TURBOMOLE V6.6 (June 2014)

Release Notes of Turbomole 6.6

a) New features:

- Reaction path optimization (new module: woelfling)
  The optimization starts with a linear synchronous transit (LST) followed by a chain-of-states method that optimizes reaction paths under the sole constraint of equally spaced structures. In contrast to Nudged Elastic Band or Growing String Method, it requires no spring forces, interpolation algorithms, or other heuristics to control structure distribution. [1]

- First order electron vibration coupling (new module: evib)

- Many body perturbation theory in the GW approximation (escf)

- Solvation effects on excited states ADC(2) with COSMO (ricc2)

- The M06 and M06-2X functionals (ridft, rdgrad, dscf, grad, aoforce, escf) The XCFun library (https://repo.ctcc.no/projects/xcfun/wiki) is now used for easier interchange of new functionals.

- CCSD(T) energy with interference-corrected MP2-F12 (ricc2)

- RI-RPA gradients available (rirpa)

- Two-component RI-RPA energies (rirpa)

- Two-component TD-DFT for spin-orbit effects (escf)

- VV10 like density based dispersion correction (ridft, rdgrad) [2]

b) Efficiency:

- MP2/COSMO is included in ricc2. The rimp2 module is removed since all functionalities are now available in ricc2.

c) Usability:

- New def2 basis sets for the Lanthanides [3]

- New scripts and tools:
  + scanprep. Prepares a scan along frozen internal coordinates
  + log2rog. Calculate the radius of gyration from MD log files
  + past. Turns coord in principal axis system and prints rotational constants
  + NumGrad, NumHess. Computes numerical gradient and second derivatives

- TmoleX 4.0:
  + A new look and feel and some code reorganisation
  + The builder is improved to more chemical intuition
  + New option in Transition State Search: Reaction Path Sampling
  + First version of an online update possibility

d) Bug fixes:

- The SMP/GA version of ridft/rdgrad can now be run with more one job on one machine
- Problem of define for small molecules in symmetry creating start orbitals fixed.

----------


TURBOMOLE V6.5 (May 2013)

New features:

- CCSD vertical excitation energies
- MP2 & CC2 polarizabilities [1]
- MP3(F12) and MP4(F12) energies
- new odft module, for all orbital-dependent Kohn-Sham DFT methods. Includes LHF and a new implementation of the exchange-only optimized effective potential (OEP-EXX) [2]

Efficiency:

- Linux version: overall faster code on newer Intel or AMD CPUs
- parallel SMP version for RI-K gradient
- enhanced parallel SMP version of ridft and rdgrad
- new SMP parallel versions of scdf, grad, ridft and rdgrad available as alternative to default parallelization
- again, IBM Platform MPI (8.2) is included in the Turbomole distribution, for details about Platform MPI see: http://www-03.ibm.com/systems/technicalcomputing/platformcomputing/products/mpi Turbomole users can run parallel calculations 'out-of-the-box' without the need to install MPI itself. Uses shared memory on one node and supports Infiniband or most other high-speed interconnects between nodes.

Usability:

- new scripts MECPprep and MECPopt for preparing and performing minimum-energy crossing point optimizations.
- new auxiliary basis sets for RI-MP2 and RI-CC (cbasen) for def2-SVPD, def2-TZVPD, def2-TZVPPD, def2-QZVPPD
  from H-Rn (without Lanthanides).
- TmoleX 3.4
  - new feature: batch jobs (graphical version of the 'calculate' script). It is now possible to define a job template with one or several different jobs (basis set, method, charge, kind of job, etc.) and apply it to a LIST of molecules. Runs either on the local system or on a remote machine.
  - new feature: simple build-in queuing system for local and remote jobs. If you tell TmoleX how many CPUs you want to use on your local or on remote systems, it is possible to start many different jobs at a time. TmoleX will only run a limited number of jobs, automatically starting jobs as soon as a CPU is free for computation.
  - new features: TDA (Tamm-Dancoff) is now supported, ESP fits and EPN (electrostatic potential at nuclei) added.
  - export of MOs to WFN, molden, and AOMix enabled.
  - improvements: easier plotting of electrostatic potential on density isosurface check work load on remote system from within TmoleX

Note: parts of the new SMP parallel features are only available under Linux 64bit.


a) New features:

DFT/TDDFT:
- RI-RPA
- non-adiabatic TDDFT surface hopping
- spin-flip TDDFT
- semi-numerical HF exchange for one- and two-component calculations
- gradients for 2c-DFT energies
- FDE, frozen density embedding (dscf module only)

post-Hartree-Fock:
- CCSD excitation energies
- O(N^4) implementation of SOS-CC2 excitation energies

b) Efficiency:

- parallel SMP version for CCSD(F12)

- parallel MPI versions of dscf and grad can skip time demanding pre-job step which determines the task distribution for large molecules by setting environment variable $SKIP_PARASTAT=yes
  NOTE: use with care, it assumes that you are not using more CPUs than symmetry non-redundant shells.

- max. number of CPUs for parallel MPI jobs increased to > 2000

- new option 'nocheck' for point charges skips check for overlapping point charges and correct symmetry. Significantly faster if many point charges are given.

