Gaussian 16 Features at a Glance

Features introduced since Gaussian 09 Rev A are in **blue**.
Existing features enhanced in Gaussian 16 are in **green**.

Fundamental Algorithms

- Calculation of one- & two-electron integrals over any contracted gaussian functions
- Conventional, direct, semi-direct and in-core algorithms
- Linearized computational cost via automated fast multipole methods (FMM) and sparse matrix techniques
- Harris initial guess
- Initial guess generated from fragment guesses or fragment SCF solutions
- Density fitting and Coulomb engine for pure DFT calculations, including automated generation of fitting basis sets
- $\mathcal{O}(N)$ exact exchange for HF and hybrid DFT
- 1D, 2D, 3D periodic boundary conditions (PBC) energies & gradients (HF & DFT)
- Shared-memory (SMP), cluster/network and **GPU-based** parallel execution

Model Chemistries

Molecular Mechanics

- Amber, DREIDING and UFF energies, gradients and frequencies
  - Custom force fields
- Standalone MM program

Ground State Semi-Empirical

- CNDO/2, INDO, MINDO3 and MNDO energies and gradients
- AM1, PM3, PM3MM, PM6 and PDDG energies, gradients and reimplemented (analytic) frequencies
- **PM7: original and modified for continuous potential energy surfaces**
- Custom semi-empirical parameters (Gaussian and MOPAC External formats)
- DFTB and DFTBA methods

Self Consistent Field (SCF)

- SCF restricted and unrestricted energies, gradients and frequencies, and RO energies and gradients
- **EDIIS+CDIIS default algorithm; optional Quadratic Convergent SCF**
- **SCF procedure enhancements for very large calculations**
- Complete Active Space SCF (CASSCF) energies, gradients & frequencies
  - Active spaces of up to **16** orbitals
- Restricted Active Space SCF (RASSCF) energies and gradients
- Generalized Valence Bond-Perfect Pairing energies and gradients
- Wavefunction stability analysis (HF & DFT)

Density Functional Theory

Closed and open shell energies, gradients & frequencies, and RO energies & gradients are available for all DFT methods.

- EXCHANGE FUNCTIONALS: Slater, Xα, Becke 88, Perdew-Wang 91, Barone-modified PW91, Gill 96, PBE, OPTX, TPSS, **revised TPSS**, BRx, PKZB, ωPBEh/HSE, PBEh
- CORRELATION FUNCTIONALS: VWN, VWN5, LYP, Perdew 81, Perdew 86, Perdew-Wang 91, PBE, B95, TPSS, **revised TPSS**, KCIS, BRC, PKZB, VP86, V5LYP
- OTHER PURE FUNCTIONALS: VSXC, HCTH functional family, τHCTH, B97-D, M06-L, SOGGA11, M11-L, MN12-L, N12, **MN15-L**
- HYBRID METHODS: B3LYP, B3P86, P3PW91, B1 and variations, B98, B97-1, B97-2, PBE1PBE, HSEh1PBE and variations, O3LYP, TPSSh, τHCTH hybrid, BMK, **AFD**, M05, M05-2X, M06, M06-HF, M062-X, **M08-HX**, **PW6B95**, **PW6B95D3**, **M11**, **SOGGA11-X**, **N12**, **N12-SX**, **MN12-SX**, **MN15**, HISSbPBE, X3LYP, BHandHLYP; user-configurable hybrid methods
- DOUBLE HYBRID: B2PLYP & mPW2PLYP and variations with dispersion, **DSDPBEP86**, **PBE0DH**, **PBEQIDH** (see also below in "Electron Correlation")
- EMPIRICAL DISPERSION: **PFD, GD2, GD3, GD3BJ**
- FUNCTIONALS INCLUDING DISPERSION: **APFD, B97D3, B2PLYPD3**
- LONG RANGE-CORRECTED: LC-ωPBE, CAM-B3LYP, ωB97XD and variations, Hirao's general LC correction
- **Larger numerical integrations grids**

Electron Correlation:

All methods/job types are available for both closed and open shell systems and may use frozen core orbitals; restricted open shell calculations are available for MP2, MP3, MP4 and CCSD/CCSD(T) energies.

