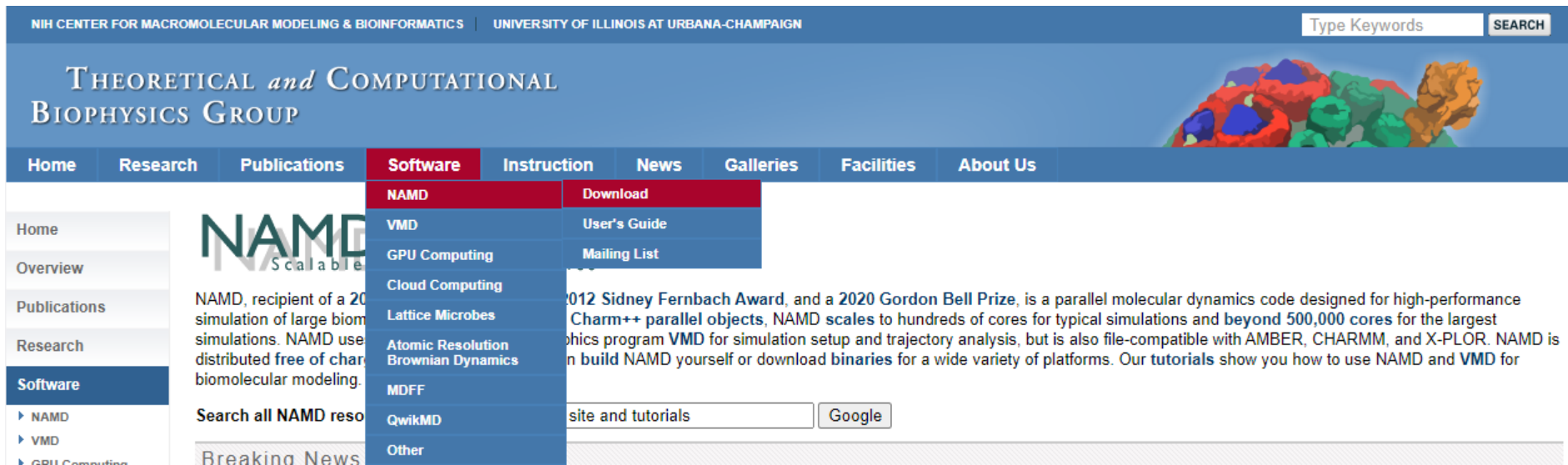


NAMDのインストール(1)

1. <https://www.ks.uiuc.edu/Research/namd/>にアクセス
2. 「Software」→「NAMD」→「Download」を選ぶ



The screenshot shows the website for the NIH Center for Macromolecular Modeling & Bioinformatics at the University of Illinois at Urbana-Champaign. The page is titled "THEORETICAL and COMPUTATIONAL BIOPHYSICS GROUP". The navigation menu includes Home, Research, Publications, Software, Instruction, News, Galleries, Facilities, and About Us. The "Software" menu is expanded, showing options for NAMD, VMD, GPU Computing, Cloud Computing, Lattice Microbes, Atomic Resolution Brownian Dynamics, MDFF, QwikMD, and Other. The "NAMD" option is selected, and the "Download" sub-menu is visible, containing "User's Guide" and "Mailing List". The main content area features a large "NAMD" logo with the tagline "Scalable" and a description of the software as a parallel molecular dynamics code designed for high-performance simulation of large biomolecular systems. A search bar is also present at the bottom of the page.

NAMDのインストール(2)

3. Version 2.14から「MacOSX-x86_64」または「Win64」を選ぶ

Version 2.14 (2020-08-05) Platforms:

- Linux-x86_64-multicore (64-bit Intel/AMD single node)
- Linux-x86_64-multicore-CUDA (NVIDIA CUDA acceleration)
- Linux-x86_64-netlrts (Multi-copy algorithms, single host or ethernet)
- Linux-x86_64-netlrts-smp-CUDA (Multi-copy algorithms, single process per copy)
- Linux-x86_64-verbs (InfiniBand, no MPI needed, supports multi-copy algorithms)
- Linux-x86_64-verbs-smp (InfiniBand, no MPI needed, supports multi-copy algorithms)
- Linux-x86_64-verbs-smp-CUDA (InfiniBand, no MPI needed, supports multi-copy algorithms)
- 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)
- Win64 (Windows 7, 8, 10, etc.)
- Win64-CUDA (NVIDIA CUDA acceleration)
- Win64-MPI (Windows HPC Server, multi-copy algorithms)
- Win64-MPI-smp-CUDA (HPC Server with CUDA)
- Source Code

NAMDのインストール(3)

4. 適当なユーザー名とパスワードを入力して「Continue ...」

Registration/Login

You will need a username and password to download software.

If this is your first download, please choose a username and password to register.
Current NAMD or VMD users, please enter your existing username and password.

Username:

Password:

Your download will continue after you have registered or logged in.

5. 右の画面で情報を埋めて「Register」

New User Registration

New User Registration for 'Tohru.Terada':

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:

Research Teaching Commerce Personal

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

Yes No

Re-enter password for confirmation:

NAMDのインストール(4)

6. 右の画面で、「I am ...」をクリック
7. ダウンロードが完了したら「開く」
 - Windowsはスライド5へ
 - macOSはスライド6へ

Software Downloads

NAMD 2.14 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>
Non-Exclusive, Non-Commercial Use License</h3>

<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.
```

I am Tohru Terada and I agree to the terms of this License

NAMDのインストール(5)

- 8. 解凍して生成されたフォルダ
「NAMD_2.14_Win64-multicore」内の
「namd2.exe」と「tcl85t.dll」をデスクトップに
コピー

NAMDのインストール(5)

8. 解凍して生成されたフォルダ
「NAMD_2.14_MacOSX-x86_64-multicore」内の
「namd2」をデスクトップにコピー

NAMD実行時の注意(1)

1. NAMD実行時に右のウィンドウが現れたら「キャンセル」
2. Dockから「システム環境設定」を選ぶ



3. 「セキュリティとプライバシー」を開く



NAMD実行時の注意(2)

4. 右のウィンドウで「このまま許可」をクリック

Big Surではこのウィンドウが現れるので「開く」

