

Installation guide for GAMESS on Windows

Feb. 15, 2017

1. Access to website link below.

http://www.msg.ameslab.gov/games/License_Agreement.html

Gordon Group/GAMESS Hom... X +

www.msg.ameslab.gov/games/License_Agreement.html

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GAMESS

GAMESS User License Agreement

All GAMESS requestors MUST agree to the following license agreement which covers all versions of GAMESS (source code, and binaries for Windows, Macintosh and ChemOffice).

With regard to the ab initio quantum chemistry code GAMESS, together with its associated graphics and utility programs, with which you have supplied me a copy, I agree to the following conditions:

1. I will not supply a copy of the code to anyone outside my institution or corporation for any reason whatsoever. Instead, I will refer any requests for copies of the program to you at ISUQCG. This in no way limits my making of copies of the code for backup purposes, or for running on more than one computer system at my institution or home.
2. I understand that copyright or ownership rights to GAMESS are retained by ISUQCG and contributors to the GAMESS package. I will not incorporate any part of GAMESS into any other program system, either for sale or for non-profit distribution, without written permission from ISUQCG.
3. I understand that no large program such as GAMESS can be considered to be bug free, and accordingly the ISUQCG supplies the GAMESS software on an "as is" basis, with no additional responsibility or liability.
4. If results obtained with GAMESS are published in the scientific literature, I will reference the program from the article M.W.Schmidt, K.K.Baldrige, J.A.Boatz, S.T.Elbert, M.S.Gordon, J.H.Jensen, S.Koseki, N.Matsunaga, K.A.Nguyen, S.J.Su, T.L.Windus, M.Dupuis, J.A.Montgomery J. Comput. Chem. 14, 1347-1363 (1993). Using specific methods included in GAMESS may require citing additional articles, as described in the manual. I agree to honor the request to cite additional papers, as appropriate.
5. This license is considered a "Research Group" license. Thus anyone directly associated with your research group is covered by the license and may share your copy of GAMESS on all of your group's computer resources.

I agree to the above terms ←

I do not agree to the above terms

Click [I agree to the above terms].

GAMESS Registration: Downlo... × +

www.msg.ameslab.gov/GAMESS/download/register/ 67%

GAMESS Registration System

Request Download

Fields in bold face type are required.

Email address:

Select desired programs below

Pre-compiled Binary Distributions

Distributions tested on their platform:

- GAMESS version August 18, 2016 R1 for Apple MacOS X
- GAMESS version August 18, 2016 R1 for Microsoft Windows**
- GAMESS version Sep 6 2001 for MacOS 7-9
- GAMESS (VigyanCD based on an obsolete version of GAMESS) version 1.0 beta for 32 bit x86 compatible PC
- GAMESS for ChemOffice version 6-9 (Does not include ChemOffice or work with more recent versions) version June 2003 for Microsoft Windows

Source Code Distributions

There is only one combined source code version of GAMESS, containing versions to compile on any of the machines listed below: You will be downloading only one tar file, so please check only the versions you will actually be using. Your choice(s) serve as a survey of the actual usage of different machine types, so please check all of the machines which you do actually intend to use.

Distributions well-tested on their platform:

- GAMESS version August 18, 2016 R1 for 32 bit (x86 compatible) under Linux
- GAMESS version August 18, 2016 R1 for 64 bit (x86_64 compatible) under Linux with gnu compilers
- GAMESS version August 18, 2016 R1 for 64 bit IA64/x86_64 under Linux with Intel compilers
- GAMESS version August 18, 2016 R1 for Apple MacOS X
- GAMESS version August 18, 2016 R1 for AXP under Tru64/Linux (sold as Digital, Compaq, or HP)
- GAMESS version August 18, 2016 R1 for Cray XI under Unicos
- GAMESS version August 18, 2016 R1 for Cray XT
- GAMESS version August 18, 2016 R1 for Fujitsu PrimePower under Solaris OE
- GAMESS version August 18, 2016 R1 for HP PA-RISC or Intel under HP-UX
- GAMESS version August 18, 2016 R1 for IBM BlueGene
- GAMESS version August 18, 2016 R1 for IBM Power/PowerPC processors under AIX and Linux
- GAMESS version August 18, 2016 R1 for IBM SP under AIX
- GAMESS version August 18, 2016 R1 for Intel Xeon Phi
- GAMESS version August 18, 2016 R1 for Microsoft Windows HPC Server 2008 using PGI compilers
- GAMESS version August 18, 2016 R1 for NEC-SX series
- GAMESS version August 18, 2016 R1 for Sun Opteron or UltraSPARC under Solaris
- GAMESS+LIBCCHEM version August 18, 2016 R1 for NVIDIA GPUs

Distributions for older systems (extra effort may be needed to run)

- GAMESS version August 18, 2016 R1 for Cray T3E under Unicos
- GAMESS version August 18, 2016 R1 for Cray vector machine under Unicos
- GAMESS version August 18, 2016 R1 for SGI MIPS under Irix

Request submission may take a few minutes. Please only click the Submit button once.