- new version of Platform MPI (8.2) is included in the Turbomole distribution, for details see:
  http://www.platform.com/cluster-computing/platform-mpi/features-benefits

c) Usability:

- new script 'DRC' for performing dynamic/intrinsic reaction coordinate calculations

- interface to the hotfcht program from R. Berger
  http://fias.uni-frankfurt.de/~berger/group/hotFCHT/index.html

- full 64bit version with 'huge' parameter set (up to 1400 atoms) for Linux
systems will be available in addition to the default version. Those binaries will use more memory and run a bit slower, but should be able to use a more or less unlimited amount of memory and disk space.

- TmoleX 3.3:
  
  + molecular builder with new simple 'paint'-tool
  + job templates can handle multi-jobs, for example
    - geometry optimization with subsequent vibrational frequencies calculation
    - optimize with small basis set, then with larger basis set,
      then run single-point MP2 or CCSD(T) energy calculation
    - run jobs using different density functionals at a time
  + combine results from different jobs, including export to Excel file
  and (for simple organic molecules) 2D graphics
  + New viewer for spectra, including broadening of lines using Lorentz or Gaussian
  + finite temperature contributions from vibrational frequencies
  + POV-Ray export of molecular orbitals
  + support of DFT-D3 with BJ damping
  + diffuse basis functions def2-SVPD, def2-TZVPD, def2-QZVPD supported
  + new FINE cavity for COSMO single-point energies can be chosen

---

TURBOMOLE V6.3.1 (June 2011) Release Notes

New features and bug fixes:

- DFT-D3 in version 6.3 had problems when using ECPs, in such cases the original code of the Grimme group has not been invoked correctly and wrong dispersion parameters have been used. With default Turbomole/Karlsruhe basis sets this did occur for all elements beyond Kr
- RI-CC2 excited state gradient problems in some rare cases where the program stopped in 6.3
- COSMO + scf in parallel jobs gave I/O problems in some cases at the end of the job
- TDDFT + COSMO need more balanced thresholds for integral screening, for very small symmetric molecules and many excited states TDDFT did not converge in 6.3
- ScalAPACK turned out to be very slow on clusters with a slow network, here the Turbomole-own parallel linear algebra routines are faster. Now users can add $parallel\_platform cluster to the control file to switch off the usage of ScalAPACK

Usability:

- TmoleX 3.2
  + includes Turbomole 6.3.1
  + new possibility to control the assignment of ECPs to the basis sets
  + problems with potential energy scans running on remote systems removed
  + various minor changes
TURBOMOLE V6.3 (March 2011) Release Notes

New features:

- parallel SMP version for + 2nd analytic derivatives (module aoforce)
- + TDDFT excited state energies and gradients (modules escf and egrad)
- + CCSD and CCSD(T) (module ricc2)
- Symmetry in CCSD and CCSD(T) for D2h and its subgroups
- Vibrational frequency calculations are now restartable (module aoforce)
- TDDFT vertical excitation energies with full COSMO solvation treatment (module escf)
- CCSD(F12*) as a more cost-efficient alternative to CCSD(F12)
- Two-component MP2-F12 energy calculations for spin-orbit coupling (module ricc2)
- Property-optimized Gaussian basis sets addition of diffuse functions to the Karlsruhe basis sets: def2-SVPD, def2-TZVPD, def2-QZVPD
- New segmented contracted basis sets for one- and two-component Dirac-Fock effective core potentials
- Support for DFT-D3 dispersion correction (original code from Grimme group), including 2nd derivatives with module aoforce (new keyword $disp3)

Efficiency:

- Platform MPI 7.1 is included in the Turbomole distribution, for details see: features-benefits

Usability:

- New parallel environment setting for SMP/multi-core systems
- New script 'evalgrad' which monitors the values of bond length, bond angle or dihedral angle of all steps of a geometry optimization or an MD run
- New toolkit 'thermocalc' to calculate batch-wise atomization energies and heats of formation with customizable computational protocols
- NumForce transfers resulting Hessian and vibrational modes to the original control file for a subsequent transition state search
- TmoleX 3.1
  - Improved molecular builder
  - More features of Turbomole supported

_______________________________________________________

TURBOMOLE V6.2 (June 2010) Release Notes

a) New features:

- Initial implementation of CCSD, CCSD(F12) variants, and CCSD(T) (module ricc2)

b) Efficiency:
• LHF is now parallelized with OpenMP (module dscf)

c) **Usability:**
- **TmoleX 3.0:**
  - the molecule builder has been re-engineered
  - MOPAC7 is included as a pre-optimizer
  - the job type selection has been laid out results oriented
  - a visualization of spectra has been implemented
  - new way of how to define and run PES scan jobs
  - more features of TURBOMOLE can be used now
- LHF supports up to h-functions and heavy elements with ECP
- "$pointval xc" option, to plot exchange-correlation potential on an user define grid
- new MoleControl version 2.1 with enhanced features and an easier installation procedure

d) **Bugfixes:**
- the sign of electronic rotatory dispersion has been corrected (module escf/egrad)
- various bugfixes for the the gobal array (GA) version (module ridft_ga/rdgad_ga)

-------------------------------

**Turbomole 6.1 Release Notes**

a) **New features:**
- N^4 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 user 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 gnupolt 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