Package Programs List

Compilers and Libraries

(Status on Apr 6, 2021.) Most packages are installed under /local/apl/lx.

Name	Version	misc info
Intel Parallel Studio XE	2020 update 2	icc 19.1.2
		icpc 19.1.2
		ifort 19.1.2
		impi 2019.0.8 (2019.8.254)
	2019 update 5	icc 19.0.5
		icpc 19.0.5
		ifort 19.0.5
		impi 2019.0.5 (2019.5.281)
	2019 update 1	icc 19.0.1
		icpc 19.0.1
		ifort 19.0.1
		impi 2019 Update 1 (2019.1.144)
	2018 update 4*	icc 18.0.5
		icpc 18.0.5
		ifort 18.0.5
		impi 2018.0.4
	2018 update 2	icc 18.0.2
		icpc 18.0.2
		ifort 18.0.2
		impi 2018.0.2
	2017 update 8	icc 17.0.8
		icpc 17.0.8
		ifort 17.0.8
		impi 2017.0.4
	2017 update 4	icc 17.0.4
		icpc 17.0.4
		ifort 17.0.4
		impi 2017.0.3
	2015 update 1	icc 15.0.1
		icpc 15.0.1
		ifort 15.0.1
		impi 5.0 Update 2
GCC	4.8.5*	
	9.3.1	Devtoolset-9 Software Collections[2]
	8.3.1	Devtoolset-8 Software Collections[2]
	7.3.1	Devtoolset-7 Software Collections[2]
	6.3.1	Devtoolset-6 Software Collections[2]
	5.3.1	Devtoolset-4 Software Collections[2]
	4.9.2	Devtoolset-3 Software Collections[2]
PGI Compilers and Tools	20.4-0*	
	18.1-1	
	17.5-0	
	16.5-0	
CUDA	11.1.105*	
	10.1.243	
	9.1.85	
	8.0.61	
	3.6.8	(default version for python3)
	3.4.10	
	2.7.5*	

Name	Version	misc info
Python[1]	3.7.7 (Anaconda3-2020.02)	
	3.7.3 (Anaconda3-2019.03)	
	2.7.16 (Anaconda2-2019.03)	
Julia	1.5.3	/local/apl/lx/julia-1.5.3/bin/julia
	1.3.1	/local/apl/lx/julia-1.3.1/bin/julia
Open MPI	4.0.2	(mpi1 and cxx support enabled)
	4.0.0	(cxx support enabled)
	3.1.0	
	2.1.3	
Singularity	3.7.1	

*: default version
[1]: you can install packages in your home directory by using "pip install (package name) --user" command. Installation of Anaconda (to the homedir) is also recommended. Miniconda might be better if you want to avoid long wait time upon loading anaconda env (current RCCS file system is not good at handling many small files).
[2]: installed under /opt/rh/devtoolset-(version-number). For example, you can load gcc-6.3.1 environment conveniently by "module load scl/devtoolset-6".

Application Software

(Aug. 23, 2021) The following packages are installed in the system. Please see the official documents/manuals for the detailed usage. These packages are installed under /local/apl/lx directory of the frotend hosts and calculation nodes. See this page for detailed information about installation.

name	description
ABINIT	Package for material science within density functional theory, using a plane wave basis set and pseudopotentials.
AlphaFold	AI program for predictions of protein structure.
AMBER	Package of molecular simulation programs.
AutoDock	Suite of automated docking tools.
CP2K	A quantum chemistry and solid state physics software package.
CRYSTAL	General-purpose programs for the study of crystalline solids.
DIRAC	Computes molecular properties using relativistic quantum chemical methods (named after P. A. M. Dirac).
GAMESS	General atomic and molecular electronic structure system.
Gaussian	Ab initio molecular orbital calculations.
GENESIS	Molecular dynamics and modeling software for bimolecular systems such as proteins, lipids, glycans, and their complexes.
GROMACS	Fast, Free and Flexible MD
GRRM	Automated Exploration of Reaction Pathways.
LAMMPS	Large-scale Atomic/Molecular Massively Parallel Simulator.
OpenMolcas	Quantum chemistry software.
Molpro	Complete system of ab initio programs.
NAMD	Scalable molecular dynamics program.
NBO/NBOView	Discovery tool for chemical insights from complex wavefunctions.
NTChem(*17)	Comprehensive new software of ab initio quantum chemistry made in AICS from scratch.
NWChem	Computational chemistry tools that are scalable both in their ability to treat large scientific computational chemistry problems
ORCA	An ab initio quantum chemistry program package
PSI4	Open-source suite of ab initio quantum chemistry programs designed for efficient, high-accuracy simulations of a variety of molecular properties.
Quantum ESPRESSO	Integrated suite of Open-Source computer codes for electronic-structure calculations and materials modeling at the nanoscale.
Reaction Plus	Program to obtain the transition state and reaction path along the user's expected reaction mechanism.
SIESTA	Efficient electronic structure calculations and ab initio molecular dynamics simulations of molecules and solids
SMASH	Scalable Molecular Analysis Solver for High performance computing systems
TURBOMOLE	One of the fastest programs for standard quantum chemical applications.
GaussView	Viewer for Gaussin 03 / 09.
Luscus	A portable GUI for MOLCAS and other quantum chemical software.
Molden	Visualization program of molecular and structure.
VMD	Molecular graphics viewer

