

zCluster Computational Software

Computational software installed on CCB clusters, and who supports and manages which software.

Question for Lulu

Can the information at the following wiki page be deleted?

- [Cluster application software specifics](#)

See also

- [Roles and responsibilities for clusters managed by ChemIT](#)

Computational Software List, by cluster

Application	Who/How manages	Scheraga	Hoffmann	Lancaster /Crane	Collum	Widom	Loring	Abruna	ChemIT
Gaussian	ChemIT	g09-C.01	g09-A.02		g09-A.02			g09-A.02	g09-C.01
gv	ChemIT		gv-508		gv-508			gv-508	gv-508
orca	ChemIT		orca_3_0_1	orca_3_0_1					orca_2_9_1
gromacs	ChemIT	gromacs-4.5.4							gromacs-4.6.5
Intel Compiler	ChemIT	11.1 20100414	11.1 20100203						intel-14
Mathematica	ChemIT						8.0		8.0
mpich	ChemIT	mpich-1.2.7p1_intel-11.1	mpich-1.2.7.p1	mpich-1.2.7.p1	mpich-1.2.7.p1		mpich-1.2.7p1_intel-10.1	mpich-1.2.7.p1	mpich-1.2.7.p1
openmpi	ChemIT	openmpi-1.4.3	openmpi-1.6.5	openmpi-1.6.5					openmpi-1.6.5_intel_14
sbgrid	ChemIT			yes					
WebMO	ChemIT				10.1.002e				
CUDA	ChemIT	CUDA5.5							
Quantum Espresso	Group?		espresso-4.0.1					espresso-5.0.1	
adf	Group?		adf2012.01						
phonopy	Group		phonopy-1.6.1						
avogadro	Group		yes						
xtalopt	Group		yes						
VASP	Group		VASP.5.3/vasp.5.lib						
Gamess	Group	gamess2009	yes						
bomb	Group		bomb27						
boss	Group		boss48						
mcpro	Group		mcpro21						
xcrysden	Group		xcrysden-1.5.53						
mpiexec	Group		mpiexec-0.83						
yaehmop	Group		yes						
LAMMPS	Group		yes						
amber	Group	amber10							
OpenMM	Group	OpenMM4.0							
shiftx2	Group	shiftx2-v107							
sparta+	Group	SPARTA+_v2.60							
mopac	Group	MOPAC2012							