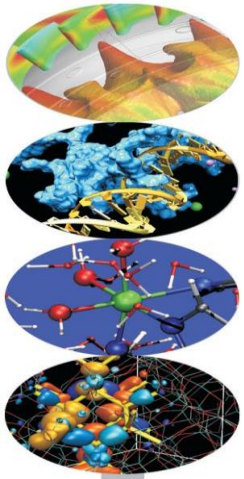
CINECA SCAI
SuperComputing Applications and Innovation

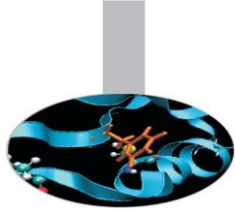


61st Ticket Meeting

HPC User Support @ CINECA
February, 14th 2022

CINECA

Content



- Status of the clusters - main events affecting production [Jan 15 – Feb 11]
- Examination of active tickets on HPC-US-SECOND queue
  - escalated to Intel support
  - escalated to NVIDIA support
  - other tickets
- Ticket statistics on queue [Jan 14 - Feb 09]
  - HPC-US-FIRST
  - HPC-US-SECOND
- Module usage on Marconi-SKL

Status of the clusters [Jan 15 – Feb 11]

Main events affecting production

Jan 20: scheduled maintenance operations on Marconi100 on January 25th
https://www.hpc.cineca.it/center_news/scheduled-maintenance-marconi100-next-tuesday-january-25th
https://www.hpc.cineca.it/center_news/reminder-scheduled-maintenance-marconi100-tomorrow-january-25th
https://www.hpc.cineca.it/center_news/m100-maintenance-completed

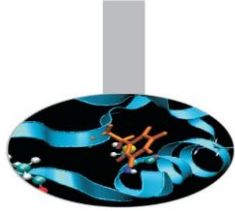
Feb 4: Issue on Marconi filesystem
https://www.hpc.cineca.it/center_news/marconi-issues-filesystems-0
https://www.hpc.cineca.it/center_news/marconi-issues-filesystems-solved-0

Feb 4: scheduled maintenance operations on Marconi on February 9th
https://www.hpc.cineca.it/center_news/marconi-scheduled-maintenance-february-9th
https://www.hpc.cineca.it/center_news/reminder-scheduled-maintenance-marconi-tomorrow-february-9th
https://www.hpc.cineca.it/center_news/marconi-maintenance-completed-2

Tickets escalated to **Intel** support

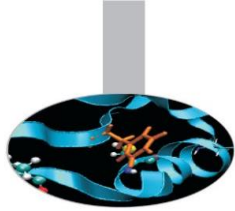
Ticket	Subject	Creation date	Last Updated by Intel	Comments
3932	Pointers to module arrays not working with SIMD (nilsm@ipp.mpg.de) serhiy.mochalskyy@ipp.mpg.de	18/09/2019 17:24:02	**31/07/2021 (Intel issue opened by CINECA)**	Intel originally found a bug on the compiler front end and solved it. They provided us an archive with the sources, BUILD script and the outputs of the reproducer that did not showed the issue. The first bug had "hidden" a second bug on the vectorizer that was triggered by the definition of the macro "USE_ARR_IN_MODULE" in the reproducer. We reported this issue to Intel that confirmed the problem and opened a new bug: Intel bug report CMPLRIL0-33599 Intel support has provided a resolution for the problem reported in the second bug: “”” We cannot use simd for a loop that has F90 pointer assignment inside. For every iteration of the loop, it is updating the same dope vector for f4a. That means there is a loop carried dependency preventing vectorization. If it is vectorized with veclen =2, for iteration 1 and 2, it is storing into the same location of the dope vector and the address code of f4a is picked up incorrectly. In order to generate the right code, it can run in a non-vector mode. However, attached is fixed.f90 which shows the right way to do it. We need to declare a structure of arrays to store the F90 pointers. In that way, every iteration is storing into different dope vectors. And, of course, the result from fixed.f90 is different because I used different computations in the loop.””” We reported to Intel support users’ feedback: “” Since I specifically made the f4a pointer private in my omp simd pragmas, it is very unexpected for them to still produce a loop carried dependency. Marking a variable as private is specifically defined as getting around it being a loop carried dependency. The struct of pointers, which fixes the problem, is exactly the kind of solution, the compiler should generate when encountering a pointer variable in a private clause. I hope this is the understanding of the Intel engineers as well, and they'll provide a fix in an upcoming release.”” **Intel oneAPI 2022.1 release has been installed on Marconi, should fix this bug, needs confirmation**