name	version	status (install date)	notes
ABINIT	8.8.3	◎ (2018/7/10)	
	7.8.2	-	
ADF(*9)		(unavailable)	
	2 (20210819)	○ (2021/8/23)☆	(latest snapshot on Aug 19, 2021)

name	version	status (install date)	notes
AlphaFold	2 (20210720)	○ (2021/7/26)☆	(latest snapshot on Jul 20, 2021)
Amber	20-update9	○ (2021/2/24)☆	P100, V100 supported
	20-update0	○ (2020/6/9)☆	P100, V100 supported
	18-bugfix16	◎ (2019/9/10)☆	P100, V100 supported
	18-bugfix12	○ (2019/2/14)☆	P100, V100 supported
	18-bugfix11-volta	○ (2019/2/14)☆	V100 supported
	18-bugfix1	○ (2018/6/4)☆	P100, V100 supported
	16-bugfix15	○ (2018/7/25)☆	P100 supported
	16-bugfix10	○ (2017/10/01)☆	P100 supported
	14-bugfix11	○ (2015/7/21)	
	12-bugfix21	○ (2013/12/10)	
AutoDock	4.2.6	-	
CP2K	8.2.0	○ (2021/6/22)	without ELPA/COSMA
	8.1.0	(skipped)	Apparently slower than previous version. (10-20%(gcc)/~30%(intel) slower even without COSMA)
	7.1.0	◎ (2020/2/27)‖ Intel/GNU	
	6.1.0	○ (2018/11/22)☆‖ Intel/GNU	P100, V100 supported
CRYSTAL	17-1.0.2(*21)	○ (2020/1/27)	
	14-1.0.4(*18)	○ (2016/5/11)	
DIRAC(*19)	19.0	○ (2021/5/19)	
	18.0	◎ (2019/5/14)	
GAMESS	2021-R1(Jun30)	○ (2021/8/19)△	
	2020-R1(Jun30)	◎ (2020/8/19)△	
	2019-R2(Sep30)	○ (2019/12/13)△	
	2018-Sep30	○ (2018/11/9)▲	
	2018-Feb14	○ (2018/3/19)▲	
	2017-Nov11	○ (2017/12/15)	
	2017-Apr20(*11)	○ (2017/10/1)	
Gaussian	16.C.01	◎ (2019/8/2)☆▲△	P100, V100 supported
	16.B.01	○ (2018/3/12)☆▲	P100 supported
	16.A.03	○ (2017/2/13)▲	
	09.E.01	◎ (2015/12/24)	
	09.D.01	○ (2013/7/25)▲	
	09.C.01	○ (2012/2/1)	
	09.B.01	○ (2012/2/7)	
GENESIS	1.6.0	◎ (2020/12/28)☆ CPU/GPU	P100, V100★ supported
	1.4.0	○ (2019/11/21)☆ CPU/GPU	P100, V100★ supported
	1.3.0	○ (2018/9/4)☆ CPU/GPU	P100, V100★ supported
	1.1.6	○ (2017/12/13)☆ CPU/GPU	P100, V100★ supported
	1.1.5	○ (2017/8/4)	
	2021.2	○ (2021/5/13)☆‖ GNU: cpu/gpu Intel: cpu/gpu	P100, V100 supported