- MP2 energies, gradients, and frequencies
- **Double hybrid DFT** energies, gradients and frequencies, with optional empirical dispersion (see list in "Density Functional Theory" above)
- CASSCF calculations with MP2 correlation for any specified set of states
- MP3 and MP4(SDQ) energies and gradients
- MP4(SDTQ) and MP5 energies
- Configuration Interaction (CISD) energies & gradients
- Quadratic CI energies & gradients; QCISD(TQ) energies
- Coupled Cluster methods: restartable CCD, CCSD energies & gradients, CCSD(T) energies; optionally input amplitudes computed with smaller basis set
  - **Optimized memory algorithm to avoid I/O during CCSD iterations**
- Brueckner Doubles (BD) energies and gradients, BD(T) energies; optionally input amplitudes & orbitals computed with a smaller basis set
- **Enhanced** Outer Valence Green's Function (OVGF) methods for ionization potentials & electron affinities
- Complete Basis Set (CBS) MP2 Extrapolation
- Douglas-Kroll-Hess scalar relativistic Hamiltonians

Automated High Accuracy Energies

- G1, G2, G3, G4 and variations
- CBS-4, CBS-q, CBS-QB3, ROCBS-QB3, CBS-Q, CBS-APNO
- W1U, W1BD, W1RO (**enhanced core correlation energy calculation**)

Basis Sets and DFT Fitting Sets

- STO-3G, 3-21G, 6-21G, 4-31G, 6-31G, 6-31G†, 6-311G, D95, D95V, SHC, CEP-*n*G, LanL2DZ, cc-pV{D,T,Q,5,6}Z, original and def2- versions of SV, SVP, TZV & QZVP, EPR-II, EPR-III, Midi!, UGBS*, MTSmall, DG{D,T}ZVP, **CBSB7**
  - **Augmented cc-pV*Z schemes: Aug- prefix, spAug-, dAug-, Truhlar calendar basis sets (original and regularized)**
- Effective Core Potentials (through second derivatives): LanL2DZ, CEP through Rn, Stuttgart/Dresden
- Support for basis functions and ECPs of arbitrary angular momentum
- DFT FITTING SETS: DGA1, DGA1, W06, older sets designed for SVP and TZVP basis sets; auto-generated fitting sets; optional default enabling of density fitting

Geometry Optimizations and Reaction Modeling

- Geometry optimizations for equilibrium structures, transition structures, and higher order saddle points, in redundant internal, internal (Z-matrix), Cartesian, or mixed internal and Cartesian coordinates
- **GEDIIS optimization algorithm**
- Redundant internal coordinate algorithm designed for large system, semi-empirical optimizations
- Newton-Raphson and Synchronous Transit-Guided Quasi-Newton (QST2/3) methods for locating transition structures
- IRCMax transition structure searches
- Relaxed and unrelaxed potential energy surface scans

- Implementation of intrinsic reaction path following (IRC), applicable to ONIOM QM:MM with thousands of atoms
- Reaction path optimization
- BOMD molecular dynamics (all analytic gradient methods); ADMP molecular dynamics: HF, DFT, ONIOM(MO:MM)
- Optimization of conical intersections via state-averaged CASSCF
- **Generalized internal coordinates for complex optimization constraints**

Vibrational Frequency Analysis

- Vibrational frequencies and normal modes (harmonic and **anharmonic**), including display/output limiting to specified atoms/residues/modes (optional mode sorting)
- Restartable analytic HF and DFT frequencies
- MO:MM ONIOM frequencies including electronic embedding
- Analytic Infrared and static and dynamic Raman intensities (HF & DFT; MP2 for IR)
- Pre-resonance Raman spectra (HF and DFT)
- Projected frequencies perpendicular to a reaction path
- NMR shielding tensors & GIAO magnetic susceptibilities (HF, DFT, MP2) and enhanced spin-spin coupling (HF, DFT)
- Vibrational circular dichroism (VCD) rotational strengths (HF and DFT; harmonic and **anharmonic**)
- Dynamic Raman Optical Activity (ROA) intensities (harmonic and **anharmonic**)
- **Raman and ROA intensities calculated separately from force constants in order to use a larger basis set**
- Harmonic vibration-rotation coupling
- **Enhanced** anharmonic vibrational analysis, including **IR intensities, DCPT2 & HDCPT2 method for resonance-free computations of anharmonic frequencies**
- Anharmonic vibration-rotation coupling via perturbation theory
- Hindered rotor analysis