Tickets escalated to NVIDIA support



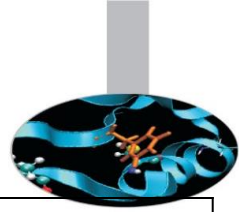
Ticket	Subject	Requestors	Created	Host	Supp. Level	Comments
18851	Problem with the nvidia compiler and -lnvc on m100	nilsm@ipp.mpg.de serhiy.mochalskyy@ipp.mpg.de	2021-06-23 11:00:02	M100	2nd NVDIA	The user report a strange behaviour referring to CUDA devices detection when adding (or not) the «-lnvc» flag for the compilation of a test code available on the latest hpc-sdk compiler suite on Marconi100 cluster. We performed some investigations that show that with and without the flag -lnvc the same libraries are linked, the only difference is in the order of the linkage. We are in contact the nvidia support for discussion.
19978	OpenACC compiler problem with function intermediates	nilsm@ipp.mpg.de serhiy.mochalskyy@ipp.mpg.de	2021-08-24 17:14:02	M100	2nd NVIDIA	The user provided a test code that is compiled using hpc-sdk/2021--binary module: “The compiler generates an intermediate, called get_arr1 , to store the result of the multiplication in line 26. This intermediate is copied to the device, as seen in the compiler output. Unfortunately, this intermediate needs to be private, as each thread needs its own copy. It is impossible to achieve that, as its name is not known, and it doesn't exist during compile time. Array b has the correct result as the result of the function call is saved in the variable c , so no intermediate is necessary. This problem emerges for all function calls to a device function that returns an array.” ***The issue was escalated to nvidia compiler engineers (a race condition is hypotized for the implicitly privatized fixed size local array). Three suggested workarounds.***

Tickets escalated to NVIDIA support



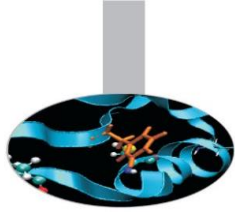
Ticket	Subject	Requestors	Created	Host	Supp. Level	Comments
19982	OpenACC compiler problem with writing back from the GPU	nilsm@ipp.mpg.de serhiy.mochalskyy@ipp.mpg.de	2021-08-24 17:44:02	M100	2nd NVIDIA	The user provided a test code that is compiled using hpc-sdk/2021--binary module; it do not generate expected results related to a copyout data clause. This problem seems related to the syntax used in the copyout data clause. To complete the analysis the issue has been reported to the nvidia support to ask for further clarifications. ***Due to initial users' request, nvidia implemented a non-OpenACC standard (see the workaround initially suggested to solve the problem). The most recent versions of the hpc-sdk toolkits restored the compliance to the standard, and have been installed on M100.***
20303	OpenACC compiler problem, unexpected implicit wait	nilsm@ipp.mpg.de serhiy.mochalskyy@ipp.mpg.de	2021-09-09 15:58:01	m100	2nd	This issue is still under investigation. We will also report it to nvidia if neccesary as soon as preliminary checks will be completed.

Other active tickets on HPC-US-SECOND



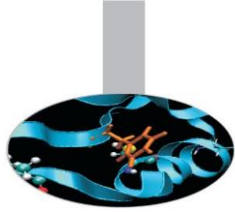
Ticket	Subject	Requestors	Created	Host	Supp. Level	Comments
18205	paraview on M100	mattwi@fysik.dtu.dk	2021-05-28 11:46:01	M100	Int.	The user reported issues when running paraview version available as module through a RCM session. To fix this is required a recompilation of paraview (we will include, if possible, the installation of the nvidia plugin index required also by this user). The installation of paraview is underway but it is showing issues. Also, we are in contact with nvidia to clarify the terms of the license required to install/run nvidia plugin index on M100 cluster.
20015	Device to device MPI communication with OpenMP4.5	asahi.yuichi@jaea.go.jp	2021-08-26 08:08:03	M100	2nd	The user report errors when trying to compile his code. This first error refers to a XLC++ version of the code that could compile and run correctly before the major update of the cluster. We helped the user into the compilation of the code by including a missing linking flag. The user confirmed that he can go on with the work. The second error reported refer to the usage of hpc-sdk compiler suite for the compilation of the same code (FATAL ERROR: “data in use_device clause was not found on device 1: host:0x2140dbf02), this is still under investigation. The user is able to work in any case that to the solution of the first problem.

