEHAVIOR (CONTINUED)

- ▶ Estimated time statistics from Aug/2016 to May/2018



THE USERS' BEHAVIOR (CONTINUED)

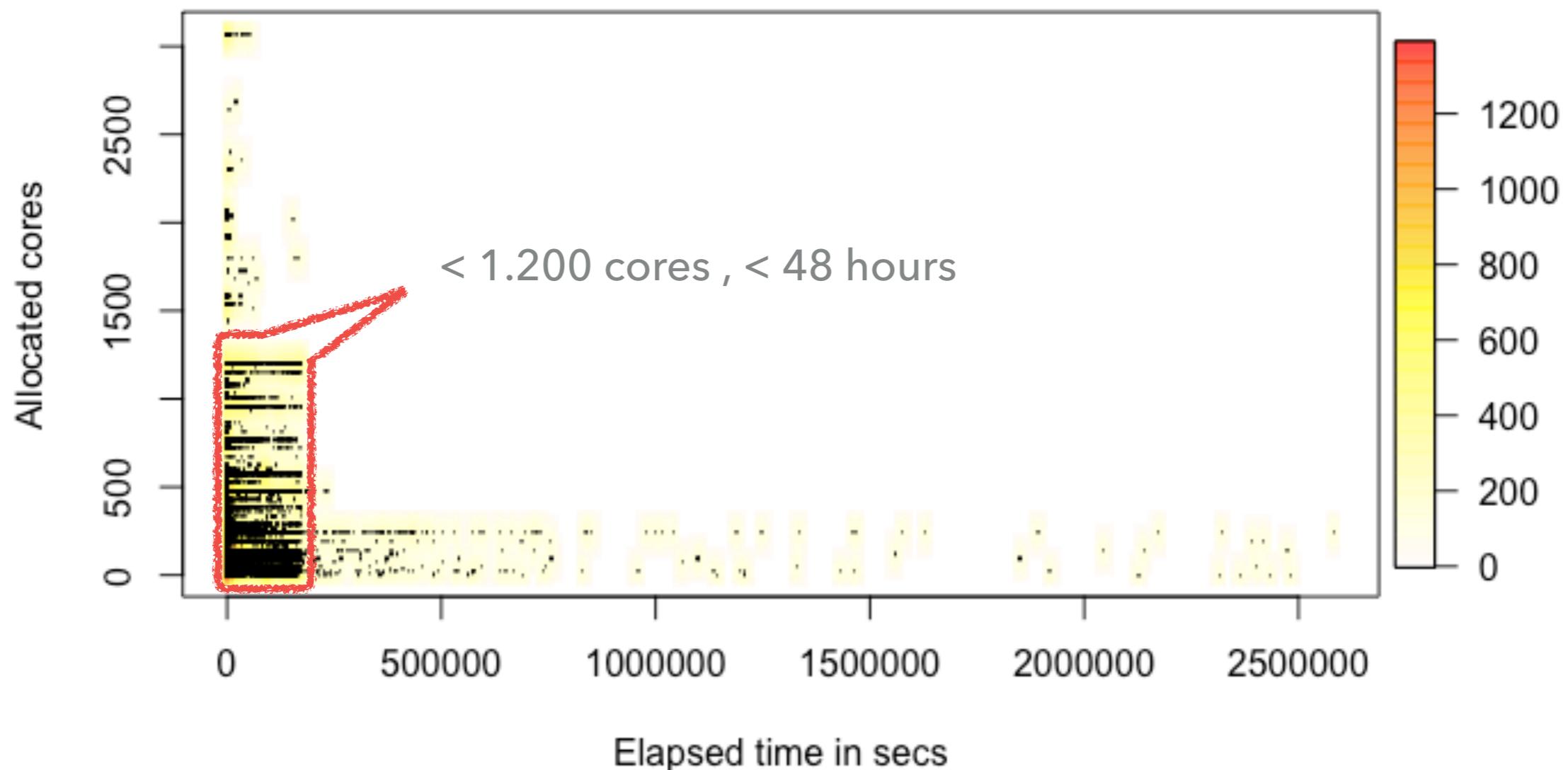
- Core allocation statistics from Aug/2016 to May/2018



