TURBOMOLE V5.10 Release Notes (January 2008)

New features:

- Vibrational Raman intensities
  using analytical derivatives of frequency-dependent TDHF and (hybrid) TDDFT polarizabilities
- Spin-Orbit Coupling
  Two-component RI-Hartree-Fock and RI-DFT calculations with Spin-Orbit-ECPs (spin-orbit coupling)
- SCS-RI-MP2 (module ricc2)
  energy and gradients (for closed-shell HF and UHF reference states, sequential and parallel implementation)
- Periodic Point Charges
  for HF and DFT, energy and gradient calculations
- DFT+D
  DFT with dispersion, method of S. Grimme (reference: see manual)
- COSMO for RI-MP2 calculations (using rimp2 module)
- Properties: Merz-Kollman ESP fit
- Spin flipping for broken symmetry treatment (module define)

Efficiency:

- RI-MP2/RI-CC2 (module ricc2)
  gradients/properties for RI-HF-based RI-MP2 and RI-CC2 calculations (i.e. RI-JK approximation for Z-vector equation and gradients)
- NumForce handles frozen cartesian coordinates (option -frznuclei)
- NumForce and jobex:
  possibility to use RI-JK together with RI-MP2/RI-CC2 (option -rijk)

Usability

- molecular orbital files can be kept in binary format
- tm2molden supports g-functions
- cube format for 3D grid files
- convert vibrational frequency output to G98 format

TURBOMOLE V5.9.1 (April 2007)

New features:

- Linux/PC and Itanium2/Linux parallel binares are now using **HP-MPI**.

    - HP-MPI comes with Turbomole, there is no need to install it
    - no license key is needed for HP MPI, Turbomole will run 'out of the box'
    - HP-MPI is able to run on several different interconnects like TCP/IP, SMP, Infiniband, Myrinet, Quadrix, ...
- statpt
    - statpt is able to fix Cartesian coordinates
    - more stable internal coordinates

Bugfixes:

- Bug with reducible E representations has been fixed
- RI-R12-MP2 bug fixed
- EM64T binaries for large input files are more stable now
- ricc2 is able to plot properties on grids like potential, electric field, el. field gradients, etc.
- NumForce bug when having fixed Cartesian coordinates fixed
- define bugs (basis set change, delete atom with ECPs, ...) fixed
- jobbsse bug with ECPs fixed
- tmole bug when scanning torsions fixed
- several minor bugs fixed

New binary version:

- Windows version of Turbomole available now - binaries are delivered together with the new
  graphical user interface **TmoleX**.

TURBOMOLE V5.9 (December 2006)

New features include:

Methods:

- RI-J for Hartree-Fock and DFT hybrid functionals: Efficiency!
- RI-JK gradients implemented and DFT hybrid functional calculations enabled
- aoforce greatly enhanced and extended - module for analytical harmonic vibrational frequencies available for basis sets up to g functions, ECPs up to g projectors enabled
- RI-CC2/RI-MP2: parallel version for ground and excited state gradients and gradients for excited state ADC(2) and CIS(D_infinity) implemented
- MD: Finite temperature canonical Born-Oppenheimer molecular dynamics using Nosé-Hoover thermostat
- NPA - Weinhold's Natural Population Analysis

- New, improved, and automated optimization method for minima and transition structures, new GDIIS method, improved overall stability and generation of internal redundant coordinates
- RI-MP2-R12: Single-point explicitly-correlated RI-MP2-R12 energies for closed- and open-shell systems.
- BSSE: Geometry optimizations can be carried out within the framework of the full function-counterpoise method to avoid basis-set superposition errors

Efficiency:

- RI-J in combination with Hartee-Fock exchange speeds up large Hartree-Fock or DFT hybrid-functional calculations
- MARI-J (Multipole Accelerated RI-J): Increased accuracy with reduced overall computational cost
- New parallel diagonalizer with better speed-up for parallel calculations
- aoforce: increased efficiency

Basis sets and auxiliary basis sets:

- Basis sets for Lanthanides and Actinides up to Lr
- RI-J auxiliary basis sets (jbasen) for def2- basis sets H-Rn and def- basis sets for Lanthanides and Actinides
- RI-JK auxiliary basis sets (jkbasen) for all triple and quadruple zeta valence basis sets, including the Lanthanides and Actinides
- New auxiliary basis sets for RI-MP2 and RI-CC2 (cbasen) for:
  - def2-QZVPP for Rb-Rn (without Lanthanides)
  - def2-SVP, def2-TZVP, def2-TZVPP for H-Rn (without Lanthanides)
  - (aug-)cc-pVXZ-PP and (aug-)cc-pwCVXZ-PP with X=D,T,Q,5 for Cu, Ag, Au and Zn, Cd and Hg
- Possibility to use auxiliary basis sets up to l functions

DFT quadrature:

- New grids for Lanthanide and Actinides up to Lr
- Grid optimization: no 'unoptimized grid' for DFT any more
- DFT grids extended for diffuse cases
- Fixed numerical problems with quadrature

TURBOMOLE V5.8 (November 2005)

New features include:

- Implementation of new basis sets for the elements H - Rn, except lanthanides, which guarantee consistent accuracy across the periodic table.

