

Emerson Center Software Collection

System Software:

AIX + XLF Fortran;
SuSe Linux Professional;
PGI
Intel

Electronic structure:

GAUSSIAN	MOLPRO
VASP	TURBOMOLE
DFTB+	DALTON
GAMESS	ORCA
ACES II M	NWCHEM
OCTOPUS	COLUMBUS

Simulation and modeling software:

GROMACS	AMBER
NAMD	VMD
ReaxFF	TINKER

Graphics and programming software:

MATLAB	Mathematica
VMD	GaussView