name	version	status (install date)	notes
GROMACS	2020.6	◎ (2021/3/8)☆‖ Intel: cpu/gpu GNU: cpu/gpu	P100, V100 supported
	2020.4	○ (2020/10/12)☆‖ I:c/I:g/G:c/G:g	P100, V100 supported
	2020.2	○ (2020/5/13)☆‖ I:c/I:g/G:c/G:g	P100, V100 supported
	2019.6	○ (2020/3/5)☆‖ I:c/I:g/G:c/G:g	P100, V100 supported
	2019.4	○ (2019/10/8)☆‖ I:c/I:g/G:c/G:g	P100, V100 supported
	2019.2	○ (2019/4/18)☆‖ I:c/I:g/G:c/G:g	P100, V100 supported
	2018.8	○ (2019/10/8)☆‖ I:c/I:g/G:c/G:g	P100, V100 supported
	2018.7	○ (2019/7/19)☆‖ I:c/I:g/G:c/G:g	P100, V100 supported
	2018.6	○ (2019/3/27)☆‖ I:c/I:g/G:c/G:g	P100, V100 supported
	2018.3	○ (2018/9/4)☆‖ I:c/I:g/G:c/G:g	P100, V100 supported
	2018.1	○ (2018/4/17)‖ I:c/G:c	GPU versions (intel and gcc) are not installed, since they fail on some tests. (tip4p for intel15-cuda8, lj-pme for gcc5-cuda8)
	2016.6	○ (2019/2/22)☆‖ I:c/I:g/G:c/G:g	P100, V100 supported
	2016.5	○ (2018/4/17)☆‖ I:c/I:g/G:c/G:g	P100, V100★ supported
	2016.4	○ (2017/10/01)☆	P100, V100★ supported
	2016.3	○ (2017/3/16)☆	P100, V100★ supported
	2016.1	○ (2017/2/2)☆	P100, V100★ supported
	5.1.5	○ (2018/4/17)☆‖ I:c/I:g/G:c/G:g	P100, V100★ supported SelectionCollectionDataTest.HandlesCharge unittest failed on intel, single precision version due to a tricky numerical error
	5.1.4	○ (2018/1/19)☆	P100, V100★ supported
	4.5.5	○ (2012/6/12)☆	
GRRM(*5)	17	◎ (2021/1/27)	(multi-node parallel enabled)
	14	○ (2015/7/29)	
	11	○ (2012/9/26)	
LAMMPS	29Oct20	◎ (2021/3/5)☆ CPU/GPU	P100, V100★ supported
	7Aug19	○ (2019/11/14)☆ CPU/GPU	P100, V100★ supported
	22Aug18	○ (2018/11/6)☆	P100 supported (lmp_rccs_gpu) V100 supported (lmp_rccs_volta)
	16Mar18(*15)	○ (2018/5/10)☆‖ Intel: cpu/gpu GNU: cpu/gpu	(2018/7/4 update), P100 supported
Molcas	8.2	(2020/1/30 license expired)	
Molpro(*2,*8)	2021.1.0	○ (2021/5/21)	(latest commit: 2021/5/12 17:52:32 +0100)
	2020.1.2	◎ (2020/10/20)‖ GNU/Intel	(Manual in pdf format (converted via wkhtmltopdf@Nov 12, 2020))
	2019.2.3	○ (2019/12/10)	
	2019.1.2	○ (2019/4/16)	
	2018.2	○ (2018/12/20)	
	2015.1-44	○ (2021/7/14)	
	2015.1-33	○ (2018/6/12)	
	2015.1-27	○ (2017/12/14)	