1) Put your email address.

2) Check 'GAMESS versionfor Microsoft Windows'

3) Click [Submit Request].

2. Download GAMESS by following the instructions in the email (see the fig. below).

Caution! The mail sometime delays in a few days.

You can download GAMESS for Windows binaries with your browser by going to:
<http://www.msg.chem.iastate.edu/GAMESS/download/Windows64.html>
Instructions are provided on that web page for downloading and unpacking the GAMESS for Windows archive. The username is: source

You will need the password listed below:

Please note that the password will be changed regularly (usually weekly on Sunday). You should therefore arrange to complete the downloading of the source in a timely manner, before the password is changed. The password this week is:

aKEGiVMQ

next week it will be:

Fud1COKg

Enjoy the program!

Programs requested:

GAMESS version August 18, 2016 R1 for Microsoft Windows

1) Copy the password to download.

2) Access to the link in the email.

Welcome to GAMESS Microsoft Windows Operating Systems.

64-Bit Windows

Notice: Native binaries for 32-bit Microsoft Windows Operating Systems are no longer supported. It can, however, be compiled from the source.

This version is the complete version of GAMESS (with Tinker, NEO, and VB2000) precompiled for use on 64-bit Windows. To download any of these Windows binaries, just click on your choice below, enter the username (which is always **source**), and the current download password, from the e-mail you should have already received. Once downloaded, you just need to double click on the .msi file, and read the instructions.

The files are Microsoft Setup and Installation types (.msi). All post Windows-2000 installations should have an msixec to run it.

Release	Download (.msi)	Compiler	Optimization Flags	Math Library	Comments
2016 R1	gameSS-64-2016-pgi-linux-mkl.msi	PGI	-Mipa=fast,safe	Intel MKL	all exam files pass
2016 R1	gameSS-64-2016-pgi-linux-pgi.msi	PGI v. 15.4	-fastsse -Mipa=fast,safe	PGI BLAS	all exam files pass
2016 R1	gameSS-64-2016-intel-linux-mkl.msi	Intel		Intel MKL	exam 43 fail

If you are unsure which .msi file to choose then please select the executable name in **BOLD**.

You should also download the directions file, [GAMESS-WINDOWS-README.pdf](#), which contains screen shots of how to install and execute GAMESS.

Recent versions of Chemdraw (in Chem Office) can prepare and then execute GAMESS input. In order to do so, please follow the installation direction files just noted. After GAMESS itself works, you need to copy the file C:\Users\Public\gameSS-64\runGms.gms to C:\Users\Public\gameSS-64\parameters.gms. The interface should then work, provided you did succeed in running GAMESS by itself, according to the direction file named above.

32-Bit Windows

If your PC is running an extremely old version of Windows, which is only a 32-bit version, we provide a very old 32-bit [binary](#). This [binary](#) is derived from the Oct 1, 2012 (R3) source code. Not everything mentioned in the manual will work, nor are bug fixes from the following years included. You will also need the [directions](#) for installing this old binary file. No one should use this old binary unless their computer is incapable of 64-bit operation!

for 32-bit Windows

3) Download the installer package

[for 64-bit Windows]

The msi file in boldface (See the fig. above)

[for 32-bit Windows]

'32-bit binary'

4) Username and password are asked. Type as follows.

username: source

password: (from the email)

See

<http://www.msg.chem.iastate.edu/GAMESS/download/GAMESS-Windows-64-Bit-README-THE-N-README-AGAIN.pdf>

<http://www.msg.chem.iastate.edu/GAMESS/download/source/Windows/32bit/WinGAMESS-setup-guide-32.pdf>

for detail.

3. Unpack .msi file

1) Move to the folder containing .msi file.

2) Double-click .msi file. The setup wizard starts.



3) Click [Next] and follow the instructions on the wizard.