- Small core ECPs for 5p and 6p elements and corresponding basis sets.
- ECP routines including g-projectors (energy and gradient only).
- Parallel multipole accelerated RI-J (MARI-J).
- Faster integral routines, especially for RI treatments.
- Improved functionality and simplified handling of tools for molecular properties, wavefunction analysis, and interfaces to visualization tools.
- Analytical excited state gradients for RI-CC2.
- Parallel RI-MP2 and RI-CC2 ground state and RI-CIS(D), RI-CC2, and RI-ADC(2) excitation energies (ricc2 module).
- Full support of the ricc2 program by the input module define.
- Additional auxiliary basis sets for RI-MP2/RI-CC2 calculations for the QZVPP (H-Kr) and cc-pwCVXZ (B-Ne, Al-Ar) orbital basis sets.
- COSMO with symmetry and more stable A-matrix setup.
- Virtual cavities for condensed phases and bond distance constraints added to molecular dynamics.
- A new and user-friendly input generator TMOLE with extended functionality (e.g. Z-matrix input, potential curve calculations).
- New DIIS methods and damping defaults for accelerated SCF convergence.
- Automatic switching from internal coordinates to Cartesians and back in case of internal coordinate failure for minimization and transition state optimization.
- Maximum number of atoms and basis functions increased to 700 and 10000 resp.

Improvements:

- better interfaces to graphics programs
- ...

available Turbomole add-ons:

- **SNF** provided by Carsten Kind, **Markus Reiher, J. Neugebauer, C. Herrmann** , and Bernd A. Hess
  The program package SNF is a parallel (PVM or MPI) program for the calculation of vibrational frequencies, IR and Raman intensities.
- **qmpot** provided by **Marek Sierka**.
  The program qmpot is able to perform transition state optimizations (and more...) using Turbomole.

TURBOMOLE V5.7 (July 2004)

New features include:

- Effective core potentials supporting basis sets with high l-quantum numbers

- Improved analytic second derivative calculations (for basis sets with up to d functions)
- Excitation energies for the algebraic diagrammatic construction through second order ADC (2)
- Visualization of ground and excited state densities and differential densities
- RI-J approximation for excited state properties, geometry optimizations, and (numerical) force constante calculations using TDDFT
- Analytical gradients for multipole accelerated RI-J (MARIJ)
- TPSS and TPSSH meta-GGA functionals (energies and gradients), including RI-J
- Gradients for the optimization of auxiliary basis functions for RI-MP2 and RI-CC2 calculations
- Basis sets of quadruple zeta valence quality for atoms H-Kr
- Improved transition state optimization; new optimizer for ground states (alternative to relax)
- Spin-unrestricted exact exchange methods using the LHF approximation
- Various other improvements, including a better documentation (user's guide)

TURBOMOLE V5.6 (December 2002)

- Excited state properties, geometry optimization, and (numerical) force constant calculations using TDDFT, CIS, and RPA
- RI-CC2 one-electron properties for ground and excited states, ground geometry optimization and force constant calculations (using numerical a hessian)
- Improved analytic second derivative calculations (including partial use of the RI approximation)
- Direct iterative methods for computing the lowest vibrational modes of a molecule
- Efficient calculation of optical rotations using TDDFT
- "O(N)-RIDFT" using the multipole accelerated RI-J approximation
- Occupation number optimization using (pseudo-Fermi) thermal smearing
- RI-JK approximation for Hartree-Fock including highly accurate optimized auxiliary basis sets

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TURBOMOLE V5.5 (January 2002)

- calculation of electronic excitation energies at the CIS, CIS(D) and CC2 level using either a closed shell RHF or a UHF SCF reference function. Employs the RI technique to approximate two-electron integrals
- Universal Force Field (UFF) for geometry optimizations at a force field level and calculation of the analytical cartesian hessian
- Gaussian version of B3-LYP (using the simplified VWN-III functional)
- analytic closed shell hessian calculation at DFT level
- efficient Block-Davidson algorithm for CIS, RPA and DFT hybrid functional excitation energies, including spin-unrestricted cases

- RI-TDDFT method for dynamic polarizabilities and rotatory dispersions
- new COSMO routines for closed and open shell calculations of the energy and the gradients
- transition states search algorithm using the reduced gradient following method
- aug-cc-pVDZ, aug-cc-pVTZ and aug-cc-pVQZ Dunning basis sets
- online documentation, FAQ and Turbomole user mailing list available
- new DFT routines with better scaling
- new and very fast linear algebra routines with low memory requirements
- better scaling of RI integral routines
- new CPHF routines for more stable force calculations
- 64Bit binaries on HP (HP-UX 11)
- no 2GB file size limit on Linux machines (Kernel 2.4 required)

TURBOMOLE V5.3 (April 2000)

- New documentation (more detailed)
- COSMO code parallelized
- Point charges: number limitation removed, contribution to the gradient implemented

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TURBOMOLE V5.2 (November 1999)

- Automatic definition of redundant internal coordinates
- Chemical shifts with DFT
- All-electron basis sets for Rb to Xe
- Standard calculations of molecules with up to 7000 basis functions (minimum storage requirements: 250 MB)

TURBOMOLE V5-1 (February 1999)

- FORTRAN-90 dynamic memory allocation
- ESCF: performance improved by simulataneous vector iteration (Block Davidson Algorithm). Calculation of chiroptical properties.
- Better grid-point distribution in DFT quadrature (up to 30% acceleration)

TURBOMOLE V4-9 (September 1998)

- RIMP2 with optimized auxiliary basis sets