Molecular Properties

- Population analysis, including per-orbital analysis for specified orbitals: Mulliken, **Hirshfeld/CM5**
- **Computed atomic charges can be saved for use in a later MM calculation**
- Electrostatic potential, electron density, density gradient, Laplacian, and magnetic shielding & induced current densities over an automatically generated grid
- Multipole moments through hexadecapole
- Biorthogonalization of MOs (producing corresponding orbitals)
- Electrostatic potential-derived charges (Merz-Singh-Kollman, CHelp, CHelpG, **Hu-Lu-Yang**)
- Natural orbital analysis and natural transition orbitals
- Natural Bond Orbital (NBO) analysis, including orbitals for CAS jobs. Integrated support for NBO3; **external interface to NBO6**
- Static and frequency-dependent analytic polarizabilities and hyperpolarizabilities (HF and DFT); numeric 2nd hyperpolarizabilities (HF; DFT w/ analytic 3rd derivs.)
- Approx. CAS spin orbit coupling between states
- Enhanced optical rotations and optical rotary dispersion (ORD)
- Hyperfine spectra components: electronic *g* tensors, Fermi contact terms, anisotropic Fermi contact terms, rotational constants, dipole hyperfine terms, quartic centrifugal distortion, electronic spin rotation tensors, nuclear electric quadrupole constants, nuclear spin rotation tensors
- ONIOM integration of electric and magnetic properties

ONIOM Calculations

- Enhanced 2 and 3 layer ONIOM energies, gradients and frequencies using any available method for any layer
- Optional electronic embedding for MO:MM energies, gradients and frequencies implemented so as to include all effects of the MM environment without neglecting terms in its coupling with the QM region
- Enhanced MO:MM ONIOM optimizations to minima and transition structures via microiterations including electronic embedding
- Support for IRC calculations
- ONIOM integration of electric and magnetic properties

Excited States

- ZINDO energies
- CI-Singles energies, gradients, & freqs.
- Restartable time-dependent (TD) HF & DFT energies, gradients and **frequencies**. **TD-DFT can use the Tamm-Dancoff approximation.**
- **SAC-CI energies and gradients**
- EOM-CCSD energies and **gradients** (restartable); optionally input amplitudes computed with a smaller basis set
- **Franck-Condon, Herzberg-Teller and FCHT analyses**
- **Vibronic spectra including electronic circular dichroism (ECD) rotational strengths (HF and DFT)**
- **Resonance Raman spectra**
- **Ciofini's excited state charge transfer diagnostic (D_{CT})**
- **Caricato's EOMCC solvation interaction models**
- CI-Singles and TD-DFT in solution
- State-specific excitations and de-excitations in solution
- **An energy range for excitations can be specified for CIS and TD excitation energies**

Self-Consistent Reaction Field Solvation Models

- New implementation of the Polarized Continuum Model (PCM) facility for energies, gradients and frequencies
- Solvent effects on vibrational spectra, NMR, and other properties
- Solvent effects for ADMP trajectory calcs.
- Solvent effects for ONIOM calculations
- Enhanced solvent effects for excited states
- SMD model for ΔG of solvation
- Other SCRF solvent models (HF & DFT): Onsager energies, gradients and freqs., Isodensity Surface PCM (I-PCM) energies and Self-Consistent Isodensity Surface PCM (SCI-PCM) energies and gradients

Ease-of-Use Features

- Automated counterpoise calculations
- Automated optimization followed by frequency or single point energy
- Ability to easily add, remove, freeze, differentiate redundant internal coords.
- Simplified isotope substitution and temperature/pressure specification in the route section
- Optimizations:
  - **Retrieve the *n*th geometry from a checkpoint file**
  - **Recompute the force constants every nth step of a geometry optimization**
  - **Reduce the maximum number of allowed steps, including across restarts**
  - **180° flips detected and suppressed for better visualization**
- Freezing by fragment for ONIOM optimizations
- Simplified fragment definitions on molecule specifications
- Many more restartable job types
- Atom freezing in optimizations by type, fragment, ONIOM layer and/or residue
- QST2/QST3 automated transition structure optimizations
- Saving and reading normal modes
- **%OldChk Link 0 command specifies read-only checkpoint file for data retrieval**
- Default.Route file for setting calculation defaults
- **Enhanced set of equivalent Default.Route directives, Link 0 commands, command line options and environment variables**

Integration with External Programs

- **NBO 6**
- COSMO/RS
- AIMPAC WfnX files
- **Antechamber**
- **ACID**
- Pickett's program
- **DFTB input files**
- **General external interface script-based automation, results post-processing, interchanging data/calculation results with other programs, and so on:**
  - **Interface routines in Fortran, Python and Perl (open source)**
  - Keyword and **Link 0 command** support

GaussView 6 Features at a Glance

Features new to GaussView 6 are in **blue**; features enhanced in GaussView 6 are in **green**.

