

Gaussian 16 Available Binary Versions for Rev. C.01 and C.02

Important Notes for All Gaussian Binary Versions:

- Beginning with Revision C.01, *Linda 9.2* is required for network parallel use of *Gaussian 16*. Earlier versions of *Linda* are incompatible. Thus, upgrading from *Gaussian 16 Rev. A.03* or *B.01 w/Linda* to *G16 Rev. C.01* or *C.02 w/Linda* or *G16 Rev. C.02 w/Linda* requires an update to *Linda 9.2*.
- The Linux RedHat and SuSE versions specified for x86_64, IA32, and IBM Power systems refer only to the *unmodified, unpatched* original media/ISO image distributions as released by the vendor.

Revision C.01 x86_64 AVX-enabled Binary Version:

- The AMD/Intel x86_64 AVX-enabled binary version includes GPU support for NVIDIA K40, K80, P100, and V100 boards with 12 GB of memory or higher. A version of NVIDIA drivers compatible with CUDA 10.0 is required to run on these GPUs with this binary version. (NVIDIA drivers can be found at www.nvidia.com/download/index.aspx).

REVISION C.01

Vendor	CPU	Shared Memory Parallel	Linda Parallel	OS Version(s)	Required Libraries & Drivers
AMD/Intel	x86_64 ("Legacy" – pre-SSE4.2)	Y	Y	openSUSE Linux 10.3, 11.4, 12.3, 13.2, Leap 42.3, 15.0; SUSE Linux Enterprise Server 11 SP4, 12 SP4, 15; Red Hat Enterprise Linux 5.11, 6.10, 7.6	
AMD/Intel	x86_64 (SSE4.2-enabled)	Y	Y	openSUSE Linux 11.4, 12.3, 13.2, Leap 42.3, 15.0; SUSE Linux Enterprise Server 11 SP4, 12 SP4, 15; Red Hat Enterprise Linux 5.11, 6.10, 7.6	
AMD/Intel	x86_64 (AVX-enabled)	Y	Y	openSUSE Linux 13.2, Leap 42.3, 15.0; SUSE Linux Enterprise Server 11 SP4, 12 SP4, 15; Red Hat Enterprise Linux 5.11, 6.10, 7.6, 8.3	Drivers compatible with NVIDIA CUDA 10.0
AMD Athlon and Intel IA32-based systems	IA32 (Pentium IV and higher); AMD Athlon	Y	Y	SuSE Linux 10.3, 11.4; Red Hat Enterprise Linux 5.6, 6.1	
Apple	EM64T (64-bit Intel Mac)	Y	Y	OS X 10.6.8, 10.7.5, 10.8.5, 10.9.5, 10.10.5, 10.11.6, 10.12.6, 10.13.6, 10.14.5	
IBM	Power 5 (64-bit)	Y	Y	AIX 5.3	
IBM	Power 7 (64-bit)	Y	Y	AIX 6.1, 7.1	xlsmp.rte 3.1.0.3
IBM	Power 7 (64-bit)	Y	Y	SuSE Enterprise Linux 11 SP2; Red Hat Enterprise Linux 6.3 (big endian)	xlsmp.rte 4.1.0.2
IBM	Power 8 (64-bit)	Y	Y	AIX 7.2	xlsmp 4.1.3.0
IBM	Power 8 (64-bit)	Y	Y	RedHat Enterprise Linux 7.3 (big endian)	xlsmp 4.1.0.2
IBM	Power 8 (64-bit)	Y	Y	RedHat Enterprise Linux 7.3 (little endian)	xlsmp 4.1.3.0
IBM	Power 9 (64-bit)	Y	Y	RedHat Enterprise Linux 7.6 (little endian)	xlsmp 5.1.1.0

Revision C.02 x86_64 AVX2-enabled Binary Version:

- Revision C.02 is an update to support the NVIDIA A100 (Ampere) GPUs. It is available for the AMD/Intel x86_64 AVX2-enabled platform only, which also supports NVIDIA K40, K80, P100, V100 and A100 GPUs with 12 GB of memory or higher. A version of NVIDIA drivers compatible with CUDA Toolkit 11.2 is required to run the Revision C.02 binaries on these GPUs (NVIDIA drivers can be found at www.nvidia.com/download/index.aspx).

