

HPRC User Software

The following points are related to the installation of software for use on the HPC cluster:

1. Generally, [software is installed/upgraded upon request only](#).
2. HPC staff will install the latest [stable](#) version of software you have require installed or upgraded.
3. HPC staff will attempt to install all software under [environment modules](#) control. Exceptions will only occur when new HPC images are deployed (rarely).
4. Software will not be installed or upgraded if there is a risk of system/service failure, as assessed by HPC and/or eResearch staff.

The most up to date version of scientific software installed on HPC cluster nodes can be obtained by logging onto `zodiac.hpc.jcu.edu.au` (using an SSH client) and using the following command:

```
module avail
```

The list of installed software will be quite long. The environment for a given software package can usually be setup using one of the commands:

```
module load <software>
module load <software>/<version>
```

where `<software>` is replaced by the module name and, if required, `<version>` is replaced by the specific version desired.

Operating Systems

JCU HPC cluster nodes are built on the **RedHat Enterprise Linux** (RHEL 6.x) operating system. There are two main reasons for this choice:

1. Hardware maintenance agreements that JCU pays for require use of a commercially support operating system.
2. JCU ICT has signed up to a RedHat CAUDIT agreement for licensing of RHEL systems and seek to maximize their return on investment.

JCU HPC also runs a small VMware ESXi cluster (2 servers) that can be used to deliver *small* Windows systems to satisfy eResearch requirements that cannot be solved on Linux (e.g., web services, databases, or Windows compute). Researchers wanting to run other flavours of Linux (e.g., Ubuntu) should look to taking advantage of NeCTAR resources.

HPC Cluster Software Catalogue

Yellow shaded shells indicate that the software version is only available through use of environment modules.

Shells	
Software	Version
bash	4.1.2
dash	0.5.5.1
ksh	20120801
tcsh	6.17

Compilers	
Software	Versions
GNU	4.4.7
	4.9.3
	5.3.0
	6.1.0

Compilers / Interpreters	
Software	Versions
java	sun-1.6.0.25 , oracle-jdk-7u67 , oracle-jdk-8u20

matlab		2008b , 2013a , 2014a , 2014b , 2015a , 2016a
perl	5.10.1	
python	2.6.6	2.7 , 2.7.3 , 3.5.1
R		2.15.1 , 3.0.0 , 3.2.2
ruby	1.8.7.374	
tcl	8.5.7	
tk	8.5.7	

Further detail on MATLAB toolboxes and R addons/plugins can be found toward the bottom of this page.

Libraries (only)

Software	Versions	
atlas	3.8.4	
blas	3.2.1	3.6.0
boost	1.41.0	1.61.0
gmp*	4.3.1	6.1.0
lapack		3.6.0
mpc*		1.0.3
mpfr*	2.4.1	3.1.4

* gmp, mpc, & mpfr libraries may be built into GNU compilers (not necessarily the above versions though).

Scientific Software

Software	Version
4ti2	1.3.2
abyss	1.3.2
allpathslg	44837
ariadne	1.3
arlequin	3.5
asap	4.0.0
bayesass	1.3
beagle	1.1.0
beast	1.6.1
BEDTools	2.15.0
bamtools	31
blast	2.2.29 , 2.3.0

Software	Version
4ti2	1.3.2
abyss	1.3.2
bayesass	1.3
BamTools	3
Software	Version(s)
4ti2	1.3.2
abyss	1.3.2
bayesass	1.3
BamTools	3
Software	Version(s)
4ti2	1.3.2
abyss	1.3.2
bayesass	1.3
BamTools	3
Software	Version(s)
targetp	
tmap	
tmhmm	
topali	
towhee	
trans-abyss	
transrate	1.0.2
trinityrnaseq	
trinotate	3.0.1
udunits	1.12.11
udunits2	2.1.19
velvet	1.2.10
w2rap-contigger	
wcslib	4.13.4
wise2	2.2.0
wwatch3	
xfig	3.2.5
yasm	1.2.0
zlib	1.2.8
zonation	3.1.9, 4.0.0

Software Catalogue

Please note that there is an almost endless list of scientific software that could be installed on HPC systems. Unless a request is received, HPC staff do not try to guess what software (inc. version) you need/want to use. While you may be able to install software yourself, generally you should avoid doing this - it is an unsustainable practice in terms of power, cost, and time (whole of JCU view). Additionally, software installed by HPC staff will reside on a different filesystem to where users home directories are located - improving performance at times of high IO load on filesystem(s) containing home directories. Extra information about software highlighted by a light green background colour is supplied at the end of this page.