THE USERS' VERSUS JOBS' BEHAVIOR

- ▶ Job geometry statistics from Aug/2016 to May/2018

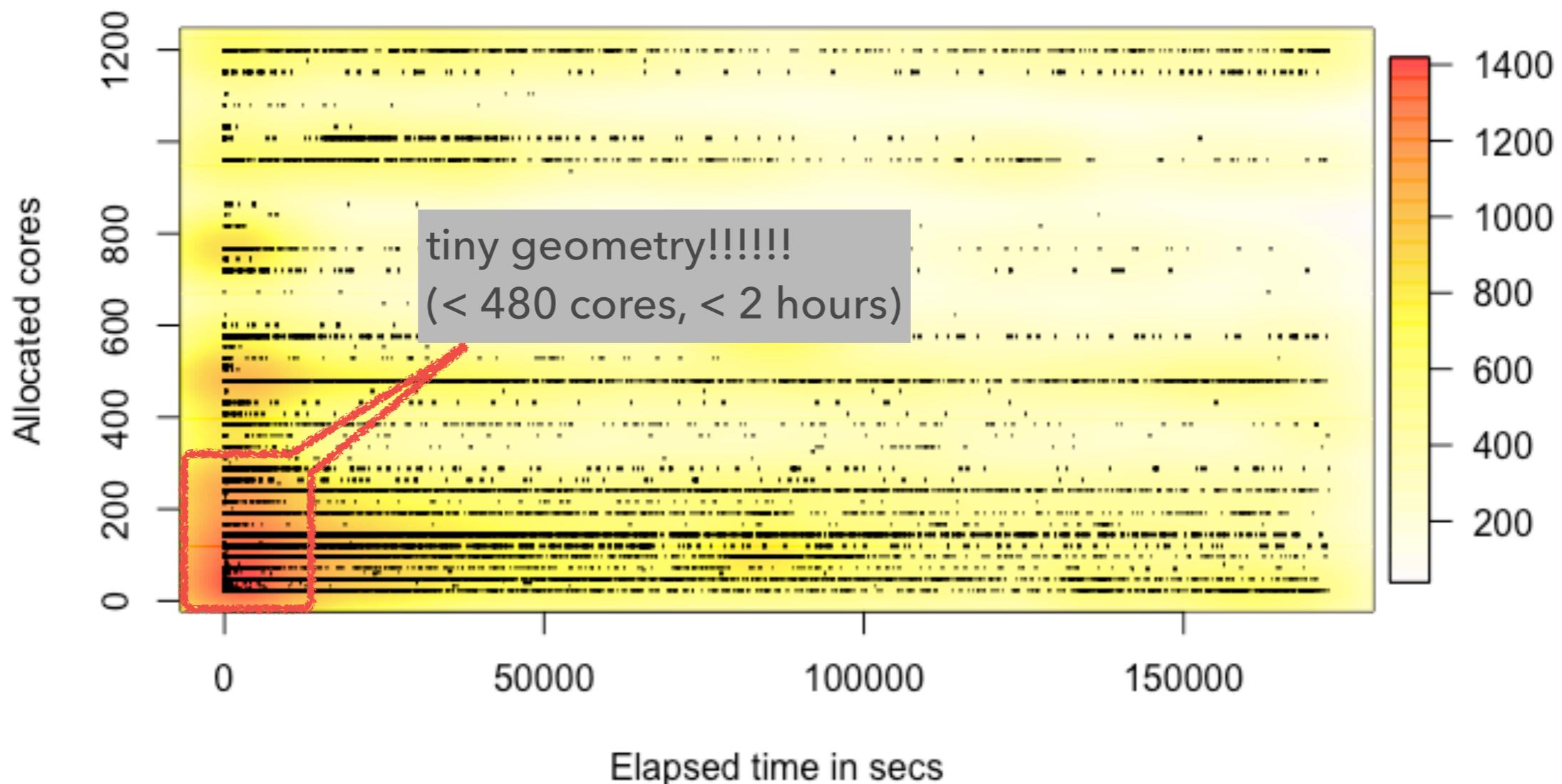
Scatterplot with smoothed density of jobs' geometry



THE USERS' VERSUS JOBS' BEHAVIOR (CONTINUED)

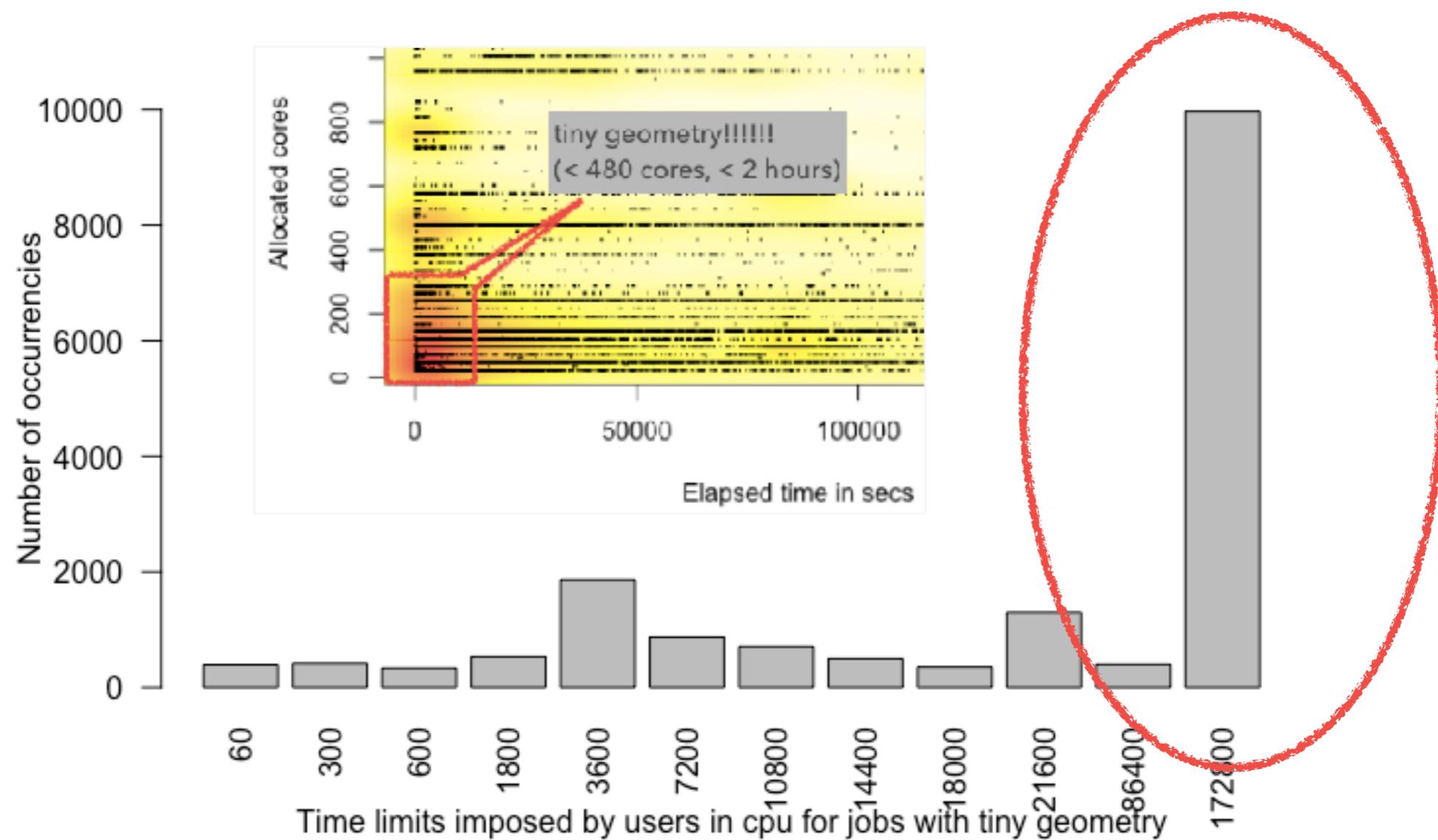
- ▶ Job geometry statistics from Aug/2016 to May/2018