Other active tickets on HPC-US-SECOND



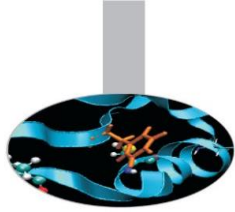
Ticket	Subject	Requestors	Created	Host	Supp. Level	Comments
21940	gcc/10 on marconi?	nicola.varini@epfl.ch	2021-11-10 18:04:01	SKL	2nd	The user has requested the installation on Marconi cluster of netcdf-fortran and hdf5 libraries, that need to be compiled with gcc/10 and mpi. The libraries have been installed and we are waiting for a feedback from the user.
23189	problema mamoria M100	giovanni.digiannatale@epfl.ch	2022-01-07 10:50:06	M100	2nd	The user is observing out of memory errors when running an ORB5 simulation, he is asking for 32 nodes for the run.The case he is running foresees 1600M particles, 32 nodes is on the edge. The user states that he can work with restarts, but has memory errors after a certain number of them. For testing purpose, he has been granted the qos_special to run with 48 nodes Ticket has been escalated to CINECA 2nd level support.
23515	Pointer issues at runtime	fwidmer@rzg.mpg.de	2022-01-18 16:54:01	M100	2nd	The user encounters errors of invalid pointers at the first simulation step of Orb5. The error happens when running simulations with collisions, while simulations without them work fine. We asked further details to the user and we suggested him to contact the EF high level support, since the issue seems code related.

Other active tickets on HPC-US-SECOND



Ticket	Subject	Requestors	Created	Host	Supp. Level	Comments
23627	QOSMaxCpuPerUserLimit	alberto.mariani@istp.cnr.it	2022-01-21 17:42:02	SKL	2nd	The user reports a problem with his jobs not starting, caused by an error that has promptly been fixed. He then moves the topic with MPI_ABORT called by GENE. We detected the part of the code that prompts the abort, it appears that the problem is on the user's side and is abot resource managing. Ticket likely to be closed soon..
23682	stale file handle Marconi	cas@ipp.mpg.de	2022-01-25 09:18:01	SKL	2nd	The user reports some cases of jobs with 128 nodes that crashed due to stale file handle. The investigation reported 2 nodes with issues that have been repaired since. The ticket is still open because the user keeps notifying similar issues with her job, the latest report being on Feb. 10th due to a general OPA instability reported also by other users.
24045	Question: rsync files	alejandro.guillevic@univ-lorraine.fr	2022-02-04 15:56:01	SKL	2nd	The user need to transfer big files from his local workstation to his scratch area on Marconi. We suggested to use the bdw_all_serial queue with rsync and to ask for a certificate to use GridFTP service.