Revision C.02 Apple M1/M2 Binary Version:

- Revision C.02 adds support for the Apple M1/M2 processors. Builds from source code are not supported.

REVISION C.02

Vendor	CPU	Shared Memory Parallel	Linda Parallel	OS Version(s)	Required Libraries & Drivers
AMD/Intel	x86_64 (AVX2-enabled)	Y	Y	openSUSE Leap 42.3, 15.x; SUSE Linux Enterprise Server 12 SP4, 15; Red Hat Enterprise Linux 8.3	Compatible with NVIDIA CUDA 11.2
Apple	M1/M2	Y	N	macOS 12.3-13.3.1	
Fujitsu	ARM A64FX (FX700, FX1000)	Y	N	Red Hat Enterprise Linux 8.4	FX700 - FUJITSU Software Compiler Package V1.0L21 (cp-1.0.21.02) FX1000 - FUJITSU Software Technical Computing Suite V4.0L20 (tcsds-1.2.36)

Gaussian 16 Available Source Code Versions for Rev. C.01

FOR REVISION C.02, SEE THE NEXT PAGE

Important Notes for Gaussian 16 Revision C.01 Source Code:

- Binaries for platforms marked with † can be built with GPU support for NVIDIA K40, K80, P100, and V100 boards with 12 GB of memory or higher. NVIDIA A100 GPUs require *Gaussian 16 Revision C.02*. A version of NVIDIA drivers compatible with CUDA 10.0 is required to run binaries built with Revision C.01 source code on these GPUs (NVIDIA drivers can be found at www.nvidia.com/download/index.aspx).
- *Linda 9.2* is required for network parallel use of *Gaussian 16 Revision C.01*. Earlier versions of *Linda* are incompatible. Thus, upgrading from *Gaussian 16 Rev. A.03* or *B.01 w/Linda* to *G16 Rev. C.01 w/Linda* requires an update to *Linda 9.2*.
- 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).
- The Linux RedHat and SuSE versions specified for x86_64, IA32, and IBM Power systems refer only to the *unmodified, unpatched* original media/ISO image distributions as released by the vendor.