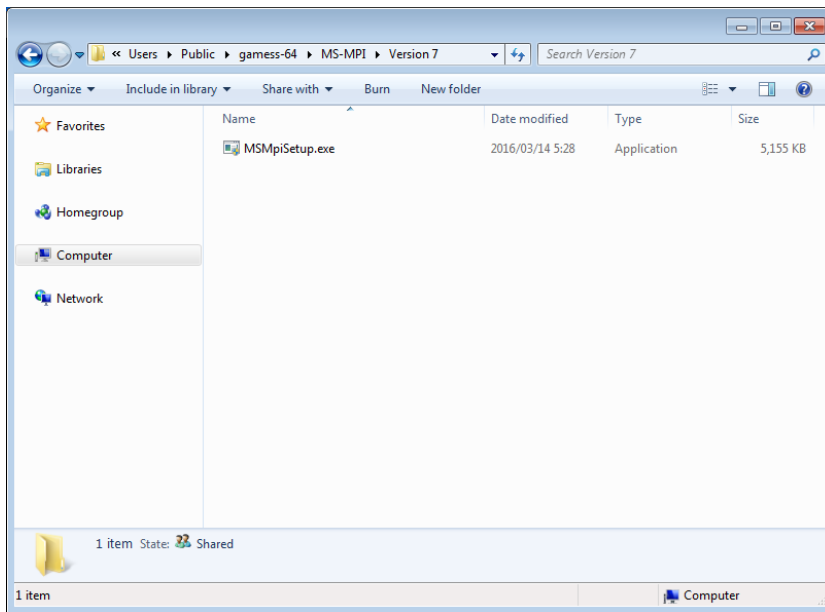
The folder to be installed must not be include white spaces.

4. MPI Installation

(for 64-bit version)

1) Move to the folder GAMESS installed (e.g. C:\Users\Public\gamess-64)

2) Move to MS-MPI\Version 7



3) Double-click MSMpiSetup.exe and follow the instruction to install MS-MPI.

4) Restart Windows.

(for 32-bit version)

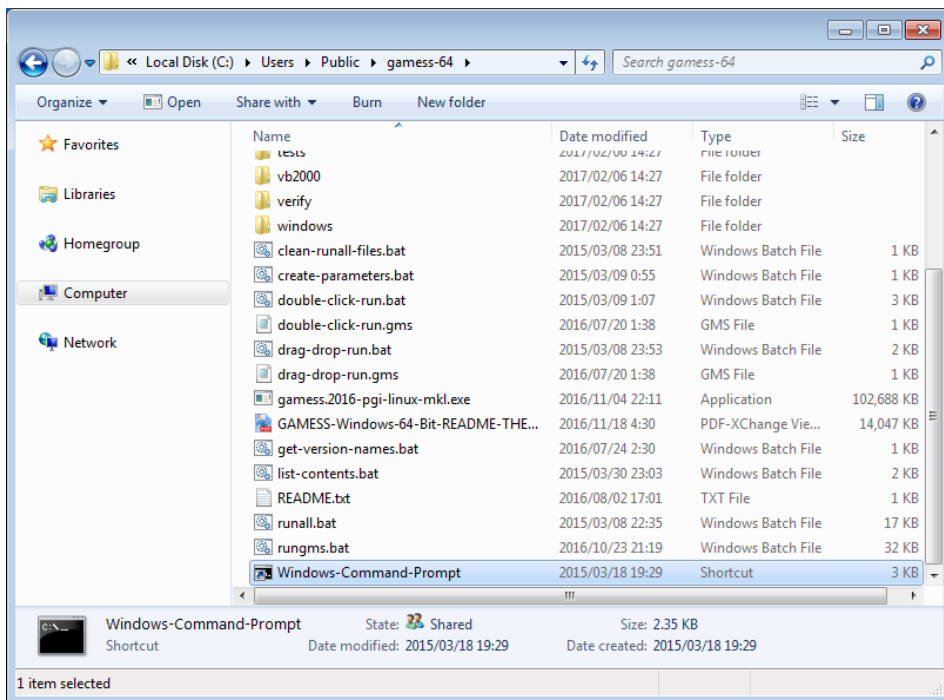
Download and install “Microsoft Visual C++ 2010 Redistributable Package (x86)” from <https://www.microsoft.com/en-US/download/details.aspx?id=5555> .

Download and install “HPC Pack 2008 R2 MS-MPI Redistributable Package with Service Pack 4” from <https://www.microsoft.com/en-US/download/details.aspx?id=14737> .

5. GAMESS Configuration

(for 64-bit version)

1) Move to the folder GAMESS installed (e.g. C:\Users\Public\gamed64)



2) Double-click Windows-Command-Prompt.

```

Windows-Command-Prompt - C:\Users\Public\gamess-64\list-contents.bat
Script          Description
=====
clean-runall-files.bat  Removes exam log, scratch, and restart files.

create-parameters.bat  Creates rungms.gms parameter file needed by
                        the rungms.bat batch script.

double-click-run.bat   Run all *.inp files from the input folder and
                        store log files in output folder defined in
                        double-click-run.gms

drag-drop-run.bat      Script that accommodates drag-and-drop of *.inp
                        files. Uses [ncpus] and [version] defined in
                        drag-drop-run.gms

get-version-names.bat  List available GAMESS binaries and version names

runall.bat [version] [ncpus]
                Run exam files in either serial or parallel

rungms.bat [input] [version] [ncpus] [ppn]
                Run a GAMESS calculation

Press any key to continue . . .
  
