Gaussian 09 Available Source Code Versions for Rev. B.01

Additional Notes for Source Code Version (see also notes above):

- An upgraded version of **Linda** is required when upgrading from *Gaussian 03* to *Gaussian 09*.
- In order to build on Intel-based Macintosh computers, the source code and tools must be installed on an HFS+ *case-sensitive* file system (or a UFS file system for systems where that is supported). Building *Gaussian 09* from source code is not supported for PowerPC-based Macintosh systems (including universal binaries). Finally, G09M binaries are not supported on Intel Macs (i.e., running under Rosetta).

Vendor	CPU	Shared Memory Parallel	Linda Parallel	OS Version(s)	Fortran	C	Libraries
AMD	AMD64 (Opteron, Athlon 64).	Y	Y	SuSE Linux 9.3, 10.3, 11.1; SuSE Linux Enterprise 10; Red Hat Enterprise Linux 5.3, 5.4	Portand Group F77 10.5 www.pgroup.com	gcc included with Linux	Atlas (included on G09 CD)
Apple	IA32 (32-bit Intel Mac)	Y	Y	OS X 10.5.8 and 10.6.4	Portand Group F77 10.5 www.pgroup.com	gcc 4.0.1 and 4.2.1	Atlas (included on G09 CD)
Apple	EM64T (64-bit Intel Mac)	Y	Y	OS X 10.5.8 and 10.6.4	Portand Group F77 10.5 www.pgroup.com	gcc 4.0.1 and 4.2.1	Atlas (included on G09 CD)
HP	Alpha	Y	Y	Tru64 5.1B	F95 V5.5A-3548	6.5-011	CXML 5.2
HP	Intel Itanium2 (IA64)	Y	N	HP-UX 11	F90 version 3.1.1	A.06.12	
IBM	eServer pSeries (RS/6000) work-stations, Power 5 (64-bit)	Y	Y	AIX 5.3	10.1	8.0	xlsmp 1.5.0.0; Atlas (included on G09 CD)
IBM	eServer pSeries (RS/6000) work-stations, Power 6 (64-bit)	Y	Y	AIX 5.3	13.1	11.1	xlsmp 2.1.0.0; Atlas (included on G09 CD)
IBM	eServer pSeries (RS/6000) work-stations, Power 5 (64-bit)	Y	Y	SuSE Linux Enterprise Server 10	10.1.1	8.0.1	Atlas (included on G09 CD)
Intel IA32 & AMD Athlon-based systems	IA32 (Pentium III and higher); AMD Athlon	Y	Y	Red Hat Ent. Linux 5.3; SuSE Linux 9.3, 10.3, 11.1; SuSE Linux Enterprise 10	Portland Group F77 10.5 www.pgroup.com	gcc included with Linux	Atlas (included on G09 CD)
Intel EM64T-based systems	Intel EM64T	Y	Y	Red Hat Ent. Linux 5.3, 5.4, 5.5; SuSE Linux 9.3, 10.3, 11.1, 11.2; SuSE Linux Enterprise 10, 11 SP1	Portland Group F77 10.5 www.pgroup.com	gcc included with Linux	Atlas (included on G09 CD)
Intel IA64-based systems	Intel Itanium2 (IA64)	Y	Y	Red Hat Enterprise 5.2; SuSE Linux Enterprise Server 9 and 10	Intel Version 11.1 Update 6 (11.1.072, Build 20100401; l_fc_p_11.1.072)	Intel Version 11.1 Update 6 (11.1.072, Build 20100401; l_cc_p_11.1.072)	Intel MKL 10.2 Update 5 (10.2.5.035)
SGI	R1x000 (64-bit)	Y	N	IRIX 6.5.4 or later	7.4	7.4	SCSL 18
Sun	AMD Opteron; EM64T; UltraSPARC	*Building from source code not yet supported; contact Gaussian Technical Support for details.*					

Gaussian 09 Available Binary Versions for Rev. B.01

Important Notes for All Gaussian Versions (Binary and Source):

- An upgraded version of **Linda** is required when upgrading from *Gaussian 03* to *Gaussian 09*.
- The Linux RedHat and SuSE versions specified for IA32, IA64 and EM64T/Operton systems refer only to the *unmodified, unpatched* original media/ISO image distributions as released by the vendor.
- PowerPC-based Macintosh computers require ***Gaussian 09M***. G09M binaries are *not* supported on Intel Macs (i.e., running under Rosetta).