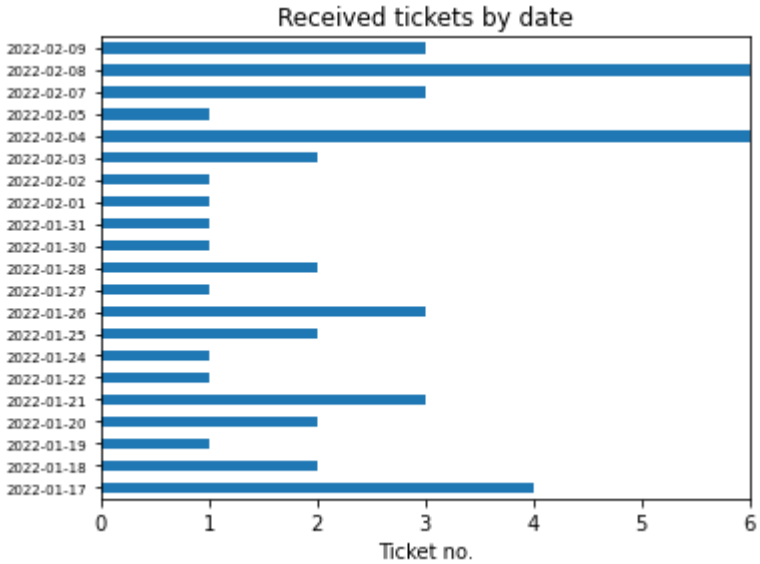
Other resolved tickets on HPC-US-SECOND

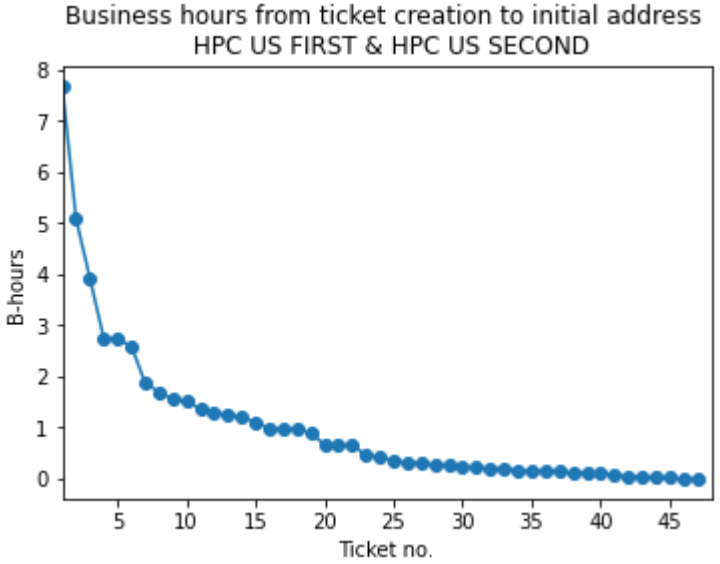


Ticket	Subject	Requestors	Created	Host	Supp. Level	Comments
20676	QdstrmImporter	huw.leggate@dcu.ie	2021-09-30 13:04:01	M100	2nd	The user reports that using nvsys the QdstrmImporter step fails for the qdstrm files.He tried also the execution of QdstrmImporter from the command line obtaining the same result. He is attempting to use openmp offloading with the default gcc 8.4.0, that appears to have been built without offloading enabled, and he suspects that may be causing the crash. While gcc 8.4.0 has been updated and now supports offloading, the problem was solved when the user modified his code so that the error with nvprof disappeaered.
22068	ottimizzazione job sottomesso	giovanni.giannatale@epfl.ch	2021-11-16 12:02:01	M100	2nd	The user is observing out of memory errors when running an ORB5 simultation, he is asking for 32 nodes for the run.The case he is running foresees 1600M particles, 32 nodes is on the edge. Closed because it continues in #23189

