Molecular Dynamics Studio Build and Installation Documentation

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Introduction

Download, build and installation of the Molecular Dynamics Studio (MDS) software requires some basic skills in using a web browser to download files, an understanding of the operating system environment you are using to build and install the software. My development environment is windows because the NanoEngineer-1 development environment actually works under Windows 7, Windows Vista, and Windows XP. There is a DLL issue under Windows 7 SP1 that requires some Python DLLs to be rebuilt under Window 7 SP1. I also use CYGWIN and MINGW could be used as well. CYGWIN provides you an X-Windows/UNIX environment on your Windows desktop for the purpose of building (compiling and linking) software in a UNIX like fashion. Source code distributed via a *.tgz or *.tar.gz file is usually for a UNIX/Linux environment. CYGWIN provides a command line terminal shell that runs bash by default. Building software in this environment simply requires running make in the directory structure created when you untar the necessary *.tgz files. The executables created in the CYGWIN environment do not use a standard Windows run-time and are dependent on the CYGWIN run-time. If you copy the necessary run-time DLLs to the System32 directory under the Windows operating system directory these DLLS will be loadable by the CYGWIN executables built by you. Specifically, this applies to the PACKMOL executable. As far as I know there are no free or even decently priced FORTRAN compilers for Windows. The MSI2LMP application was modified to run under Windows using Microsoft Visual Studio. It was a whim to build the application for Windows and perhaps I should create a UNIX make.

Download NanoEngineer-1

NOTE: My testing shows this installation will work for Windows XP, Windows Vista and Windows 7 (no service pack). I am also working on getting NanoEngineer-1 with modifications running on OS X and Linux.

1. Download the self-extracting NanoEngineer-1 software I started with on this project by downloading the version on the Molecular Dynamics Studio site.

- OR -

Go to the http://www.nanoengineer-1.net site and download NanoEngineer-1

2. Click NanoEngineer-1 v1.1.1 Suite (Windows)

3. Once download is complete: double click on self-extracting installer

4. Install in the default location or provide a different location.

Default installation location: C:\Program Files\Nanorex\NanoEngineer-1 v1.1.1

NOTE: for 64-bit window the "Program Files" directory becomes "Program Files(x86)"

NanoEngineer-1 Modifications Installation

1. Download the library.zip file from the Molecular Dynamics Studio site on sourceforge.

   Use your browser to visit the following URL. Click on library.zip and the download will begin.

   https://sourceforge.net/projects/moleculardynami/files/NanoEngineer/

2. Change directory to the installation directory:

   cd \install_dir   if the default directory is the install directory then

   cd \Program Files\Nanorex\NanoEngineer-1 v1.1.1

3. Change directory to the **program** subdirectory: **cd program**

4. Rename the **library.zip** file to **original_library.zip: rename library.zip original_library.zip**

5. Copy the **library.zip** file to **c:\install_dir\program**

Download Original PACKMOL

1. Download the original PACKMOL source

   Use your browser to visit the following URL. Click on the [Download](#) link at the following URL.

   http://www.ime.unicamp.br/~martinez/packmol/

 2. Register and click the "submit" button.

3. Download the source code since you must build the executable to include the modifications.

   Click on the packmol.tar.gz

4. Untar the resulting file:

   $ tar -zxvf packmol.tar.gz

5. Change directory into the new directory, packmol, created from step 2.

   $ cd packmol

6. Rename the packmol.f and io.f files to old_packmol.f and old_io.f

   $ **rename packmolnew.f old_packmolnew.f**

   $ **rename io.f old_io.f**

Download PACKMOL Modifications

1. Download the packmol_mmp_mods.tar file from the Molecular Dynamics Studio site on sourceforge.

   https://sourceforge.net/projects/moleculardynami/files/PACKMOL/

2. Copy the downloaded packmol_mmp_mods.tar to where the original PACKMOL source was downloaded.

3. Untar the file

   $ **tar -xvf packmol_mmp_mods.tar**

Build PACKMOL with Modifications

Now that the modified files are in place you can now build the modified PACKMOL.

1. Change directory into the packmol directory.

   $ **cd packmol**

2. Run the make command. Make must be able to file the FORTRAN compiler and linker for the operating system you are building under. If you install CYGWIN or MINGW as per their installtion instructions using make in the bash shell provided by CYGWIN and the CMD shell for MINGW should work directly.

   $ **make**

3. If you have trouble building PACKMOL then use the configure script from the author of PACKMOL to locate your FORTRAN compiler and reconfigure the make file. See the original PACKMOL documentation.

Install PACKMOL on Windows Platform

1. Copy the packmol executable to C:\Windows\System32

2. If this is a CYGWIN created executable then you must copy cygg_s-1.dll, cyggfortran-3.dll cygwin1.dll to C:\Windows\System32.

Install PACKMOL on Linux/UNIX Platform

1. Create /usr/local/app/packmol directory as root

   $ mkdir /usr/local/app/packmol

2. Copy packmol /usr/local/app/packmol

   $ cd packmol /usr/local/app/packmol

3. Change directory to the new executable directory

   $ cd /usr/local/app/packmol

4. Give everyone executable rights to the packmol executable

   $ chmod 755 packmol

5. Add /usr/local/app/packmol directory to the environment file in /etc. Some UNIX knowledge is required if your UNIX is different.

Download The Old Version of MSI2LMPFrom the Molecular Dynamics Studio

1. Download the msi2lmp.tar.gz from the Molecular Dynamics Studio site on sourceforge. All *.h and *.c files are required. The file are required to read the MMP file format and to process COMPASS-like force fields - specifically the CFF91 force field. The LAMMPS version of MSI2LMP is continuing to be updated and in October, 2012 it was updated to handle a triclinic MD cell geometry.

   https://sourceforge.net/projects/moleculardynami/files/MSI2LMP/

2. Untar the msi2lmp.tar.gz file into a new working directory. The tar file contains all the files needed to build the special version of MSI2LMP needed in MD Studio.

Build MSI2LMP with Modifications

Now that the modified files are in place you can now build the modified PACKMOL.

1. Change directory into the src directory.

   $ cd src

2. Run the make command. Make must be able to file the C compiler and linker for the operating system you are building under. If you install CYGWIN or MINGW as per their installation instructions using make in the bash shell provided by CYGWIN and the CMD shell for MINGW should work directly.

   $ make (Linux/UNIX/CYGWIN/MINGW)

Building the software for Windows requires a Windows-based C compiler and linker and you must build your own project file. None of this is hard and I will provide details soon.

Install MSI2LMP on Windows Platform

1. Copy the msi2lmp.exe executable to C:\Windows\System32

I will provide CYGWIN/MINGW details soon.

Install MSI2LMP on Linux/UNIX Platform

1. Create /usr/local/app/msi2lmp directory as root

   $ mkdir /usr/local/app/msi2lmp

2. Copy msi2lmp /usr/local/app/msi2lmp

   $ cd msi2lmp /usr/local/app/msi2lmp

3. Change directory to the new executable directory

   $ cd /usr/local/app/msi2lmp

4. Give everyone executable rights to the msi2lmp executable

   $ chmod 755 msi2lmp

5. Add /usr/local/app/msi2lmp directory to the environment file in /etc. Some UNIX knowledge is required if your UNIX is different.