Examine Molecular Structures

- Rotate, translate and zoom in 3D in any display using mouse operations and/or a precision positioning toolbar
- View numeric value for any structural parameter
- Use multiple synchronized or independent views of same structure (customizable)
- Manipulate multiple structures as an ensemble
- Display formats: wire frame, tubes, ball & stick/bond type, space fill (CPK) style
- View per-atom labels for element, serial number, NMR shielding (when available)
- Visualize depth with fog feature
- Display stereochemistry info
- Highlight, display or hide atoms based on rich selection capabilities (optionally persistent)

Build/Modify Molecules

- Convenient palettes for atoms, functional groups, rings, amino acids (central fragment, amino- or carboxyl-terminated) and nucleosides (central fragment, C3'-, C5'-terminated, free forms)
- Custom fragment libraries
- Import standard molecule file formats:
  - PDB, **including ones created by AMBER**. Optionally include/discard waters, apply standard residue bonding on PDB import.
  - Gaussian input (**.gjf** and **.com**), output (**.log** and **.out**), checkpoint (**.chk** and **.fchk**), cube (**.cub**), and frequency (**.gfrq**) files
  - Sybyl **.mol2**, **.ml2**; include/convert **.mol2** lone pairs
  - MDL files: **.mol**, **.rxn**, **.sdf**
  - Crystallographic Information files: **.cif**
  - Optionally include intermediate structures from optimizations, scans, etc.
- Accurately add hydrogens automatically or manually to an entire molecule or a selection
- **An advanced open dialog, allowing options to be customized and retained across sessions:**
  - **Reading intermediate geometries**
  - **Using the bond table and weak bond inclusion**
  - **Gaussian input & log file load orders**
  - **PDB and .mol2 file settings**
  - **Saving the formatted checkpoint file**
- Modify bond type/length, bond angles, dihedral angles
- Rationalize structures with an advanced clean function
- Recompute bonding on demand
- Increase **or decrease** symmetry of molecular structure; constrain structure to specific point group
- Mirror invert structure
- Invert structure about selected atom
- Place atom/fragment at centroid of selected atoms
- Define named groups of atoms via:
  - Click, marquee & **brush** selection modes
  - Complex filters combining atom type, number, MM settings, ONIOM layer
  - Select by PDB residue and/or secondary structure (e.g., helix, chain)
  - Expand selections by bond or proximity
  - Use groups for display purposes and in Gaussian input
- Specify nonstandard isotopes
- Customize fragment placement behavior
- **Specify custom bonding parameters**

Graphical Setup for Specific Calculations

Specify input for complex calculations via simple mouse/spreadsheet operations:

- Build unit cells for polymers, 2D surfaces and crystals (periodic boundary conditions)
  - Constrain to specific space group symmetry
- Assign atoms to ONIOM layers by
  - Direct selection
  - Bond proximity to specified atom
  - Absolute distance from specified atom
  - PDB file residue, secondary structure
  - Complex selection criteria
- View/specify MM atom types and charges
- Add/redefine redundant internal coordinates
- Specify frozen atoms/coordinates during optimizations
- Set atom equivalences for QST2/QST3 TS optimizations
- Manipulate MOs: Select, rearrange/reoccupy orbitals for CASSCF, etc.
- Define fragments for fragment guess/counterpoise calculations
  - Assign fragment-specific charges & spin multiplicities
- Include PDB data in molecule specification
- Select normal modes for frequency calculations
- Specify atoms for NMR spin-spin coupling
- **Search for conformations using the GMMX add-on**
- **Full AMPAC integration if software is installed**