Vendor	CPU	Shared Memory Parallel	Linda Parallel	OS Version(s)	Fortran	C	Libraries & Drivers
AMD/Intel	x86_64 ("Legacy" – pre-SSE4.2)	Y	Y	openSUSE Linux 10.3, 11.4, 12.3, 13.2, Leap 42.3; SUSE Linux Enterprise Server 11 SP4, 12 SP4; Red Hat Enterprise Linux 5.11, 6.10, 7.6	Portland Group F77 17.7 www.pgroup.com	gcc included with Linux	Atlas (included on G16 CD)
AMD/Intel	x86_64 (SSE4.2-enabled)	Y	Y	openSUSE Linux 11.4, 12.3, 13.2, Leap 42.3; SuSE Linux Enterprise Server 11 SP4, 12 SP4; Red Hat Enterprise Linux 5.11, 6.10, 7.6	Portland Group F77 17.7 www.pgroup.com	gcc included with Linux	Atlas (included on G16 CD)
AMD/Intel	x86_64 (AVX-enabled) †	Y	Y	openSUSE Linux 13.2, Leap 42.3; SuSE Linux Enterprise Server 11 SP4, 12 SP4; Red Hat Enterprise Linux 6.10, 7.6	Portland Group F77 18.10 www.pgroup.com	gcc included with Linux	Atlas (included on G16 CD); drivers compatible with NVIDIA CUDA 10.0
AMD/Intel	x86_64 (AVX2-enabled) †	Y	Y	openSUSE Linux 13.2, Leap 42.3; SuSE Linux Enterprise Server 11 SP4, 12 SP4; Red Hat Enterprise Linux 6.10, 7.6	Portland Group F77 18.10 www.pgroup.com	gcc included with Linux	Atlas (included on G16 CD); drivers compatible with NVIDIA CUDA 10.0
AMD Athlon & Intel IA32-based systems	IA32 (Pentium IV and higher); AMD Athlon	Y	Y	SuSE Linux 10.3, 11.4; Red Hat Enterprise Linux 5.6, 6.1	Portland Group F77 16.5 www.pgroup.com	gcc included with Linux	Atlas (included on G16 CD)
Apple	EM64T (64-bit Intel Mac)	Y	Y	OS X 10.9.5, 10.10.5, 10.11.6, 10.12.6, 10.13.6	Portland Group F77 18.10 www.pgroup.com	XCode corresponding to OS X version	Atlas (included on G16 CD)
IBM	Power 7 (64-bit)	Y	Y	AIX 6.1, 7.1	XLF 13.1.0.12	XLC 11.1.0.12	xlsmpl 3.1.0.3; Atlas (included on G16 CD)
IBM	Power 7 (64-bit)	Y	Y	SuSE Enterprise Linux 11 SP2; Red Hat Enterprise Linux 6.3	XLF 13.1.0.7	XLC 11.1.0.7	xlsmpl 2.1.0.7; Atlas (included on G16 CD)
IBM	Power 8 (64-bit)	Y	Y	AIX 7.2	XLF 15.1.3.4	XLC 13.1.3.4	xlsmpl 4.1.3.0; Atlas (included on G16 CD)
IBM	Power 8 (64-bit)	Y	Y	RedHat Enterprise Linux 7.3 (big endian)	XLF 15.1.0.2	XLC 13.1.0.2	xlsmpl 4.1.0.2; Atlas (included on G16 CD)
IBM	Power 8 (64-bit)	Y	Y	RedHat Enterprise Linux 7.3 (little endian)	XLF 15.1.3.0	XLC 13.1.3.0	xlsmpl 4.1.3.0; Atlas (included on G16 CD)
IBM	Power 9 (64-bit)	Y	Y	RedHat Enterprise Linux 7.6 (little endian)	XLF 16.1.1.0	XLC 16.1.1.0	xlsmpl 5.1.1.0; Atlas (included on G16 CD)

Gaussian 16 Available Source Code Versions for Rev. C.02

Important Notes for Gaussian 16 Revision C.02 Source Code:

- Binaries for the AMD/Intel x86_64 AVX2-enabled platform can be built with GPU support for NVIDIA K40, K80, P100, V100 and A100 boards with 12 GB of memory or higher. A version of NVIDIA drivers compatible with CUDA 11.2 is required to run binaries built with the Revision C.02 source code (NVIDIA drivers can be found at www.nvidia.com/download/index.aspx).
- Other binaries may also be built from the Revision C.02 source code DVD. Although their functionality has not changed, the build procedure for the other AMD/Intel x86_64-based binary versions has been modified to use the compilers in the NVIDIA HPC SDK. Their requirements are listed in the second table below.
- *Linda 9.2* is required for network parallel use of *Gaussian 16 Revision C.01*. Earlier versions of *Linda* are incompatible. Thus, upgrading from *Gaussian 16 Rev. A.03* or *B.01 w/Linda* to *G16 Rev. C.01 w/Linda* requires an update to *Linda 9.2*.
- 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).
- The Linux RedHat and SuSE versions specified for x86_64, IA32, and IBM Power systems refer only to the *unmodified*, *unpatched* original media/ISO image distributions as released by the vendor.

