What's New in Gaussian 16

New Modeling Capabilities

- **TD-DFT** analytic second derivatives for predicting vibrational frequencies/IR and Raman spectra and performing transition state optimizations and IRC calculations for excited states.
- **EOMCC** analytic gradients for performing geometry optimizations.
- Anharmonic vibrational analysis for VCD and ROA spectra: see **Freq=Anharmonic**.
- Vibronic spectra and intensities: see **Freq=FCHT** and related options.
- Resonance Raman spectra: see **Freq=ReadFCHT**.
- New DFT functionals: **M08HX**, **MN15**, **MN15L**.
- New double-hybrid methods: DSDPBEP86, PBE0DH and PBEQIDH.
- **PM7** semi-empirical method.
- Adamo excited state charge transfer diagnostic: see **Pop=DCT**.
- The EOMCC solvation interaction models of Caricato: see **SCRF=PTED**.
- Generalized internal coordinates, a facility which allows arbitrary redundant internal coordinates to be defined and used for optimization constraints and other purposes. See **Geom=GIC** and *GIC Info*.

Performance Enhancements

- NVIDIA K40 and K80 GPUs are supported under Linux for Hartree-Fock and DFT calculations. See the *Using GPUs* tab for details.
- Parallel performance on larger numbers of processors has been improved. See the *Parallel Performance* tab for information about how to get optimal performance on multiple CPUs and clusters.
- Gaussian 16 uses an optimized memory algorithm to avoid I/O during CCSD iterations.

There are several enhancements to the GEDIIS optimization algorithm.

- **CASSCF** improvements for active spaces ≥ (10,10) increase performance and make active spaces of up to 16 orbitals feasible (depending on the molecular system).
- Significant speedup of the core correlation energies for **W1** compound model.
- Gaussian 16 incorporates algorithmic improvements for significant speedup of the diagonal, second-order self-energy approximation (D2) component of composite electron propagator (CEP) methods as described in [DiazTinoco16]. See **EPT**.