Prepare and Run Gaussian Calculations

- Create input files via a menu-driven interface:
  - Select job/method/basis from pop-up menus; related options appear automatically
  - Supports all major **Gaussian 16 features**
  - Convenient access to commonly-used general options
  - **Additional input can be entered**; input sections in imported files are retained
  - **Preview input file before saving/submitting**
- Select solvent and specify other parameters for calculations in solution
- **Specify Link 0 commands**
- **Specify settings for multiprocessor and cluster/network parallel jobs**
- Use calculation schemes to set up jobs from templates
- "Quick launch" Gaussian jobs with a single mouse click
- Molecule specification created automatically
  - Optional connectivity section
- Stream log files in a text-searchable window
- Monitor/control local Gaussian and utility processes
- **Integrated, customizable queuing system**
- Initiate remote jobs via a script
- Generate job-specific input automatically:
  - PBC translation vector for periodic structures like polymers and crystals
  - Orbital alterations
  - Multiple molecule specifications for QST2/QST3 transition state searches
  - **Fragment guess and counterpoise per-fragment charge and spin multiplicity**
- **Apply calculation settings to a group of molecules with one click**
- **Save/submit identical jobs for a group of molecules in a single step, using unique file names**

Examine & Visualize Gaussian Results

- **Select which jobs to open from multi-step results files**
- Show calculation results summary, including basic information, **optimization step data and thermochemical results**
- **Display results tables for a molecule group**
- Examine atomic charges: numerical values, color atoms by charge, dipole moment vector
- **Visualize atomic properties, predicted bond lengths and predicted bond orders**
- Create surfaces and contours for molecular orbitals, electron density, electrostatic potential, spin density, NMR shielding density
  - Display formats: 3D solid, translucent or wire mesh; 2D contour
  - Color surfaces by a separate property
  - Specify the desired contour plane
  - Load cubes created by Gaussian; save computed cubes for future reuse; perform operations on cubes
- Animate normal modes:
  - Indicate motion via displacement vector, dipole derivative unit vector
  - Displace structures along normal mode
  - Select subset of modes for display
  - Save generated normal modes back to checkpoint file
  - **Scale frequencies**
  - **Save animations as MP4 movies, with options for speed, aspect ratio, looping, time delay between frames and frames/loop**

- Display spectra: IR, Raman, NMR, VCD, ROA, UV-Visible, etc.
  - **Select Harmonic and/or Anharmonic results**
  - **Customize plot displays**
  - **Display multiple data sets on a single spectra plot, with optional conformational averaging**
- Substitute isotopes in frequency analysis
- Specify incident light frequency for frequency-dependent calculations
- **Display results from Gaussian trajectory calculations**
- **View energy plot of conformational search result set**
- NMR Results:
  - Report absolute NMR chemical shifts or relative to reference compound
  - Export NMR summary data as text
- Animate structure sequences: geometry optimizations, IRC reaction paths, potential energy surface scans, BOMD and ADMP trajectories
  - Single play or continuous looping; play in reverse
  - **Save animations as MP4 movies, with options for speed, aspect ratio and frame & endpoint delays**
  - Plots of related data are also produced
- Display 3D surface plots for 2-variable scan calculations
- Customize plot and spectra displays by zooming, scaling, inverting, etc.
  - Add molecular properties to plots
  - **Advanced plot customization; line color, canvas and background color, title, x- and y- axis settings, etc.**
  - **Mixture Editor for multiple overlaid plots**
- Save any image to a file (including customizations):
  - Produce web graphics: JPEG, PNG and other formats
  - Produce publication quality graphics files and printouts: TIFF, JPEG, vector graphics EPS
  - Create images at arbitrary size and resolution
  - Select full color or high quality grey scale formats
  - **Specify custom colors and/or background**
- Save plots as images or textual data files
- Save animations in GIF, MNG, **MP4** format or as individual frames
- **Display PCM solvation cavity as a surface**

Customize GaussView

Set/save preferences for most aspects of GaussView functionality:

- Control building toolbars individually
- Colors: per-element, molecule window background, surfaces, transparency
- Builder operation: atom and fragment join methods, adding hydrogens when needed, automated full or partial clean operations, etc.
- Gaussian 16 calculation settings
- **Gaussian job execution methods**
- Display modes
- Window placement and visibility
- Icon sizes
- File/directory locations
- **Image capture and printing defaults**
- **Animation settings and movie defaults**
- Clean function parameters
- Charge distribution display defaults
- **Custom bonding parameters**
- GaussView Tips facility
- Windows file extension associations
- **Dialog-specific help system**

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