

Linux サーバ版 GAMESS インストールマニュアル

2022 年 4 月 15 日

本マニュアルの目的

本マニュアルでは、単独ユーザが独占的に Linux サーバ (CentOS 7.7) を使用して GAMESS ジョブを実行するための環境構築方法、および Winmostar のリモートジョブ機能による計算手順を示しています。つまり複数ユーザが共同使用する計算サーバ等は対象外です。また単独ノードでの複数コアによる並列計算のみを想定しており、複数ノードにまたがる並列計算は対象としておりません。そのため計算環境構築は全てユーザのホームディレクトリ配下で行うことを想定しています。共用サーバ上での環境構築および複数ノードによる環境構築方法につきましては別途お問い合わせください。

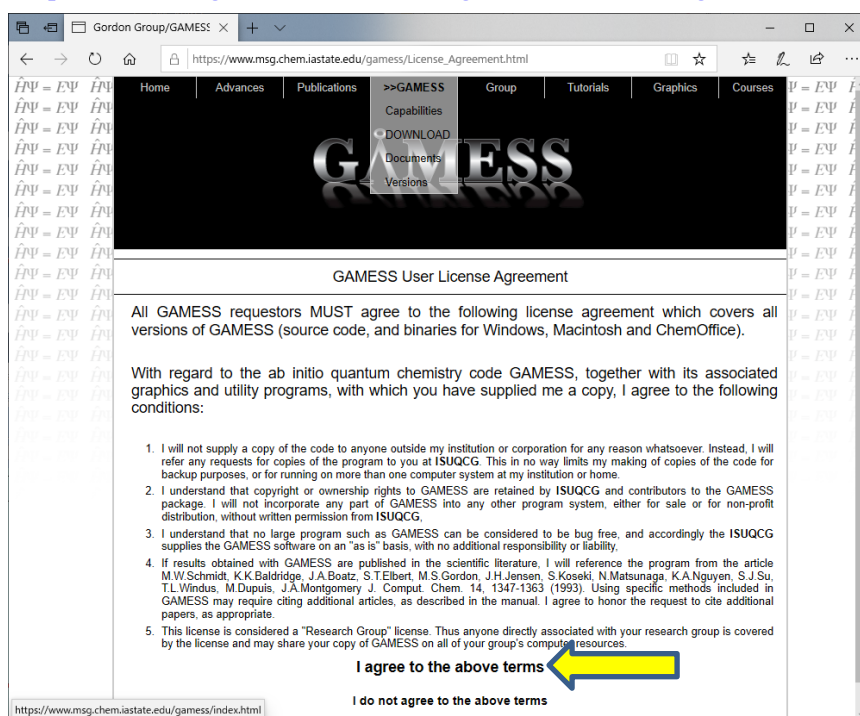
なお、本マニュアルでは Linux サーバでジョブスケジューラ TORQUE¹が使用できる状態であることを前提としています。また以下の命名としています。

サーバホスト名 : remote_server

ユーザ名 : winmostar_user

1. GAMESS のサイト内の[GAMESS User License Agreement]サイトにブラウザ(Chrome, Firefox など)を用いてアクセスする。

https://www.msg.chem.iastate.edu/games/License_Agreement.html



同意できる場合は、「I agree to the above terms」をクリックする。

¹ <http://www.adaptivecomputing.com/products/open-source/torque/> yum 等を用いて導入する。

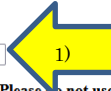
- 1) Email address を入力する
- 2) Linux 版(64 bit)を入手の場合は GAMESS versionfor 64 bit x86_64 under Linux with GNU compilers にチェックを入れる
- 3) Submit Request をクリックする

GAMESS Registration System

Request Download

Fields in bold face type are required.

Email address:



*** Apple iCloud mail server blocks emails from our domain. Please do not use an *@cloud.com email.

*** Other mail server are also blocking emails from our domain. Please do not use an *@mail.ru email.

*** If a week goes by without seeing a registration approval then please consider registering with a different email domain (gmail.com, hotmail.com, yahoo.com) or check your SPAM box.