Ticket Statistics Jan 14 - Feb 09

HPC-US-FIRST & HPC-US-SECOND

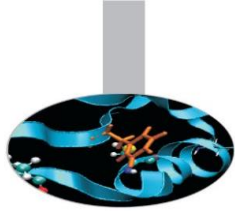


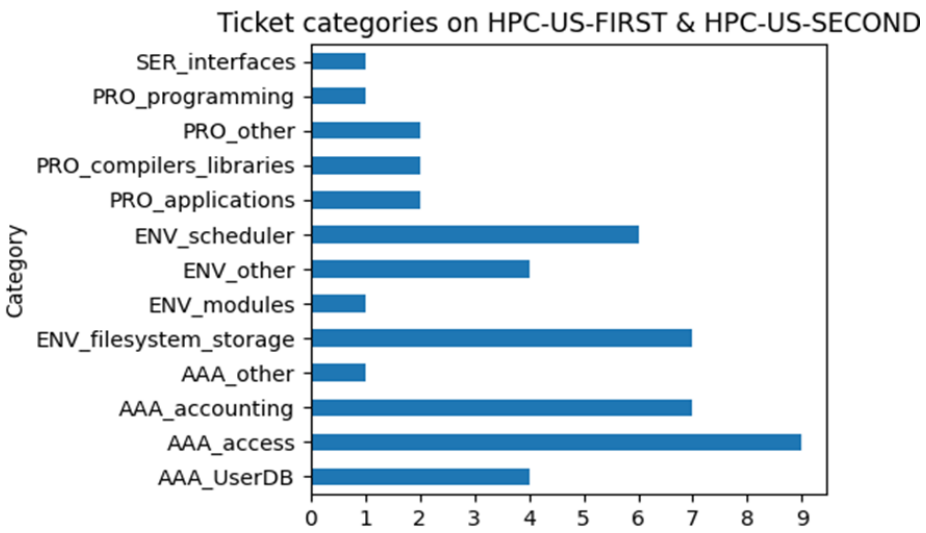


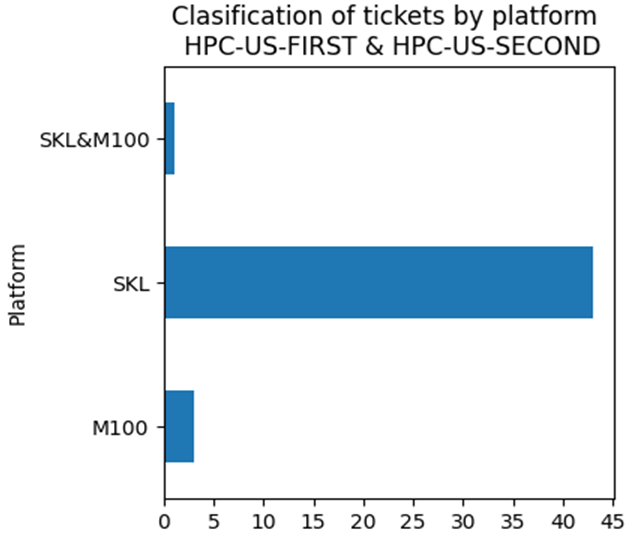
TOTAL	-> **47** tickets
- HPC-US-FIRST	-> **31**
- escalated to HPC-US-SECOND	-> **16**