Scatterplot with smoothed density of jobs' geometry for smaller jobs



(BACK TO) THE USERS' BEHAVIOR

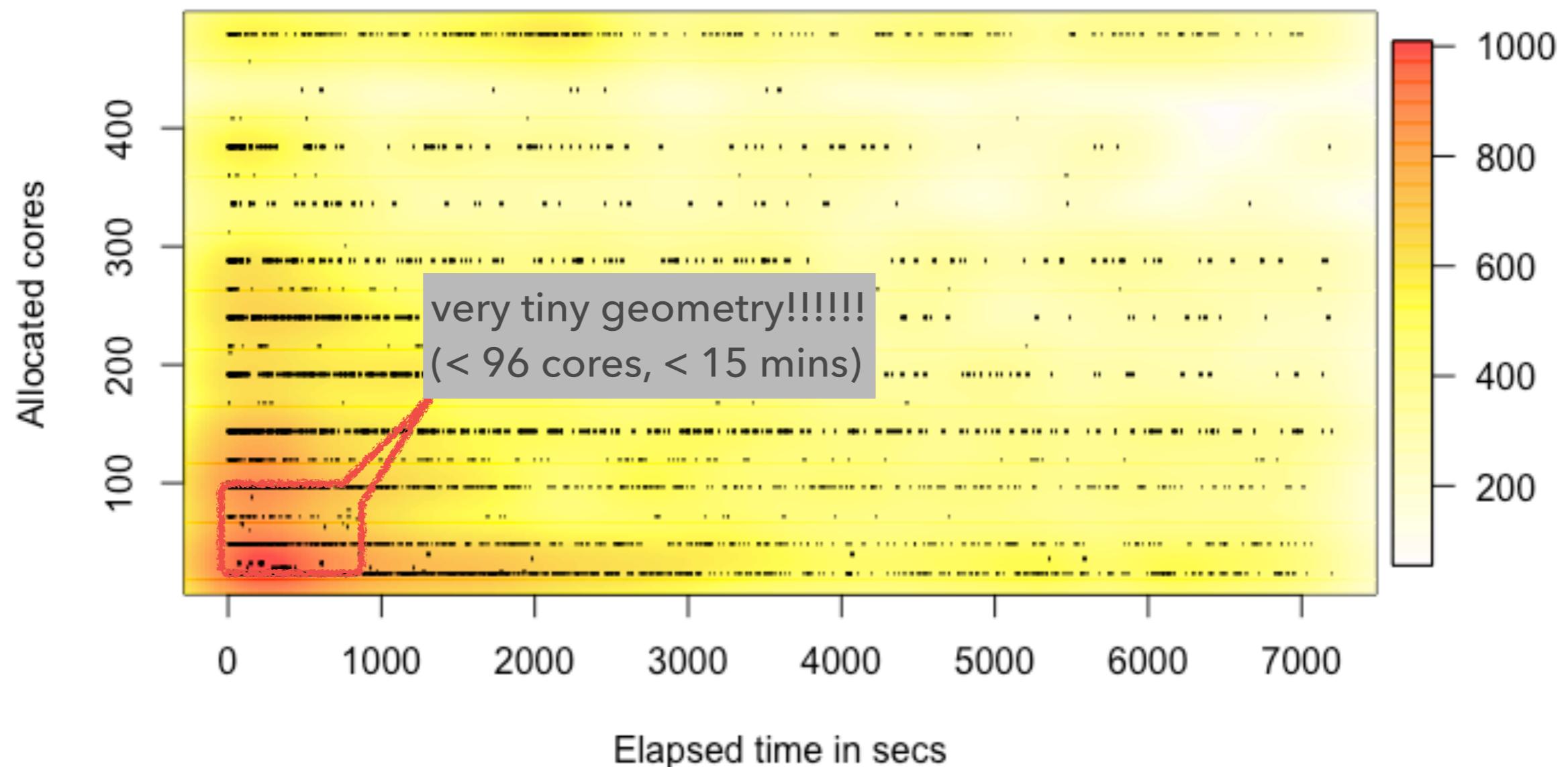
- ▶ Estimated time statistics from Aug/2016 to May/2018



THE USERS' BEHAVIOR (CONTINUED)