Select desired programs below

Pre-compiled Binary Distributions

Distributions tested on their platform:

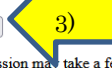
- GAMESS version September 30, 2019 R2 for Apple MacOS X
- GAMESS version September 30, 2020 R2 for Microsoft Windows

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 September 30, 2020 R2 for DoD HPCMP TI-22
- GAMESS version September 30, 2021 R2 Patch 1 for 64 bit ARM under Linux using armflang compilers
- GAMESS version September 30, 2021 R2 Patch 1 for 64 bit ARM under Linux using GNU compilers
- GAMESS version September 30, 2021 R2 Patch 1 for 64 bit ARM under Linux using NVIDIA HPC SDK
- GAMESS version September 30, 2021 R2 Patch 1 for 64 bit ARM under Linux using unlisted compilers
- GAMESS version September 30, 2021 R2 Patch 1 for 64 bit x86_64 under Linux using AMD compilers
- GAMESS version September 30, 2021 R2 Patch 1 for 64 bit x86_64 under Linux using GNU compilers
- GAMESS version September 30, 2021 R2 Patch 1 for 64 bit x86_64 under Linux using Intel compilers
- GAMESS version September 30, 2021 R2 Patch 1 for 64 bit x86_64 under Linux using Intel OneAPI compilers
- GAMESS version September 30, 2021 R2 Patch 1 for 64 bit x86_64 under Linux using NVIDIA HPC SDK
- GAMESS version September 30, 2021 R2 Patch 1 for 64 bit x86_64 under Linux using PGI compilers
- GAMESS version September 30, 2021 R2 Patch 1 for 64 bit x86_64 under Linux using unlisted compilers
- GAMESS version September 30, 2021 R2 Patch 1 for Apple MacOS X using GNU compilers
- GAMESS version September 30, 2021 R2 Patch 1 for Apple MacOS X using Intel compilers
- GAMESS version September 30, 2021 R2 Patch 1 for Apple MacOS X using PGI compilers
- GAMESS version September 30, 2021 R2 Patch 1 for Apple MacOS X using unlisted compilers
- GAMESS version September 30, 2021 R2 Patch 1 for HPE Cray
- GAMESS version September 30, 2021 R2 Patch 1 for IBM Power processors under Linux
- GAMESS version September 30, 2021 R2 Patch 1 for Microsoft Windows under Cygwin using GNU compilers
- GAMESS version September 30, 2021 R2 Patch 1 for Microsoft Windows under WSL using GNU compilers
- GAMESS version September 30, 2021 R2 Patch 1 for Microsoft Windows using Intel compilers
- GAMESS version September 30, 2021 R2 Patch 1 for Microsoft Windows using Intel OneAPI compilers
- GAMESS version September 30, 2021 R2 Patch 1 for Microsoft Windows using PGI compilers
- GAMESS version September 30, 2021 R2 Patch 1 for Microsoft Windows using unlisted compilers
- GAMESS version September 30, 2021 R2 Patch 1 for [Deprecated] 32 bit (x86 compatible) under Linux
- GAMESS version September 30, 2021 R2 Patch 1 for NVIDIA GPUs



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

- 4) 初回は登録フォームが表示される。太字の欄をすべて入力し、再度 Submit Request をクリックする

GAMESS Registration System

User Registration Required

It seems that this is your first time downloading GAMESS software. Please fill in the following form so we have an idea of who's using GAMESS.

Fields in **bold face type** are required.

Email address:
Email address again:
First name:
Last name:
Organization:
Country:
Use for GAMESS:

Select desired programs below

Pre-compiled Binary Distributions

Distributions tested on their platform:

5) 以下のような受付完了の画面が表示される

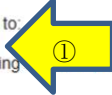
GAMESS Registration System

Request Accepted



Your download request has been accepted. E-mail has been sent to your address containing instructions for downloading the requested software. If these email(s) do not arrive in the next few days, contact gamess@si.msg.chem.iastate.edu. Note that the email will have a from address of gamess@si.msg.chem.iastate.edu and a reply to address of gamess@si.msg.chem.iastate.edu. If you do not receive the email reply within the next hour please check your spam folder or otherwise verify that the email reply has not been filtered by your email software.

