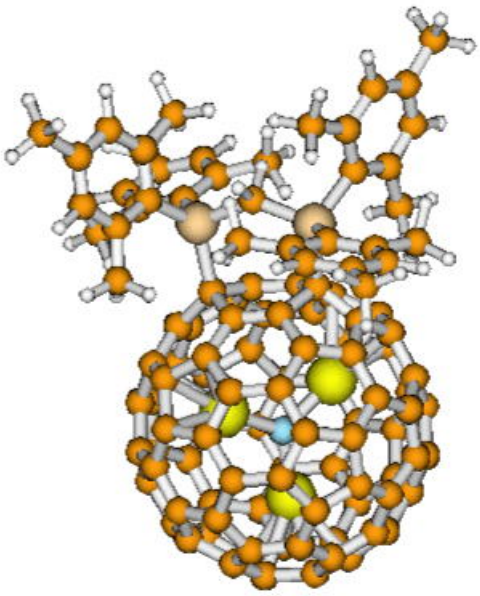
GAMESS Calculation on Altix4700

A New Fast I/O calculation server of Super Fast Molecular Simulator(Altix 4700) is attractive system for its large scale memory space and fast Disk I/O. We show the examples indicating real-performance by GAMESS electron-state calculations.

1．MP2 Gradient: Metal endohedral fullerene derivatives

$Sc_3NSi_2C_{117}H_{46}$ (C1) 846 electrons system / 6-31G 1267bases

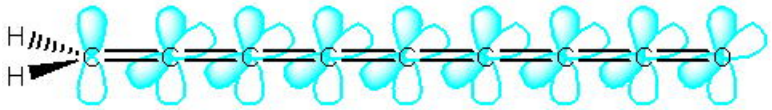


256 CPU core /4.0 TB memory	16.4 hours (cpu efficiency: 92%)

2. CASSCF Energy: Cumulene (n=8)

H_2C_8O (Cs) 58 electrons system / 6-31G(d) 139bases

CASSCF (18 electrons、17 orbital) 295,490,500 determinant CI

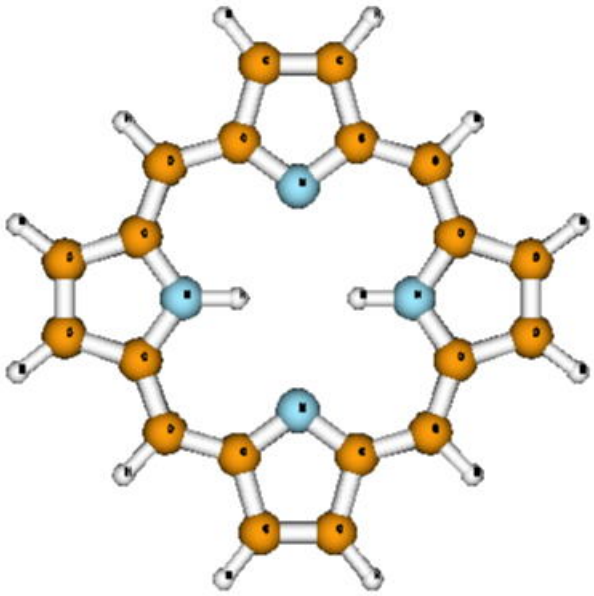


32 CPU core /1.6 TB memory	9 hours/iteration

3. CASSCF Gradient: Free Base Porphyrin

$C_{20}N_4H_{14}$ (D2h) 162 electrons system / cc-pVDZ 406 bases

CASSCF (18 electrons, 16 orbitals) 32,718,400 determinant CI



32 CPU core /189 GB memory	8.3 hours (15 iterations, cpu efficiency: 89%)

* These jobs are thanks to the cooperation of Mike Schmidt (Iowa State University), Ishimura, Nagase (IMS), and Shirai (Toyota Central R&D Labs).