- ▶ Estimated time statistics from Aug/2016 to May/2018

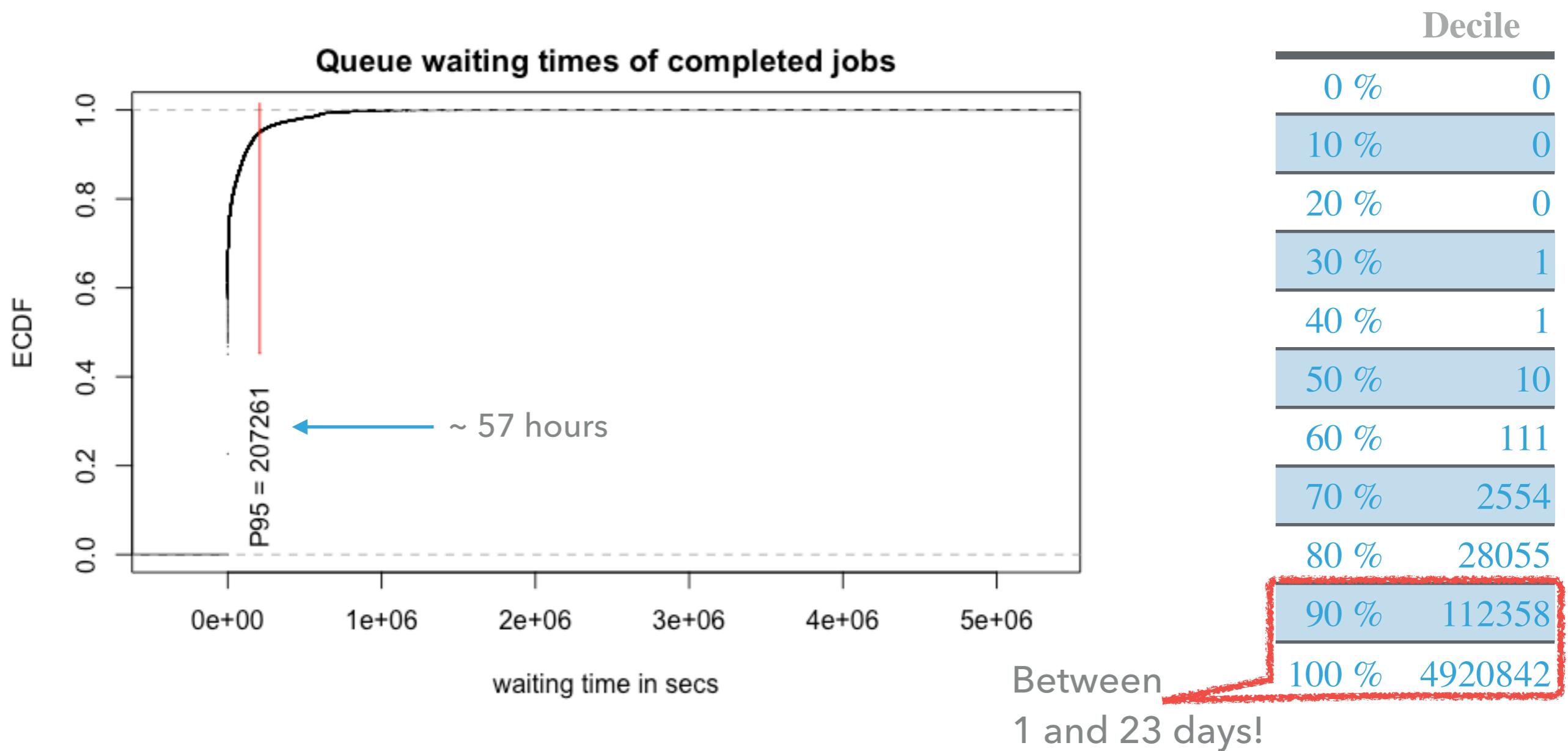
Scatterplot with smoothed density of jobs' geometry for cpu_dev partition