Ticket statistics Jan 14 - Feb 09

HPC-US-FIRST & HPC-US-SECOND

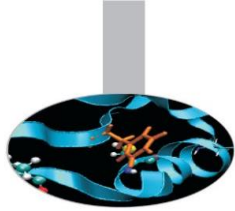


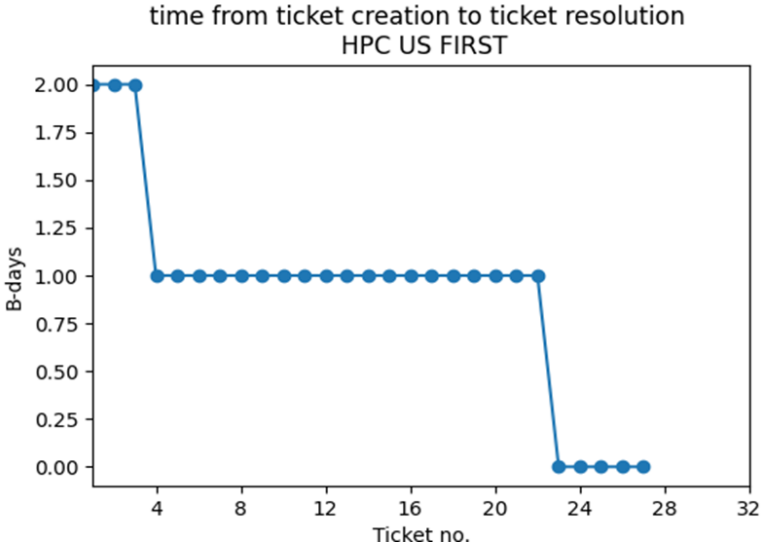


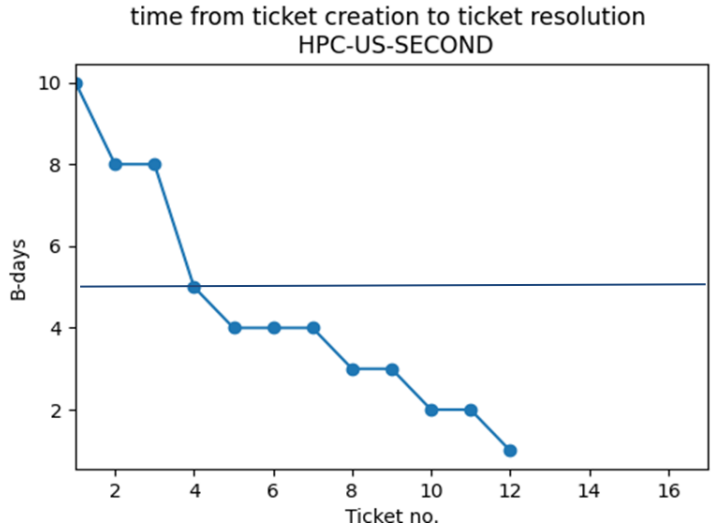


Ticket statistics Jan 14 - Feb 09

HPC-US-FIRST & HPC-US-SECOND



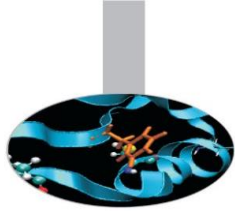




27 resolved tickets

12 resolved tickets

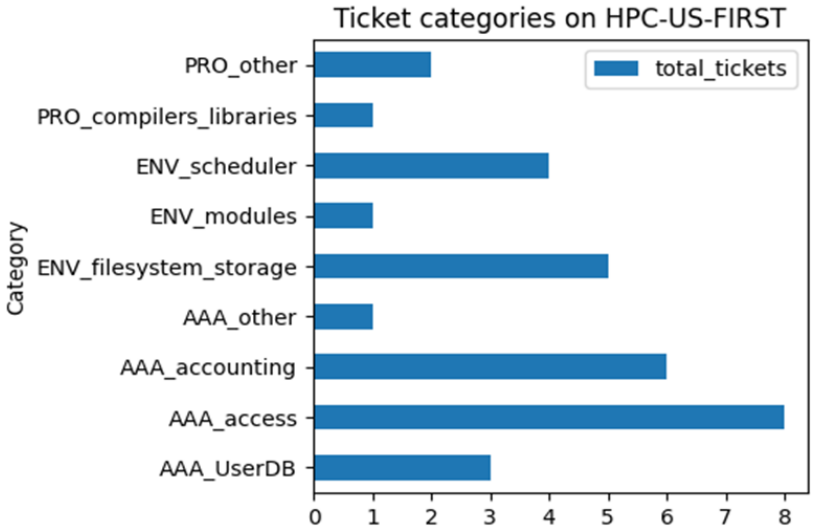
Ticket statistics Jan 14 - Feb 09

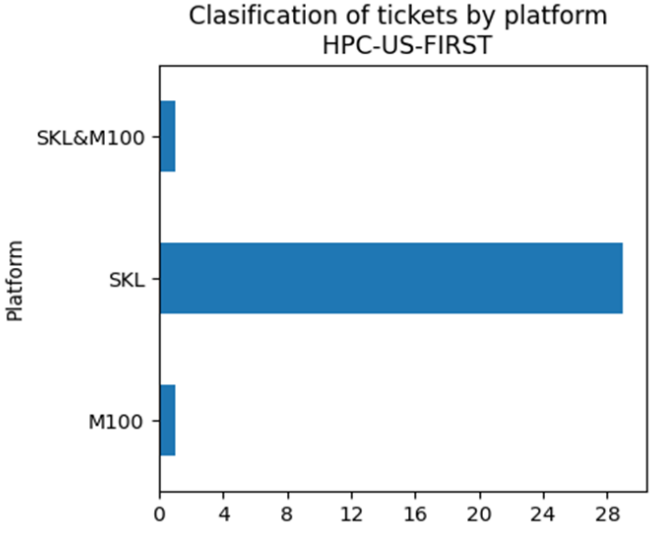


Ticket SECOND	Days	Creation time	Requestor	Subject	Notes
23493	10	2022-01-18 09:54:02	marco.veranda@igi.cnr.it	domanda compilazione gfortran + OpenAcc su M100	The user has problems when compiling his code with gnu 8 and OpenACC support, related to the version of the compiler too old to accept some falgs for the architecture. The problem is solved by moving to the hpc-sdk compiler suite.
23825	8	2022-01-28 11:52:02	adisi@ipp.mpg.de	extension project ROBIN	The user asks for an extension of 1M hours to the budget of his project. The request has been forwarded to the Allocation Committee, that denied it due to the current Eurofusion call coming to a close.
23884	8	2022-01-31 09:44:01	hari.umashankar@ubc.ca	VASP 5.4.4 license on M100 cluster	The user asks for being added to the group of users that can use VASP5 on M100, being in possession of a licence. After having granted access, he received assistance about the setup of their simulation job.