REVISION C.02 PLATFORM WITH NVIDIA A100 SUPPORT

Vendor	CPU	Shared Memory Parallel	Linda Parallel	OS Version(s)	Fortran	C	Libraries & Drivers
AMD/Intel	x86_64 (AVX2-enabled)	Y	Y	openSUSE Linux 15.x, Leap 42.3; SuSE Linux Enterprise Server 12 SP4; Red Hat Enterprise Linux 8.3	NVIDIA HPC SDK 21.3 developer.nvidia.com/hpc-sdk	gcc included with Linux	Atlas (included on G16 CD); drivers compatible with NVIDIA CUDA 11.2

REVISION C.02 PLATFORMS WITH NEW BUILD PROCEDURE

Vendor	CPU	Shared Memory Parallel	Linda Parallel	OS Version(s)	Fortran	C	Libraries
AMD/Intel	x86_64 ("Legacy" – pre-SSE4.2)	Y	Y	openSUSE Linux 15.x, Leap 42.3; SuSE Linux Enterprise Server 12 SP4; Red Hat Enterprise Linux 8.3	NVIDIA HPC SDK 21.3 developer.nvidia.com/hpc-sdk	gcc included with Linux	Atlas (included on G16 CD)
AMD/Intel	x86_64 (SSE4.2-enabled)	Y	Y	openSUSE Linux 15.x, Leap 42.3; SuSE Linux Enterprise Server 12 SP4; Red Hat Enterprise Linux 8.3	NVIDIA HPC SDK 21.3 developer.nvidia.com/hpc-sdk	gcc included with Linux	Atlas (included on G16 CD)
AMD/Intel	x86_64 (AVX-enabled)	Y	Y	openSUSE Linux 15.x, Leap 42.3; SuSE Linux Enterprise Server 12 SP4; Red Hat Enterprise Linux 8.3	NVIDIA HPC SDK 21.3 developer.nvidia.com/hpc-sdk	gcc included with Linux	Atlas (included on G16 CD)

REVISION C.02 PLATFORMS UNCHANGED FROM REVISION C.01

Vendor	CPU	Shared Memory Parallel	Linda Parallel	OS Version(s)	Fortran	C	Libraries
AMD Athlon & Intel IA32-based systems	IA32 (Pentium IV and higher); AMD Athlon	Y	Y	SuSE Linux 10.3, 11.4; Red Hat Enterprise Linux 5.6, 6.1	Portland Group F77 16.5 www.pggroup.com	gcc included with Linux	Atlas (included on G16 CD)
Apple	EM64T (64-bit Intel Mac)	Y	Y	OS X 10.9.5, 10.10.5, 10.11.6, 10.12.6, 10.13.6	Portland Group F77 18.10 www.pggroup.com	XCode corresponding to OS X version	Atlas (included on G16 CD)
IBM	Power 7 (64-bit)	Y	Y	AIX 6.1, 7.1	XLF 13.1.0.12	XLC 11.1.0.12	xlsmpl 3.1.0.3; Atlas (included on G16 CD)
IBM	Power 7 (64-bit)	Y	Y	SuSE Enterprise Linux 11 SP2; Red Hat Enterprise Linux 6.3	XLF 13.1.0.7	XLC 11.1.0.7	xlsmpl 2.1.0.7; Atlas (included on G16 CD)
IBM	Power 8 (64-bit)	Y	Y	AIX 7.2	XLF 15.1.3.4	XLC 13.1.3.4	xlsmpl 4.1.3.0; Atlas (included on G16 CD)
IBM	Power 8 (64-bit)	Y	Y	RedHat Enterprise Linux 7.3 (big endian)	XLF 15.1.0.2	XLC 13.1.0.2	xlsmpl 4.1.0.2; Atlas (included on G16 CD)
IBM	Power 8 (64-bit)	Y	Y	RedHat Enterprise Linux 7.3 (little endian)	XLF 15.1.3.0	XLC 13.1.3.0	xlsmpl 4.1.3.0; Atlas (included on G16 CD)
IBM	Power 9 (64-bit)	Y	Y	RedHat Enterprise Linux 7.6 (little endian)	XLF 16.1.1.0	XLC 16.1.1.0	xlsmpl 5.1.1.0; Atlas (included on G16 CD)