**BUT WHY SHOULD
USERS BOTHER?**

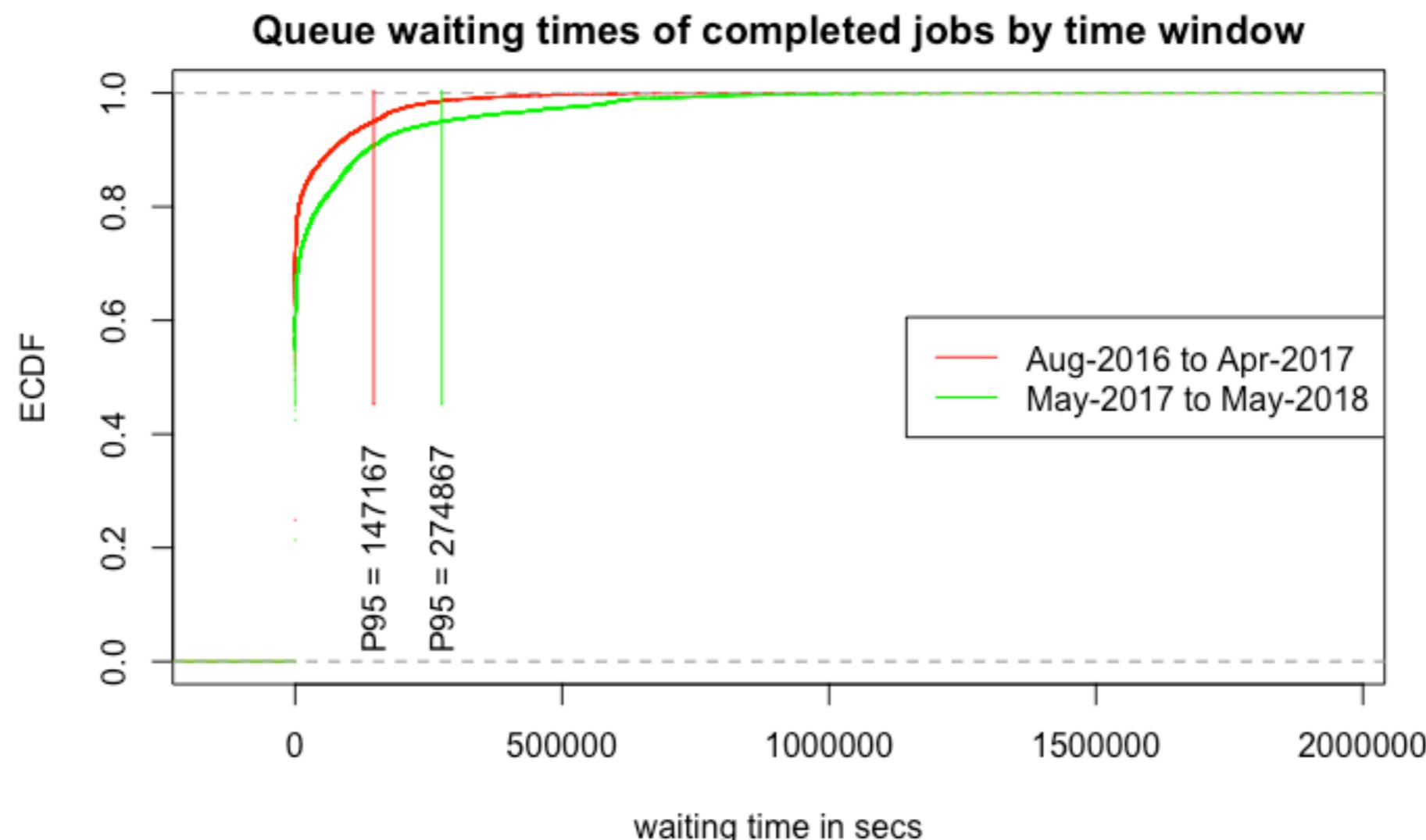
THE SYSTEMS' BEHAVIOR

- ▶ Queue waiting time statistics from Aug/2016 to May/2018



THE SYSTEMS' BEHAVIOR (CONTINUED)

- ▶ Split statistics from Aug/2016 to Apr/2017 (after 1st call) and from May/2017 to May/2018 (after 2nd call)





Design by [Harry Movie Art](#)

CAN WE HELP?

REVISITING THE SCHEDULING POLICIES

Partition	Max W.C.T (hours)	<u>Min # cores</u>	Max # cores	Max # executing jobs per user	Max # enqueued jobs per user
cpu	48	504	1200	4	24
nvidia	48	504	1200	4	24
phi	48	504	1200	4	24
mesca2	48	1	240	1	6
cpu_dev	≥ 0,3	24	480 96	1	1
nvidia_dev	≥ 0,3	24	480 96	1	1
phi_dev	≥ 0,3	24	480 96	1	1
cpu_scal	18	1224	3072	1	8
nvidia_scal	18	1224	3072	1	8
cpu_long	744	24	240	1	1
nvidia_long	744	24	240	1	1
cpu_small	2	24	480	4	24
nvidia_small	2	24	480	4	24

REVISITING THE SCHEDULING POLICIES (CONTINUED)

- ▶ "Non-exclusive mode" for mesca2 partition
- ▶ Default time estimation = $1/2$ max W.C.T.

Entered in operation in June/2018

THE JOBS' BEHAVIOR

- ▶ Overall statistics from Jun/2018 to Sep/2018



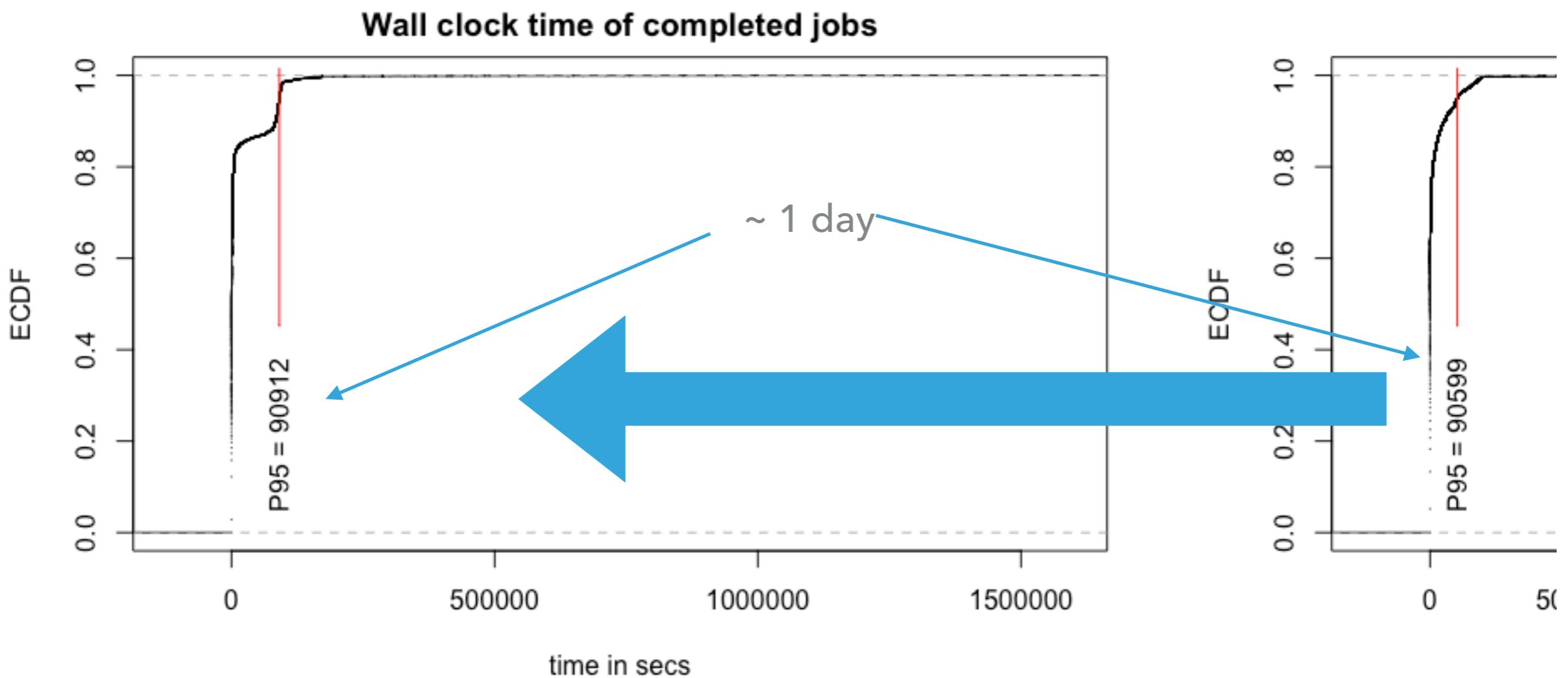
- ▶ Percentage of completed jobs in each partition

Partition name	Total number of jobs	% of total
cpu	34856	49,89 %
cpu_dev	21858	31,29 %
...		