name	version	status (install date)	notes
	2015.1-19	○ (2017/10/1)	
	2012.1-37	○ (2016/4/19)	
NAMD	2.13	◎ (2018/12/7)☆ CPU/GPU	P100, V100 supported
	2.11	○ (2017/10/1)☆	P100, V100★ supported
NBO	7.0-7	◎ (2020/1/6)	
	7.0-2	○ (2019/1/23)	
	6.0-18	◎ (2018/3/16)	
	6.0-15	○ (2018/2/6)	
NTChem(*17)	2013.12.1.1	○ (2021/6/3)	
	2013.5.0	◎ (2015/4/20)	
NWChem	6.8	◎ (2018/1/22)	
OpenMolcas	20.10	◎ (2020/12/7)	
		○ (2019/6/7)	master branch on June 4, 2019
ORCA(*20)	4.2.1	○ (2020/1/8)	
Parallel CONFLEX(*9)			
PSI4	1.1	◎ (2018/1/12)	
Quantum ESPRESSO	6.7	◎ (2021/1/5)☆ CPU/GPU	P100, V100 supported
	6.5	○ (2020/7/9)	
	6.3	○ (2018/12/17)	
	6.1	○ (2017/9/14)	
	5.4	○ (2018/12/17)	
	5.1.2	○ (2015/4/8)	
ReactionPlus	1.0	◎ (2018/1/22)	
SIESTA	4.0.2	◎ (2019/3/14)	
	3.1(*16)	○ (2012/8/16)	
SMASH	2.2.0	○ (2017/5/16)	
TURBOMOLE(*3)	7.5	◎ (2020/7/30)	
	7.4.1	○ (2020/3/2)	
	7.4	○ (2019/8/20)	
	7.3	○ (2018/7/23)	
	7.2.1	○ (2017/12/12)	
	7.2	○ (2017/8/4)	
VASP(*4)		(unavailable)	

name	version	command name / path	install date
GaussView	6.1.1	gview6	◎ (2019/10/29)
	6.0.16	/local/apl/lx/g16b01/gv/gview.sh	○ (2017/2/2)
	5.0.9	gview5	◎ (2013/3/13)
Luscus	0.8.6	/local/apl/lx/luscus086/bin/luscus	◎ (2019/6/10)
Molden	5.7	/local/apl/lx/molden/bin/molden	◎ (2016/11/22)
NBOView2	2	/local/apl/lx/nboview2/nboview2	◎ (2018/2/6)
VMD	1.9.3	/local/apl/lx/vmd193/bin/vmd	◎ (2018/2/19)

◎: installed. Simplified alias (such as g16) is also available.
○: installed. Version number (such as g16a03) has to be specified explicitly.
▲: compatible with NBO 6.0
△: compatible with NBO 7.0
☆: GPU version available
★: Not a native build for this architecture. Performance might be limited due to its nature.
‖: GCC and Intel versions available

Notices

(*2) molpro license will be expired on Sep 15, 2022. The license will be renewed every year.
(*3) Only non-commercial users in Japan can use this. The license will be expired in Jan, 2022. The license will be renewed every year.
(*4) VASP considers a small research group as a unit of licensee. We cannot install it in this center due to the policy. Users should get the license by yourselves.
(*5) English guide for GRRM17 is available at https://afir.sci.hokudai.ac.jp/documents/manual/54. Japanese guide for this center (for GRRM14/for GRRM11) is also available.
(*8) SMILES (a package for molecular integrals with Slater functions) is enabled.

(*9) We cannot install ADF and Parallel CONFLEX due to their very high license fee.
(*11) Parallel executioin of exam13.inp results in a fail. This is due to the bug in the parallel computation of higher order electrostatic moments. (already reported to the official)
(*15) Package list and result of tests for each version can be found in (CPU(intel) / GPU(intel) / CPU(gcc) / GPU(gcc)).
(*16) The following papers must be cited when you publish papers involving SIESTA 3.x calculations.

1. “Self-consistent order-N density-functional calculations for
   very large systems”, P. Ordejón, E. Artacho and J. M. Soler,
   Phys. Rev. B (Rapid Comm.) 53, R10441-10443 (1996).
2. “The SIESTA method for ab initio order-N materials simulation”
   J. M. Soler, E. Artacho,J. D. Gale, A. García, J. Junquera,
   P. Ordejón, and D. Sánchez-Portal, J. Phys.: Condens. Matt. 14,
   2745-2779 (2002).

(*17) You have to cite some papers when you publish papers with NTChem results. Please read official page and documentation(japanese) of NTChem. Documentation and tutorial files are also available in /local/apl/lx/ntchem/doc of the frontend nodes.
(*18) To use CRYSTAL14, license agreement is required for each user. Once the agreement is arrivied at RCCS, you will be able to use CRYSTAL14.
(*19) References listed in this page must be cited when you publish results obtained with DIRAC.
(*20) User registration is required for ORCA. Please read this page for further details.
(*21) To use CRYSTAL17, license agreement is required for each user. Once the agreement is arrivied at RCCS, you will be able to use CRYSTAL17.

Attachment	Size
CRYSTAL14 license agreement	281.59 KB
CRYSTAL17 license agreement	255.88 KB