Vendor	CPU	Shared Memory Parallel	Linda Parallel	OS Version(s)	Required Libraries
AMD	AMD64 (Opteron, Athlon 64)	Y	Y	SuSE Linux 9.3, 10.3, 11.1; SuSE Linux Enterprise 10; Red Hat Enterprise 5.3, 5.4	
Apple	IA32 (32-bit Intel Mac)	Y	Y	OS X 10.5.8 and 10.6.4	
Apple	EM64T (64-bit Intel Mac)	Y	Y	OS X 10.5.8 and 10.6.4	
HP	Alpha	Y	Y	Tru64 5.1B	CXML 5.2
HP	Intel Itanium2 (IA64)	Y	N	HP-UX 11	
IBM	eServer pSeries (RS/6000) workstations, Power 5 (64-bit)	Y	Y	AIX 5.3	xlsmp.rte-1.5.0.0 or higher - 1.8 does not work
IBM	eServer pSeries (RS/6000) workstations, Power 6 (64-bit)	Y	Y	AIX 5.3	xlsmp.rte-2.1.0.0
IBM	eServer pSeries (RS/6000) workstations, Power 5 (64-bit)	Y	Y	SuSE Linux Enterprise Server 10	xlf.rte-10.1.1 xlsmp.rte-1.6.1
Intel IA32 & AMD Athlon-based systems	Intel IA32 (Pentium IV or higher) and AMD Athlon	Y	Y	Red Hat Enterprise Linux 5.3; SuSE Linux 9.3, 10.3, 11.1; SuSe Linux Enterprise 10	
Intel EM64T-based systems	Intel EM64T	Y	Y	Red Hat Enterprise Linux 4.7, 5.3, 5.4, 5.5; SuSE Linux 9.3, 10.3, 11.1, 11.2; SuSE Linux Enterprise 10, 11 SP1	
Intel IA64-based systems	Intel Itanium2 (IA64)	Y	Y	Red Hat Enterprise Linux 5.2 SuSE Linux Enterprise Server 9 and 10	
SGI	R1x000 (64-bit)	Y	N	IRIX 6.5.4 or later	SCSL 18
Sun	AMD64 (Opteron)	Y	Y	Solaris 10	
Sun	EM64T	Y	Y	Solaris 10	
Sun	UltraSPARC	Y	Y	Solaris 10	

Gaussian 09 Revision B.01 Release Notes

19 August 2010

Contents

Feature and Usage Notes

- If CIS frequencies are to be used with the Herzberg-Teller or Franck-Condon-Herzberg-Teller analysis, the CIS frequencies must be done numerically (**Freq=Numer** rather than **Freq**). This is because the transition dipole derivatives are not computed during the analytic force constant evaluation. The corresponding HF frequency calculation on the ground state, which is also required, can be done analytically as usual.
- CIS and CASSCF frequencies with PCM solvation must also be done numerically using **Freq=Numer**.
- The linear scaling (FMM-based) algorithms are now Linda-parallel, so Linda parallel jobs on large molecules do not need to specify **NoFMM**, and will run faster with the default algorithms chosen by the program.
- **Opt=GDIIS** is still present but deprecated; the new default optimization algorithm (**Opt=GEDIIS**) is better than GDIIS for the few cases where GDIIS was better than the G03 default (**Opt=RFO**).
- Optimizations of large molecules which have many very low frequency vibrational modes with DFT will often proceed more reliably when a larger DFT integration grid is requested (**Int=UltraFine**).
- Density fitting can be made the default for jobs using pure DFT functionals by adding the **DenFit** keyword to the route section (-#-) line in the **Default.Route** file. Fitting is faster than doing the Coulomb term exactly for systems up to several hundred atoms (depending on basis set), but is slower than exact Coulomb using linear scaling techniques (which are turned on automatically with exact Coulomb) for very large systems.
- The default IRC algorithm has changed; refer to the *User's Guide* for details. The default is to report only the energies and reaction coordinate at each point on the path; if geometrical parameters along the path are desired, these should be defined as redundant internal coordinates via **Geom=ModRedundant** or as input to the IRC code via **IRC(Report=Read)**.
- The references for variations of the M06 functional were swapped and incomplete. The correct references are: M06HF [Zhao06b,Zhao06c], M062X [Zhao08]. The M05 functionals are also still available: M05 [Zhao05] and M052X [Zhao06].