Partition name	Total number of jobs	% of total
cpu_small	11204	55 %
cpu_dev	4621	23 %
cpu	1606	8 %
nvidia_dev	1009	5 %
nvidia_sma ll	878	4 %
nvidia_long	286	1 %
nvidia	270	1 %
cpu_long	182	1 %
mesca2	142	1 %
cpu_scal	22	0 %
nvidia_scal	17	0 %

THE JOBS' BEHAVIOR (CONTINUED)

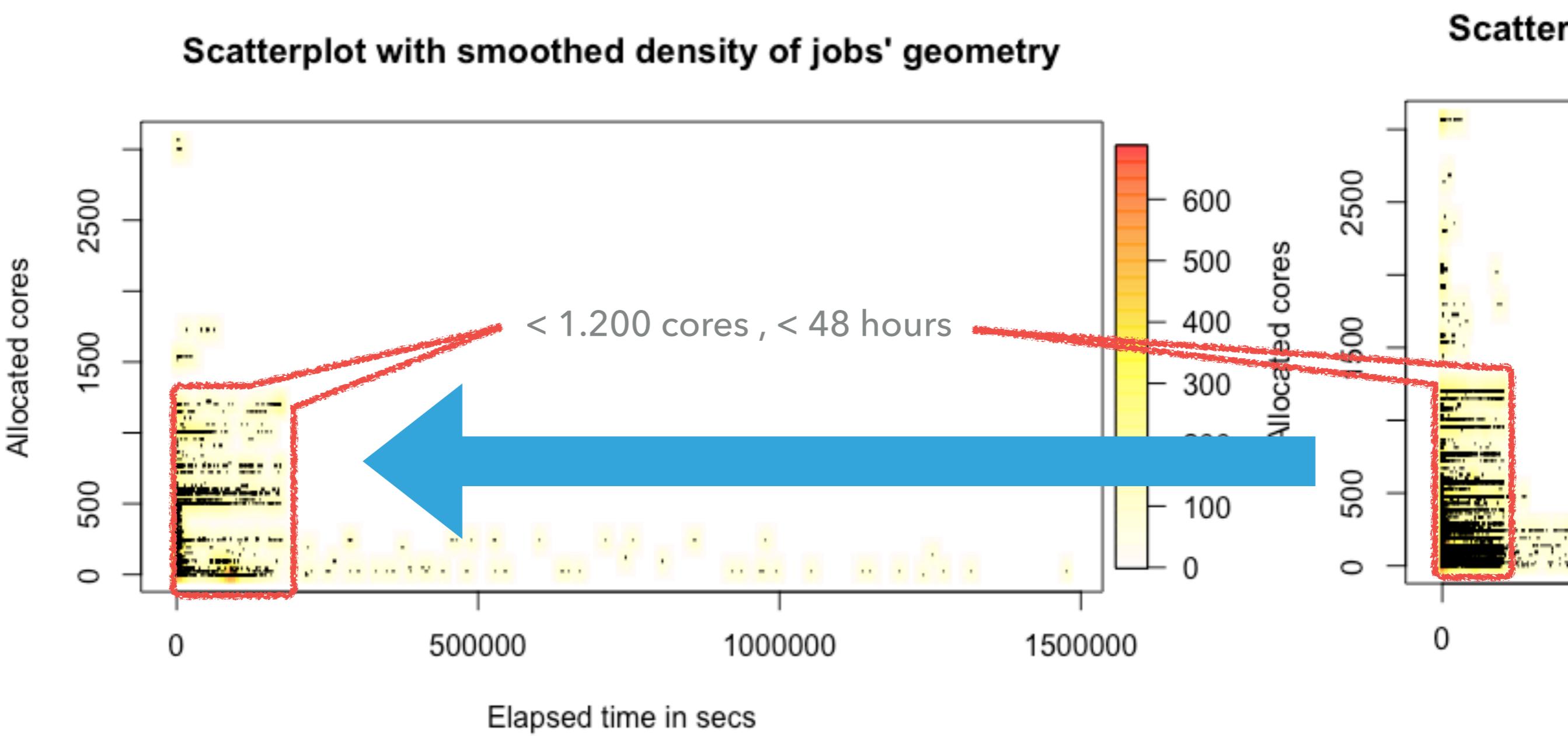
- ▶ Wall-clock time statistics from Jun/2018 to Sep/2018