Ticket statistics Jan 14 - Feb 09

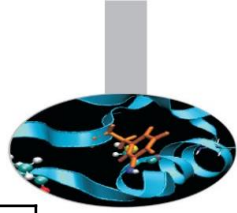
HPC-US-FIRST





Ticket statistics Dec 12 – Jan 13

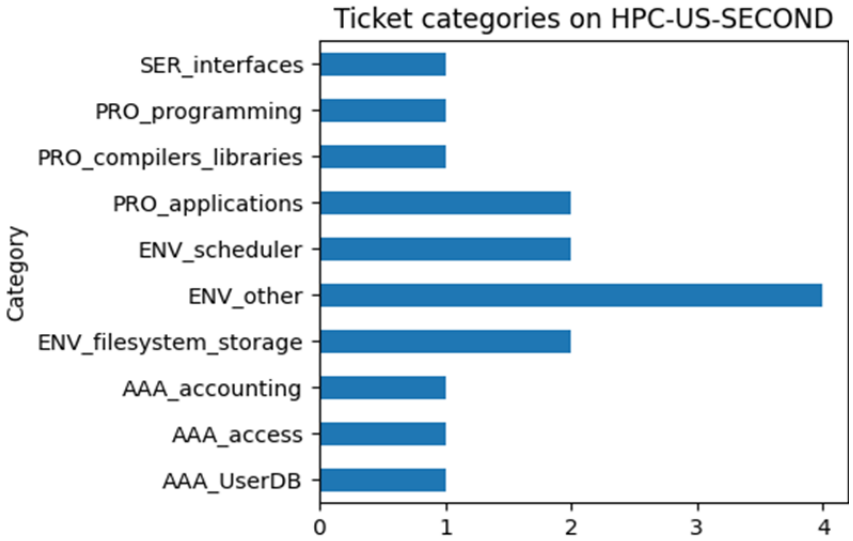
HPC-US-FIRST

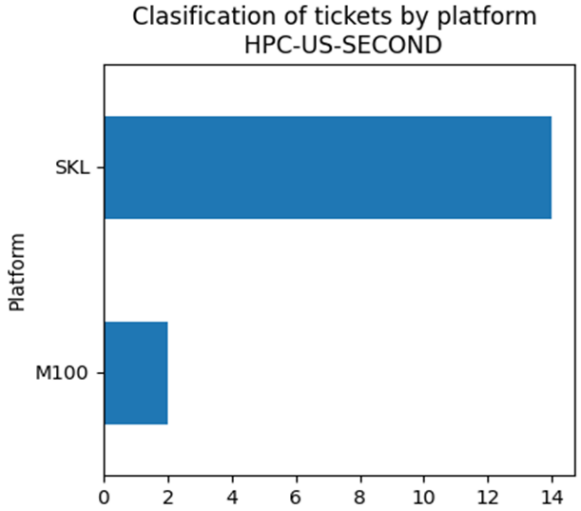


HPC-US-SECOND			By status			By platform		
			open	resolved		M100	SKL	SKL&M100
Information	AAA_access			1			1	
	AAA_accounting		1	5			6	
	AAA_other			1			1	
	ENV_filesystem_storage			1		1		
	ENV_scheduler			1			1	
Problem	AAA_access		1				1	
	ENV_filesystem_storage			3			3	
	ENV_scheduler			2			2	
	PRO_compilers_libraries			1			1	
	PRO_other			2			2	
Service Request	AAA_UserDB		1	2			3	
	AAA_access			6			5	1
	ENV_filesystem_storage			1			1	
	ENV_modules		1				1	
	ENV_scheduler			1			1	
total	**31**		**4**	**27**		**1**	**29**	**1**

Ticket statistics Jan 14 - Feb 09

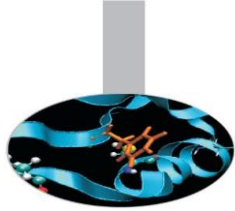
HPC-US-SECOND





Ticket statistics Jan 14 - Feb 09

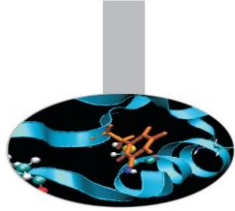
HPC-US-SECOND



HPC-US-SECOND		By status		By platform	
		open	resolved	M100	SKL
Information	AAA_UserDB		1		1
	SER_interfaces		1		1
Problem	AAA_access		1	1	
	ENV_filesystem_storage	1			1
	ENV_other	1	3		4
	ENV_scheduler	1	1		2
	PRO_applications	1			1
	PRO_compilers_libraries		1	1	
Service Request	AAA_accounting		1		1
	ENV_filesystem_storage		1		1
	PRO_applications		1		1
	PRO_programming		1		1
total	**16**	**4**	**12**	**2**	**14**

Module usage on Marconi-SKL

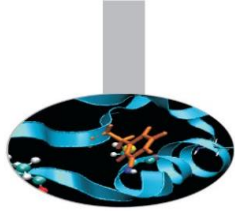
January 2022



category	modulename	partition	qos	module_load_count	elapsed_timelimit_sum
application	openfoam	skl_fua_prod	normal	2	1,42
	openfoam-ext	skl_fua_prod	normal	6	1,38
	qe	skl_fua_prod	normal	540	78,17
	starccm+	skl_fua_dbg	normal	4	2,17
		skl_fua_prod	normal	190	160,37
	vasp	skl_fua_prod	normal	451	198,71

