

Turbomole 6.1 Release Notes

a) New features:

- N⁴ spin scaling SOS-RI-MP2 (module ricc2)
- faster MP2-F12 (module ricc2)
- (One-electron) transition moments between excited states in CC2
- Douglas-Kroll-Hess Energies in C1
- OpenMP versions of ricc2 and dscf
(currently only Linux/PC 64bit binaries available)
- new parallel version of ridft and rdgrad, especially for SMP systems
(currently only Linux/PC 64bit binaries available)
BETA version - passes all tests, but needs to be watched in production runs !

including:

- parallel linear scaling exact HF-exchange for DFT hybrid functionals (energy and gradients)
- parallel RI-K routines for energy calculations, faster pre-step for parallel RI-MP2 and RI-CC2 calculations
- no master process needed any more

There is a new website which describes how to test the new parallel version and what to do if an error occurs:

<http://www.cosmologic.de/parallel-faq.html>

The web site will be opened on Monday, 26th October 2009

b) Efficiency:

- up to 30% faster binaries for current AMD CPUs
- better speed up of new parallel versions compared to the standard MPI version, especially on SMP systems (ridft, rdgrad, and ricc2)
- standard MPI version with reduced CPU usage for the master process

c) Usability:

- TmoleX 2.2 with several bug fixes for running Turbomole jobs on remote systems

d) Bugfixes:

- DFT-D aoforce calculations (for some structures 6.0 gave wrong frequencies)
- external E-Field crash on AMD CPUs fixed (ridft)
- wfn output files containing f functions fixed with \$wfn option
- initial start velocity of molecular dynamics set ups now oriented to what the user has entered as temperature (mdprep)
- fixed crashes on some CPU types of Intel and AMD when using highly optimized linear algebra routines by using the latest Intel MKL library (Intel: spin-orbit calculations, AMD: aoforce)
- NumForce and TmoleX fixes for parallel runs or remote jobs when having tcsh as default shell on target machines
- Ir basis set in Turbomole 6.0 had a missing s function in def-TZVP
- new keyword (\$lastdiag) increases the accuracy of the output of orbital energies for very small HOMO-LUMO gaps - helpful for TDDFT calculations which complain about the violation of the Aufbau principle

Turbomole 6.0, Release Notes

a) New features:

SCS-CC2 for ground and excited states. Energies, excitation energies, gradients, transitions moments, and first order properties (module ricc2).

Support of meta-GGA functionals (TPSS and TPSSh) in second analytical derivative calculations (module aoforce).

Usage of difference density for DFT quadrature (see efficiency).

MP2-F12 (module ricc2).

Gradients for point charges in ricc2 (for QM/MM).

MP2-COSMO gradients (module rimp2).

MoleControl: a workflow management script kindly provided by BASF SE (see usability).

b) Efficiency:

Difference density speeds up DFT ground state energy calculations with ridft (serial version only).

Change of the default optimizer from relax to statpt: More stable performance in critical cases, handles fixed coordinates more flexible.

Improved efficiency in second analytical derivative calculations.

Parallel gradients and response properties on ADC(2) level fully working.

c) Usability:

MoleControl runs and controls Turbomole jobs using Python scripts. Many users have written their own scripts and programs to organize their calculations. The idea of this project is to provide a standardized interface for such workflow developments. It is intended, that the scripts are expanded by the users and exchanged in the community.

Input generation with define is done by MoleControl, users have to provide coordinates and the type of job only.

Analysis of 2-component wavefunctions.

the vibration script produces a gnuplot input file, which displays IR spectra (vibration -spectrum).

extended export of orbitals to the AOMix program (script t2aomix).

COSMO calculations with a scaled isodensity cavity for post-SCF thermodynamic properties with the COSMOtherm program.

Simplified setup of COSMO calculations (just add \$cosmo to the control file), making cosmoprep obsolete.

Simplified properties and wavefunctions analysis (-proper).

Added more basis sets to the library like: d-aug-cc-pVXZ, 6-311G-type, 6-31G-type

Default settings in parallel version changed:

- \$numprocs and \$parallel_platform keywords obsolete,
- fully direct task distribution now reduces I/O in dscf,
- improved interoperability of serial and parallel version

d) Bugfixes:

aoforce with hybrid functionals and RI-J

spin flip

parallel PEECM

2-component DFT with RIJK

parallel NumForce