THE USERS' VERSUS JOBS' BEHAVIOR

- Job geometry statistics from Jun/2018 to Sep/2018

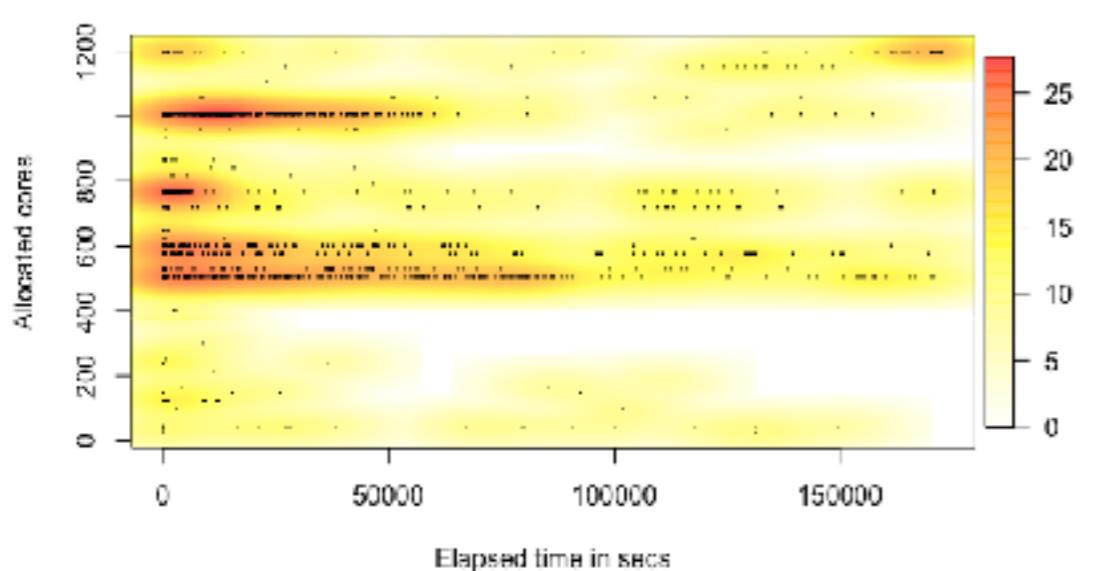
Scatterplot with smoothed density of jobs' geometry



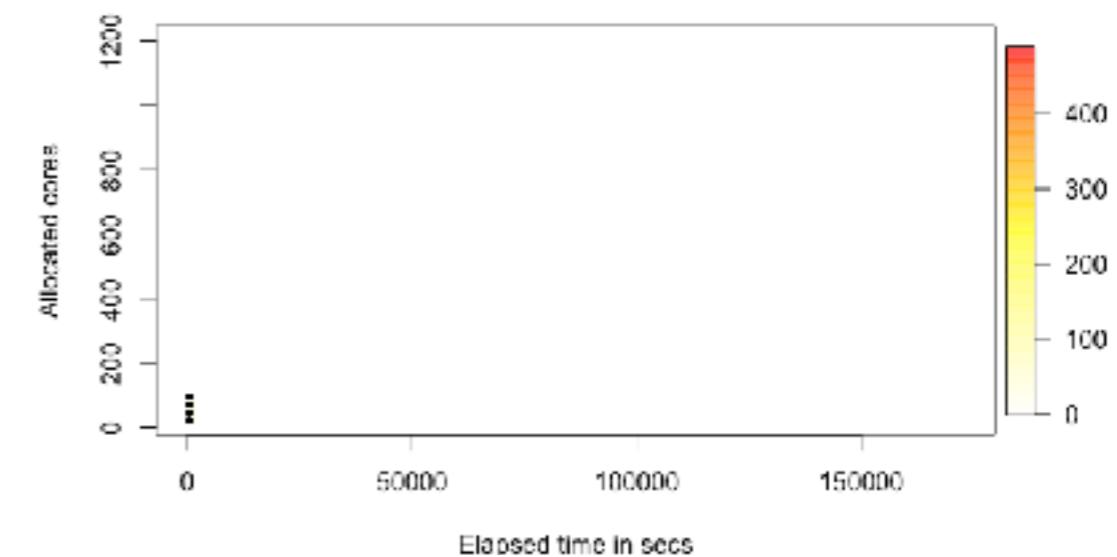
THE USERS' VERSUS JOBS' BEHAVIOR (CONTINUED)

► Job geometry statistics from Jun/2018 to Sep/2018

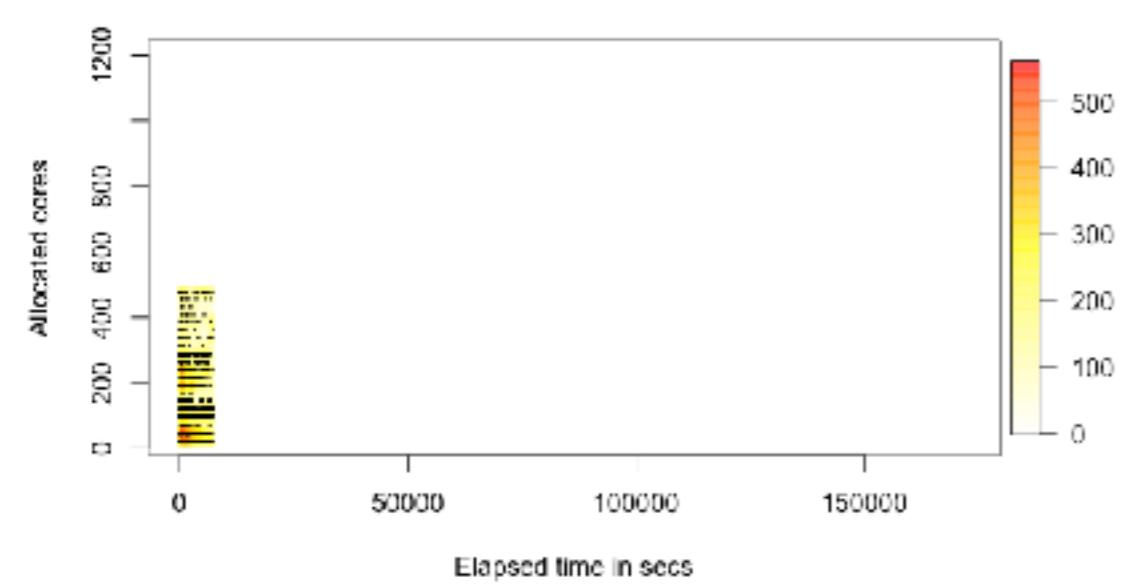
Scatterplot with smoothed density of jobs' geometry for cpu partition