Module usage on Marconi-SKL

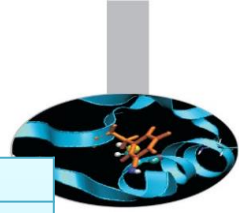
January 2022



category	modulename	partition	qos	module_load_count	elapsed_timelimit_sum
compiler	gnu	skl_fua_dbg	normal	8	1,15
		skl_fua_prod	normal	1682	864,81
	intel	skl_fua_dbg	normal	2	1,49
		skl_fua_prod	normal	145	75,7
			skl_qos_fualowprio	2	1,09
		skl_sys_test	qos_test	16	4,68
	intelmpi	skl_fua_dbg	normal	2	1,49
		skl_fua_prod	normal	143	74,69
			skl_qos_fualowprio	2	1,09
		skl_sys_test	qos_test	16	4,68
	julia	skl_fua_prod	skl_qos_fuabprod	10	6,01
	openmpi	skl_fua_dbg	normal	7	0,97
		skl_fua_prod	normal	1636	858,45
	python	bdw_all_serial	normal	40	34,4
		skl_fua_prod	normal	202	102,64
			skl_qos_fuabprod	88	62,21

Module usage on Marconi-SKL

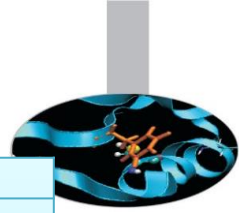
January 2022



category	modulename	partition	qos	module_load_count	elapsed_timelimit_sum
tool	anaconda	bdw_all_serial	normal	39	33,39
		skl_fua_prod	normal	15	6,63
			skl_qos_fuabprod	32	20,87
	cmake	bdw_all_serial	normal	14	12,08
		skl_fua_dbg	normal	6	4,25
		skl_fua_prod	normal	155	61,49
			skl_qos_fuabprod	4	2,14
			skl_qos_fualprod	158	30,92
	cubegui	skl_fua_prod	normal	139	73,57
			skl_qos_fuabprod	58	29,63
	idl	bdw_all_serial	normal	31	27,24
		skl_fua_dbg	normal	7	2,54
		skl_fua_prod	normal	20	10,72
			skl_qos_fualowprio	2	1,09
	scalasca	skl_fua_prod	normal	139	73,57
			skl_qos_fuabprod	58	29,63
	scorep	skl_fua_prod	normal	139	73,57
			skl_qos_fuabprod	58	29,63
	vtune	skl_fua_dbg	normal	20	8,62
		skl_fua_prod	normal	9	2,7

Module usage on Marconi-SKL

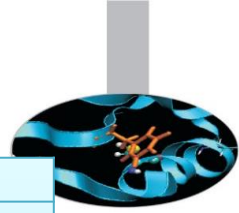
January 2022



category	modulename	partition	qos	module_load_count	elapsed_timelimit_sum
library	blas	bdw_all_serial	normal	31	27,24
		skl_fua_dbg	normal	24	6,12
		skl_fua_prod	normal	598	252,99
			skl_qos_fualowprio	34	13,92
	boost	skl_fua_prod	normal	11	4,08
	cubelib	skl_fua_prod	normal	139	73,57
			skl_qos_fuabprod	58	29,63
	fftw	bdw_all_serial	normal	14	12,08
		skl_fua_dbg	normal	37	8,96
		skl_fua_prod	normal	1143	579,45
			skl_qos_fuabprod	176	116,59
			skl_qos_fualowprio	36	15,01
			skl_qos_fualprod	158	30,92

Module usage on Marconi-SKL

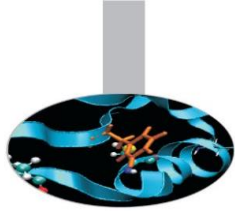
January 2022



category	modulename	partition	qos	module_load_count	elapsed_timelimit_sum
library	hdf5	skl_fua_dbg	normal	286	50,69
		skl_fua_prod	normal	1920	978,84
			skl_qos_fuabprod	150	93,99
			skl_qos_fualprod	225	41,63
	lapack	bdw_all_serial	normal	31	27,24
		skl_fua_dbg	normal	24	6,12
		skl_fua_prod	normal	515	222,78
			skl_qos_fualowprio	34	13,92
	metis	skl_fua_prod	normal	6	1,38
	mkl	skl_fua_dbg	normal	1	1,02
		skl_fua_prod	normal	138	72,69
			skl_qos_fualowprio	2	1,09
		skl_sys_test	qos_test	16	4,68

Module usage on Marconi-SKL

January 2022



category	modulename	partition	qos	module_load_count	elapsed_timelimit_sum
library	nag	bdw_all_serial	normal	2	2,01
	netcdf	skl_fua_dbg	normal	240	45,34
		skl_fua_prod	normal	828	282,76
			skl_qos_fuabprod	92	64,36
			skl_qos_fualprod	67	10,7
	netcdf-cxx4	skl_fua_dbg	normal	206	41,31