2. 以下のようなメールが届く（届くまでに数日かかることがある）。送られて来たメールの指示に従って GAMESS をダウンロードする。

- ① ダウンロードリンク先をクリックする。下図に示すサイトが立ち上がる。
- ② ダウンロードするためのパスワードをメモしておく。

You can download the WinGAMESS binaries with your browser by going to: <http://www.msg.chem.iastate.edu/GAMESS/download/WinGAMESS.html>  ①
Instructions are provided on that web page for downloading and unpacking the GAMESS 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:   ②
next week it will be:

- ③ `gamess-current.tar.gz` をクリックする。ユーザ名とパスワードの入力を要求されるので、以下のように入力する。

ユーザ名 : source

パスワード : (メールに記述されたもの)

You should have already filled out the GAMESS user registration and received an email reply with the current password for downloading the source code. If you have not received the current password click [here](#) to begin the registration process.

Downloading the latest version of GAMESS:

You can download the GAMESS source with your browser by clicking on the link below. Once you click on the link you will be prompted for the username and password, the username is always:

source

and the password is in the email reply you have received. Note that the password is changed weekly.

The download is for the current GAMESS release: [gameSS-current.tar.gz](#)
MD5 (gameSS-current.tar.gz) = 5b019733bd4054cdb27a0d84dbbd5d1a



If your browser attempts to view this file instead of saving to disk, try holding down the Shift key when you click the link.

If you have problems with your download, please make sure that you have noticed that the user name is always 'source', and that the case-sensitive password changes every week. Most download problems are a result of one or both of these. In case you are trying to use an expired password, please repeat your registration to learn the current password, by clicking [here](#).

DoD HPCMP TI-22: Sept 30, 2020 R2 Public Release:

- ④ `gameSS-current.tar.gz` を SCP など で Linux サーバのホームディレクトリに転送する。

(ここから Linux サーバ上での操作)

3. 条件設定の前に Linux サーバの環境を調べる。

- ① Intel もしくは AMD の CPU 以外の Linux マシンの場合、もしくは使用 Linux が 64 ビットか 32 ビットかが分からない場合、次のコマンドで環境を調べる。

```
uname -a
```

- ② 使用するコンパイラのバージョンを調べる。

```
gfortran の場合 : gfortran -v
```

```
Intel Fortran コンパイラの場合 : ifort -v
```

4. ファイルの展開及びビルド条件設定(configuration)を行う。

- ① 圧縮ファイルを展開する。

```
tar xzvf gameSS-current.tar.gz
```

- ② configuration を起動する。

```
cd ~/gameSS
```

```
./config
```

- ③ [return]キーを押す。

```
[winmostar_user@remote_server]$ ./config
```

This script asks a few questions, depending on your computer system, to set up compiler names, libraries, message passing libraries, and so forth.

You can quit at any time by pressing control-C, and then <return>.

Please open a second window by logging into your target machine, in case this script asks you to 'type' a command to learn something about your system software situation. All such extra questions will use the word 'type' to indicate it is a command for the other window.

After the new window is open, please hit <return> to go on.

- ④ マシン種を指定する。本マニュアルでは linux64 としているが、Intel もしくは AMD の CPU かつ 64 ビット Linux 以外の場合、3.①で調べたマシン種を入力する。

GAMESS can compile on the following 32 bit or 64 bit machines:

