

Windows 版 NAMD インストールマニュアル

2017/6/14

1. NAMD のインストール

- ① 以下のサイトにアクセスし、「Win64」のリンクをクリックする。

<http://www.ks.uiuc.edu/Development/Download/download.cgi?PackageName=NAMD>

32bit 環境の場合は Win32 をクリックする。

Download NAMD:

NAMD is a parallel, object-oriented molecular dynamics code designed for high-performance simulation of large package VMD. Visit the **NAMD website** for complete information and documentation.

Selecting an archive below will lead to a user registration and login page. Your download will continue after you

Version Nightly Build (2017-06-14) Platforms:

- Linux-x86_64-multicore (64-bit Intel/AMD single node)
- Linux-x86_64-multicore-CUDA (NVIDIA CUDA acceleration)
- Source Code

Version 2.12 (2016-12-22) Platforms:

- Linux-x86_64-multicore (64-bit Intel/AMD single node)
- Linux-x86_64 (64-bit Intel/AMD with ethernet)
- Linux-x86_64-TCP (TCP may be better on gigabit)
- Linux-x86_64-ibverbs (InfiniBand via OpenFabrics OFED, not for Omni-Path, no MPI needed)
- Linux-x86_64-ibverbs-smp (InfiniBand plus shared memory, no MPI needed)
- Linux-x86_64-multicore-CUDA (NVIDIA CUDA acceleration)
- Linux-x86_64-ibverbs-smp-CUDA (NVIDIA CUDA with InfiniBand)
- Linux-x86_64-netlrts (Multi-copy algorithms)
- Linux-x86_64-verbs (Multi-copy algorithms on InfiniBand)
- Linux-x86_64-verbs-smp (Multi-copy algorithms on InfiniBand)
- Linux-x86_64-verbs-smp-CUDA (Multi-copy algorithms on InfiniBand)
- Linux-KNL-multicore (Intel Xeon Phi KNL processor single node)
- MacOSX-x86_64 (Mac OS X for 64-bit Intel processors)
- MacOSX-x86_64-CUDA (NVIDIA CUDA acceleration)
- MacOSX-x86_64-netlrts (Multi-copy algorithms)
- Win32 (Windows XP, etc.)
- Win64 (Windows 7, 8, 10, etc.)
- Win64 CUDA (NVIDIA CUDA acceleration)

- ② Registration/Login 画面で「Username」、「Password」に適当に決めたユーザ名とパスワードを入力し、「Continue with registration or download」をクリックする。

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Registration/Login

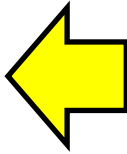
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- ③ New user Registration 画面で、必要な情報を入力して、「Register」をクリックする。

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New User Registration

New User Registration for 'namd_winmostar':

First and Last Name:

Email Address:

Affiliation:

Academic Government Industrial Other (specify)

The number of people using TCBG software at my site is:

1 2-4 5-10 11-20 21 or more

I use TCBG software primarily for:

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The work I do with TCBG software is funded (at least partially) by NIH:

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Re-enter password for confirmation:

- ④ Software Download 画面で「I am *** and I agree to the terms of this License」をクリックする。zip ファイルのダウンロードが始まる。

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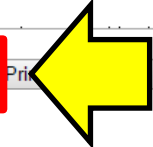
You may avoid logins for 6 months by saving a cookie on your browser:

NAMD 2.12 for Win64

To download this software you must agree to abide by the terms of the following license:

```
<h3>University of Illinois<br>
NAMD Molecular Dynamics Software<br>
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<pre>
Upon execution of this Agreement by the party identified below ("Licensee"),
The Board of Trustees of the University of Illinois ("Illinois"), on behalf
of The Theoretical Biophysics Group ("TBG") in the Beckman Institute, will
provide the NAMD molecular dynamics software ("NAMD") in Executable Code
and/or Source Code form ("Software") to Licensee, subject to the following
terms and conditions. For purposes of this Agreement, Executable Code is the
compiled code, which is ready to run on Licensee's computer. Source code
consists of a set of files which contain the actual program commands that are
compiled to form the Executable Code.
```



- ⑤ zip ファイルを解凍する。解凍したフォルダ(例えば NAMD_2.12_Win64-multicore)を適当なフォルダ(例えば C:¥)に移動する。

以上