```

3) Press any key to continue.

4) Type create-parameters.bat and press Enter. rungms.gms will be generated. Press any key to continue.

```

Windows-Command-Prompt
drag-drop-run.bat      Script that accomodates drag-and-drop of *.inp
                      files. Uses [ncpus] and [version] defined in
                      drag-drop-run.gms
get-version-names.bat  List available GAMESS binaries and version names
runall.bat [version] [ncpus]
                      Run exam files in either serial or parallel
rungms.bat [input] [version] [ncpus] [ppn]
                      Run a GAMESS calculation
Press any key to continue . . .
C:\Users\Public\games-64>create-parameters.bat
GAMESSDIR=C:\Users\Public\games-64
AUXDATADIR=C:\Users\Public\games-64\auxdata
RESTARTDIR=C:\Users\Public\games-64\restart
SCRATCHDIR=C:\Users\Public\games-64\scratch
Finished rungms.gms parameter file
Press any key to continue . . .
C:\Users\Public\games-64>

```

5) To test GAMESS, type 'runall.bat 2016-pgi-linux-mkl 1' and press Enter. '2016-pgi-linux-mkl' is the version of GAMESS installed. If you do not know that, type 'get-version-names.bat' and press Enter and see the displayed version.

```

Windows-Command-Prompt
Running exam19
Running exam20
Running exam21
Running exam22
Running exam24
Running exam26
Running exam28
Running exam29
Running exam30
Running exam31
Running exam33
Running exam34
Running exam35
Running exam36
Running exam37
Running exam38
Running exam40
Running exam41
Running exam43
Running exam44
-----
FIN
-----
C:\Users\Public\games-64>

```

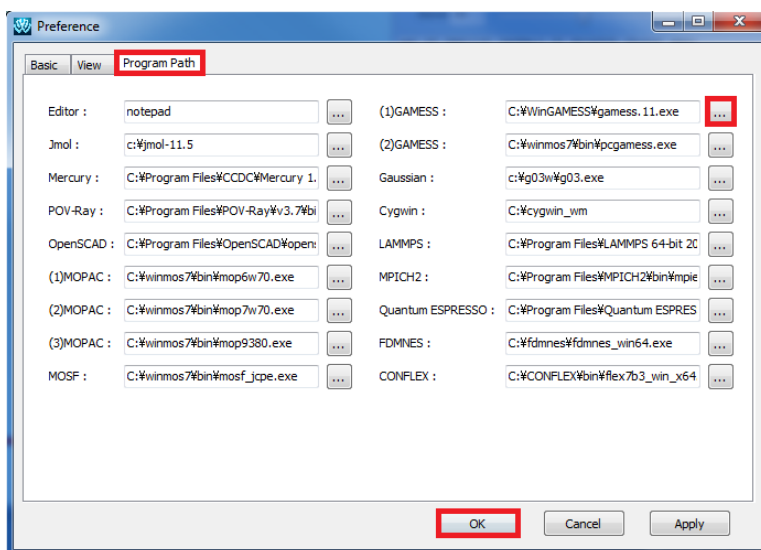
6) To test GAMESS parallel execution, type 'runall.bat 2016-pgi-linux-mkl 2' and press Enter.

(for 32-bit version)

- 1) Move to the folder GAMESS installed (e.g. C:\¥ games.32)
- 2) Modify parameters in parameters.gms for the installed folder.

6. Setting PATH

- 1) Launch Winmostar and select [Tools]-> [Preference]. In Preference window, select [Program Path] panel, click [...] button at (1)GAMESS and choose the executable file. Then, click [OK].

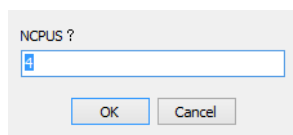


for 64-bit: e.g. games.2016-pgi-linux-mkl.exe

for 32-bit: e.g. games.11-32.exe

7. Setting CPU cores

1) Select [QM1]-> [GAMESS Keywords]-> [NCPUS] in the menu-bar. Set number of cores to use GAMESS calculation.



2) (if Job Manager is available) Select [Others] -> [Job Manager]. Specify the number of cores to use as 'MaxCores'.