- hpe-cray-ex - HPE Cray's EX architecture (e.g., narwhal, spock)
- hpe-cray-cs - HPE Cray's CS architecture (e.g., tulip)
- cray-xt - Cray's XT massively parallel system, running CNL
- cray-xc - Cray's XC massively parallel system (e.g., DoE Theta, DoD Onyx)
- fj-a64fx - Fujitsu PRIMEHPC with A64FX cpus and Fujitsu Compilers (e.g., FX1000, FX700)
- ibm64 - IBM, Power8 chip or newer, running AIX or Linux (e.g., DoE Summit, DoD Hokulea)
- linux32 - Linux (any 32 bit distribution), for x86
- linux64 - Linux (any 64 bit distribution), for x86_64, ia64, or arm64 chips, using gfortran, ifort, or perhaps PGI compilers.
- mac64 - Apple Mac, any chip, running OS X 10.5 or newer
- win64 - Windows 64-bit (Windows 10)
- singularity - GAMESS Singularity container image

type 'uname -a' to partially clarify your computer's flavor.

please enter your target machine name: [linux64](#)

- ⑤ ダウンロードした GAMESS セットアップファイル群が存在している directory を指定する。最後の行の [] 内の directory でよければ、[return] キーを押すだけでよい。

```
Setting up GAMESS compile and link for GMS_TARGET=linux64
GAMESS software is located at GMS_PATH=/home/winmostar_user/games
```

```
Please provide the name of the build location.
This may be the same location as the GAMESS directory.
```

```
GAMESS build directory? [/home/winmostar_user/games]
```

- ⑦ GAMESS の実行バイナリモジュールのバージョン番号を指定する。最後の行の[]内の 00 であれば、[return]キーを押すだけでよい。(数値は任意でよく、ここでは 00 としている。この場合、実行バイナリモジュールのファイル名は「gamess.00.x」 となる。) ²

² ここで指定するバージョン (本マニュアルでは 00) は、GAMESS 開発元の提供バージョンとは関係無い。GAMESS の提供バージョンは、output file に印字される。

gfortran is very robust, so this is a wise choice.

Please type 'gfortran -dumpversion' or else 'gfortran -v' to detect the version number of your gfortran.

This reply should be a string with at least two decimal points, such as 4.9.4 or 6.3.0.

The reply may be labeled as a 'gcc' version, but it is really your gfortran version.

Please enter only the first decimal place, such as 4.9: [4.8](#)

- ⑩ [Return]キーを押す。

(省略)

Enter your math library choice from one of the options below:

'acml', 'atlas', 'libflame', 'mkl', 'openblas', 'pgiblas', 'armpl', 'none'

: [mkl](#)

MKLが入っている `directory` のパスを入力する。`config` が自動的に調べて、`Found:`の行に書かれるため、通常はそのパスを書く。

If you have a slow network, like Gigabit Ethernet (GE), or
if you have so few nodes you won't run extensively in parallel, or
if you have no MPI library installed, or
if you want a fail-safe compile/link and easy execution,
choose 'sockets'
to use good old reliable standard TCP/IP networking.

If you have an expensive but fast network like Infiniband (IB), and
if you have an MPI library correctly installed,
choose 'mpi'.

If you wish to use a combination of TCP/IP networking for small
messages and MPI for large messages in a 'mixed' fashion,
choose 'mixed'.

communication library ('serial','sockets' or 'mpi' or 'mixed')? [sockets](#)

- ⑬ 様々なオプションに関する質問が続くが、本マニュアルではすべて no を入力する。

```
Checking the results of your sample GAMESS calculations,
the output files (exam??.log) will be taken from .
All jobs terminated normally, now checking detailed numerical results
exam01: Eerr=0.0e+00 Gerr=0.0e+00.                               Passed.
exam02: Eerr=0.0e+00 Gerr=0.0e+00 Serr=0.0e+00 Lerr=1.8e-03+6.6e-05. Passed.
(省略)
exam47: Serr=0.0e+00 Perr=6.0e-10.                               Passed.
exam48: E0err=0.0e+00 E1err=0.0e+00 Gerr=0.0e+00.             Passed.
All 48 test results are correct!
```

9. Linux サーバにログインし直し、以下のコマンドを実行してインストールした `runngms` が表示されることを確認する。

```
which runngms
```

以上