	Access Command	Version		Access Command	Version		Access Command	Version			
B	module load bfast	0.6.5a		module load blacs	1.1		module load blas	3.2.1		module load blast	2.2.29
	module load blcr	0.8.5		module load bowtie	1.0.0		module load bowtie2	2.2.4		module load bwa	0.7.4
C	module load caftools	2.0.2		module load cap3			module load carthagene	1.2.2		module load casacore	1.4.0
	module load cd-hit	4.6.1		module load cernlib	2006		module load cfitsio	3.030		module load chlorop	1.1
	module load clipper	2.1		module load clustalw	2.0.12		module load cluster	1.49		module load cns	1.3
	module load coils	2.2		module load colony2			module load consel	0.1k		module load cricmap	2.504a
	module load crimap_Monsanto			module load cufflinks	2.2.1						
D	module load dx	4.4.4									
E	module load elph	1.0.1		module load EMBOSS	5.0.0		module load enmtools	1.3		module load express	
F	module load fasta			module load fastme			module load fastStructure			module load ffmpeg	
	module load fftw			module load fftw2			module load fftw3				
G	module load garli			module load gdal			module load glimmer			module load glimmer	
	module load GMT			module load gnuplot			module load gpp4			module load grass	
	module load gromacs			module load gsl							
H	module load hdf	4.2.5		module load hdf5	1.8.5		module load hmmer				
I	module load ima2										
J	module load jmodeltest										
L	module load lagan			module load lamarc			module load lapack			module load lisa	
M	module load Macaulay2			module load matlab			module load maxent			module load maxima	
	module load migrate			module load mira			module load molphy			module load mpich2	
	module load mrbayes			module load mrmotest			module load msbayes				
N	module load ncl			module load netcdf			module load netpbm			module load netphos	
	module load numpy										
O	module load oases			module load octave			module load ogdi			module load openmpi	
P	module load pari			module load paup			module load proj			module load pvm	
R	module load R			module load r8s			module load rsem			module load rplots	
S	module load scalapack			module load scipy			module load seadas			module load seg	
	module load signalp			module load sprng			module load ssaha2			module load structure	
	module load suitesparse										

Wine <http://www.winehq.org/>

https://upc-bugs.lbl.gov/blcr/doc/html/BLCR_Users_Guide.html

<https://github.com/bli25wisc/rsem>

M

MATLAB Components/Toolboxes

Component	License allows	Toolbox	License allows
MATLAB	50 user connections	Control System	50 user connections
MATLAB Coder	50 user connections	Optimization	50 user connections
Simulink	50 user connections	Signal Processing	50 user connections
Simulink Coder	50 user connections	Symbolic Math	50 user connections
Simulink Control Design	50 user connections	System Identification	50 user connections
		Mapping	5 user connections
		Neural Network	5 user connections
		Statistics	5 user connections
		Distributed Computing	4 user connections
		Fuzzy Logic	4 user connections
		Global Optimization	4 user connections
		Image Processing	4 user connections
		MATLAB Compiler	4 user connections
		Wavelet	4 user connections