Missing, Corrected and Updated References

Boese02 A. D. Boese and N. C. Handy, "New exchange-correlation density functionals: The role of the kinetic-energy density," *J. Chem. Phys.*, **116** (2002) 9559-69.

Cammi00a R. Cammi, C. Cappelli, S. Corni, and J. Tomasi, "On the calculation of infrared intensities in solution within the polarizable continuum model," *J. Phys. Chem. A*, **104** (2000) 9874-79.

Clemente08 F. Clemente, T. Vreven, and M. J. Frisch, in *Quantum Biochemistry*, Ed. C. Matta (Wiley VCH, 2008).

Collins02 M. A. Collins, "Molecular potential-energy surfaces for chemical reaction dynamics," *Theor. Chem. Acc.*, **108** (2002) 313-24.

Fukui81 K. Fukui, "The path of chemical-reactions — The IRC approach," *Acc. Chem. Res.*, **14** (1981) 363-68.

Henderson09 T. M. Henderson, A. F. Izmaylov, G. Scalmani, and G. E. Scuseria, "Can short-range hybrids describe long-range-dependent properties?" *J. Chem. Phys.*, 131 (2009) 044108.

Izmaylov06 A. F. Izmaylov, G. Scuseria, and M. J. Frisch, "Efficient evaluation of short-range Hartree-Fock exchange in large molecules and periodic systems," *J. Chem. Phys.*, 125 (2006) 104103: 1-8.

Marenich09 A. V. Marenich, C. J. Cramer, and D. G. Truhlar, "Universal solvation model based on solute electron density and a continuum model of the solvent defined by the bulk dielectric constant and atomic surface tensions," *J. Phys. Chem. B*, 113 (2009) 6378-96.

Zhao05 Y. Zhao, N. E. Schultz, and D. G. Truhlar, "Exchange-correlation functional with broad accuracy for metallic and nonmetallic compounds, kinetics, and noncovalent interactions," *J. Chem. Phys.*, **123** (2005) .

Zhao06 Y. Zhao, N. E. Schultz, and D. G. Truhlar, "Design of density functionals by combining the method of constraint satisfaction with parametrization for thermochemistry, thermochemical kinetics, and noncovalent interactions," *J. Chem. Theory and Comput.*, **2** (2006) 364-82.

Zhao06a Y. Zhao and D. G. Truhlar, "A new local density functional for main-group thermochemistry, transition metal bonding, thermochemical kinetics, and noncovalent interactions," *J. Chem. Phys.*, **125** (2006) 194101: 1-18.

Zhao06c Y. Zhao and D. G. Truhlar, "Density Functional for Spectroscopy: No Long-Range Self-Interaction Error, Good Performance for Rydberg and Charge-Transfer States, and Better Performance on Average than B3LYP for Ground States," *J. Phys. Chem. A*, **110** (2006) 13126-30.

Gaussian 09 User's Reference Errata

- The following are missing from the list of links (pp. 38-39):
  L117 Performs IPCM calculations.
  L610 Numerical integration (for testing integral codes).
  The following links included in the list are not part of Gaussian 09: L909, L921, L922.
- The "thresh" keyword described in the discussion of selecting normal mode output on pages 107 and 289 is not available.
- The reference to Opt=DiagFull on page 116 should be Freq=DiagFull.

Gaussian 09 IOps Reference Errata

The description of IOps(1/111-113) is incorrect. Here is the corrected version:

IOp(1/111)

L103: Step-size to use with steepest descent when L103 is having trouble.

-N Scale up to RMS step of N/1000 if DXRMS is less.
-1 Effectively disables the scaling.
0 Default (50).
N Scale up or down to maximum change in a variable of N/1000.

L101: Temperature for thermochemistry.

0 Default (standard temperature, unless read in).
N N/1000 degrees.
-N N/1000000 degrees.

IOp(1/112)

Pressure for thermochemistry.

0 Default (1 atmosphere, unless read in).
N N/1000 atmospheres.
-N N/1000000 atmospheres.

IOp(1/113)

Scale factor for harmonic frequencies for use in thermochemistry and harmonic vibration-rotation analysis.

0 Default (1 unless specified by IOp in overlay 7 or read in).
N N/1000000.

Note that IOp(1/114) is not defined.