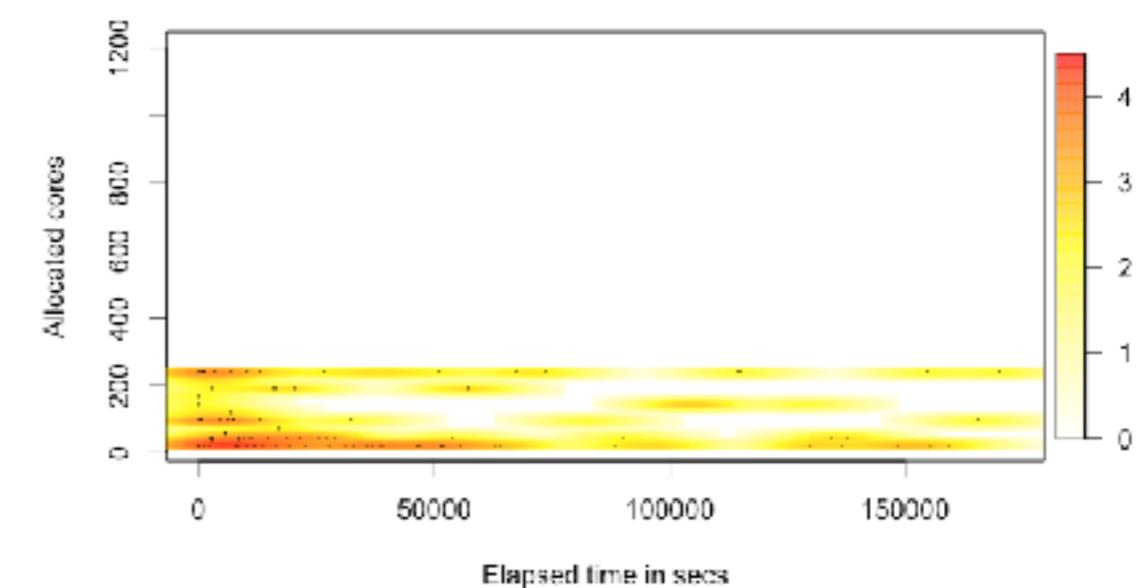
Scatterplot with smoothed density of jobs' geometry for cpu_dev partition



Scatterplot with smoothed density of jobs' geometry for cpu_small partition

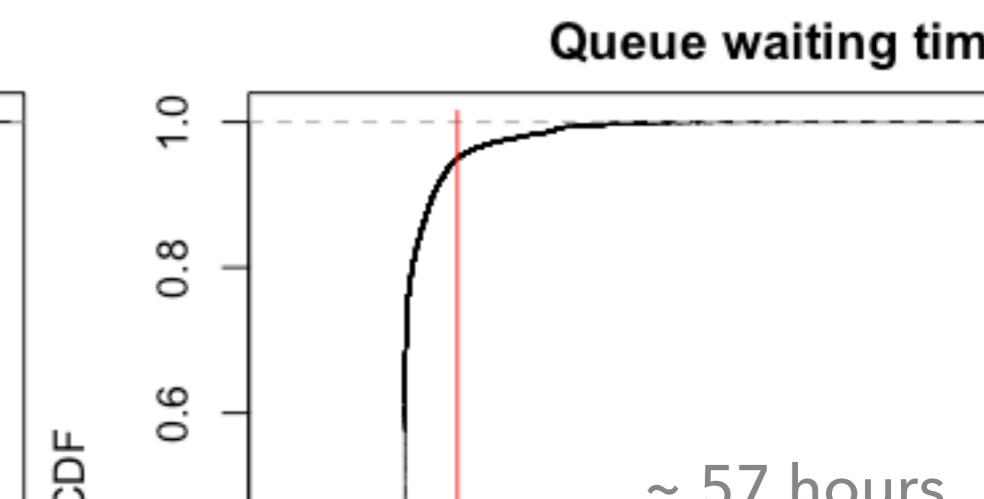


Scatterplot with smoothed density of jobs' geometry for cpu_long partition



THE SYSTEMS' BEHAVIOR

- ▶ Queue waiting time statistics from Jun/2018 to Sep/2018



Between
7 hours and 12 days!

SUMMARY AND OUTLOOK

THE SINAPAD EXPERIENCE

- ▶ Demand is **clear**, updating is **flaky**
- ▶ Mismatch between **policy and action**
- ▶ SINAPAD formal establishment X
modus operandi of funding agencies



[James Green](#) on January 25, 2016 at 10:00 am

THE SDUMONT EXPERIENCE

- ▶ **Gap** between CSE researchers/technologists and the application researchers is still huge
 - ▶ Efforts do exist (e.g. **HPC4e** project) but are not the norm
- ▶ Keeping the system operating the **best as possible** is a daunting task:
 - ▶ **Recommendation** systems
 - ▶ **Self-tuning** policies
 - ▶ Again, CSE researchers to the rescue!



[James Green](#) on January 25, 2016 at 10:00 am



Laboratório
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Ministério da
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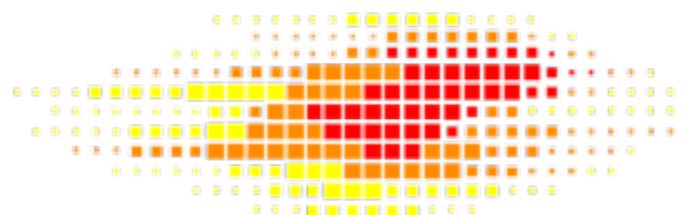
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[HTTP://SDUMONT.LNCC.BR](http://sdumont.lncc.br)

[HTTPS://WWW.FACEBOOK.COM/SISTEMA-NACIONAL-DE-PROCESSAMENTO-
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THANK YOU!

OBRIGADO!



WSCAD 2018