R

R Packages

A: abind, acepack, actuar, ade4, ade4TkGUI, adehabitat, AER, akima, alr3, anchors, ape
B: base, bdsmatrix, biglm, BIOMOD, Biobase, bitops, boot, BufferedMatrix
C: car, caTools, chron, CircStats, class, clim.pact, cluster, coda, codetools, coin, colorspace, compiler, CompQuadForm, coxme, cubature
D: DAAG, datasets, DBI, degreenet, deldir, Design, digest, diptest, DynDoc, dynlm
E: e1071, Ecdat, effects, ellipse, ergm, evaluate, expm
F: fBasics, fCalendar, fEcofin, fields, flexmix, foreach, foreign, Formula, fSeries, fts, fUtilities
G: gam, gbm, gclus, gdata, gee, geoR, geoRglm, ggplot2, gpclib, gplots, graphics, grDevices, grid, gtools
H: hdf5, hergm, hexbin, Hmisc, HSAUR
I: igraph, ineq, inline, ipred, iquantitator, ISwR, iterators, itertools, its
K: kernlab, KernSmooth, kinship
L: latentnet, lattice, leaps, limma, lme4, lmtest, locfit, logspline
M: mapproj, maps, maptools, mAr, marray, MASS, Matrix, matrixcalc, MatrixModels, maxLik, mboost, mclust, MCMCpack, mda, MEMSS, methods, mgcv, mice, misc3d, miscTools, mitools, mix, mlbench, mlmRev, mlogit, modeltools, moments, MPV, msm, multcomp, multicore, mutatr, mvtnorm
N: ncdf, network, networksis, nlme, nnet, norlrmix, np, numDeriv, nws
O: oz
P: parallel, party, PBSmapping, permute, pixmap, plm, plyr, png, prabclus, proto, pscl
Q: qtl, quadprog, quantreg
R: RandomFields, randomForest, RANN, RArcInfo, raster, rbenchmark, rcolony, RColorBrewer, Rcpp, RcppArmadillo, ReadImages, relevent, reshape, rgdal, rgenoud, rgeos, rgl, Rglpk, rjags, rlecuyer, rmeta, robustbase, ROCR, RODBC, rpanel, rpart, RSQLite, RUnit
S: sampleSelection, sandwich, scatterplot3d, SDMTTools, sem, sfmisc, sgeostat, shapefiles, shapes, slam, sm, sna, snow, snowFT, sp, spam, SparseM, spatial, SpatialTools, spatstat, spdep, splancs, splines, statmod, statnet, stats, stats4, stringr, strucchange, subselect, survey, survival, systemfit
T: tcltk, tcltk2, TeachingDemos, testthat, timeDate, timeSeries, tis, tkrplot, tools, tree, tripack, truncreg, trust, TSA, tseries, tweedie
U: urca, utils
V: vcd, vegan, VGAM, VIM
W: waveslim, wavethresh, widgetTools
X: XML, xtable, xts
Z: Zelig, zoeppritz, zoo

Linux Shells

The following Linux shells are available on HPC systems (`bash` is the default):

<code>bash</code>	<code>csch</code>	<code>dash</code>	<code>ksh</code>	<code>tcsh</code>	<code>zsh</code>
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Compression Utilities

The following archiving/compression applications are available on HPC systems:

<code>7za</code>	<code>bzip2</code>	<code>gzip</code>	<code>pbzip2</code>	<code>tar</code>	<code>unzip</code>	<code>xz</code>	<code>zip</code>
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Note that the versions of `zip` and `unzip` installed on HPC have an upper size limit of 2GB. Most active HPC users consume significantly more than 2GB of disk space. If you need assistance with using `tar`, please contact HPC staff.

Information for ITR staff

1. Environment module files are located in `/sw/modules`
2. Most scientific software is installed in `/sw/<software>/<version>/`
3. Components used by programmers (e.g., stand-alone libraries) are generally installed in `/sw/common/`. Installation of frequently required libraries is additionally done onto local system disks (using `yum`), if libraries are available in repositories.
4. *Live* upgrades of software should only be performed when no login/compute node is using the software. Compute nodes should be reimaged rather than have live upgrades performed. The login node may need to be live upgraded, due to jobs always running on this system.
5. Some packages (e.g., BLCR) are rebuilt from source RPMs. BLCR, in particular, needs to be recompiled for each new kernel installed.

Operating Systems

The following table provides information about operating systems used on physical servers managed (in some way) by HPC staff.

Operating System	Primary service(s) provided	Typically accessed from
RedHat Enterprise Linux 6.x	HPC login nodes	Desktop or Laptop computers
	HPC compute nodes	HPC login nodes
SUSE Linux Enterprise Server 11.x	CIFS fileshares	Desktop or Laptop computers
	NFS fileshares	HPC login and compute nodes
Windows 2012 Server	CIFS fileshares	Desktop or Laptop computers (Cairns)

Vendors usually require an enterprise O/S be installed on physical servers if you have purchased maintenance.

JCU researchers wishing to host servers/storage in a datacentre **must** contact ITR management before purchasing is even considered.

All virtual machines (VMs) offered by HPC are, by default, provided as *Infrastructure as a Service* (IaaS). VM owners are responsible for daily maintenance operations on their VMs. For security reasons, all systems are registered for application of automatic updates. HPC staff will apply patches /updates (from RedHat and EPEL repositories only) to VMs where the automatic update process fails.

Internal (conducted by ITR) and external security audits take place on all publicly visible systems at times determined by ITR management. VM owners are responsible for fixing any security concerns identified in these audits. HPC staff may be consulted or be asked to provide assistance with such fixes.