**AMBER INSTALLATION PROCESS RECAP**

1. **XCode has been installed with Version 2406**

(base) indahlangit@Indahs-MacBook-Pro build % xcode-select -v

xcode-select version 2406.

(base) indahlangit@Indahs-MacBook-Pro build % sudo xcodebuild -license

Password:

xcode-select: error: tool 'xcodebuild' requires Xcode, but active developer directory '/Library/Developer/CommandLineTools' is a command line tools instance

(base) indahlangit@Indahs-MacBook-Pro build % xcode-select --install

xcode-select: note: Command line tools are already installed. Use "Software Update" in System Settings or the softwareupdate command line interface to install updates

(base) indahlangit@Indahs-MacBook-Pro build % xcode-select -p

/Library/Developer/CommandLineTools

1. **XQuartz has been installed**
2. **Gfortran has been installed: gcc version 14.2.0 (Homebrew GCC 14.2.0\_1)**

(base) indahlangit@Indahs-MacBook-Pro build % gfortran -v

Using built-in specs.

COLLECT\_GCC=gfortran

COLLECT\_LTO\_WRAPPER=/opt/homebrew/Cellar/gcc/14.2.0\_1/bin/../libexec/gcc/aarch64-apple-darwin23/14/lto-wrapper

Target: aarch64-apple-darwin23

Configured with: ../configure --prefix=/opt/homebrew/opt/gcc --libdir=/opt/homebrew/opt/gcc/lib/gcc/current --disable-nls --enable-checking=release --with-gcc-major-version-only --enable-languages=c,c++,objc,obj-c++,fortran,m2 --program-suffix=-14 --with-gmp=/opt/homebrew/opt/gmp --with-mpfr=/opt/homebrew/opt/mpfr --with-mpc=/opt/homebrew/opt/libmpc --with-isl=/opt/homebrew/opt/isl --with-zstd=/opt/homebrew/opt/zstd --with-pkgversion='Homebrew GCC 14.2.0\_1' --with-bugurl=https://github.com/Homebrew/homebrew-core/issues --with-system-zlib --build=aarch64-apple-darwin23 --with-sysroot=/Library/Developer/CommandLineTools/SDKs/MacOSX14.sdk

Thread model: posix

Supported LTO compression algorithms: zlib zstd

gcc version 14.2.0 (Homebrew GCC 14.2.0\_1)

1. **Cmake has been installed with Version 3.31.5**

(base) indahlangit@Indahs-MacBook-Pro build % cmake --version

cmake version 3.31.5

CMake suite maintained and supported by Kitware (kitware.com/cmake).

1. **Cmake configuration successful**

(base) indahlangit@Indahs-MacBook-Pro build % cmake .. \

-DCOMPILER=CLANG \

-DCMAKE\_C\_COMPILER=$(which clang) \

-DCMAKE\_CXX\_COMPILER=$(which clang++) \

-DCMAKE\_Fortran\_COMPILER=$(which gfortran) \

-DCMAKE\_INSTALL\_PREFIX=/Users/indahlangit/downloads/amber24 \

-DDISABLE\_TOOLS="packmol\_memgen;moft" \

-DDOWNLOAD\_MINICONDA=FALSE

-- **Compilers:**

-- C: AppleClang 15.0.0.15000309 **(/usr/bin/clang)**

-- CXX: AppleClang 15.0.0.15000309 **(/usr/bin/clang++)**

-- Fortran: GNU 14.2.0 **(/opt/homebrew/bin/gfortran)**

-- **Building Tools:**

-- addles ambpdb antechamber cew cifparse cphstats cpptraj emil etc fe-toolkit few gbnsr6 gem.pmemd kmmd leap lib mdgx mm\_pbsa mmpbsa\_py nabc ndiff-2.00 nfe-umbrella-slice nmode nmr\_aux paramfit parmed pbsa pdb4amber pmemd pymsmt pysander pytraj quick reduce rism sander saxs sebomd sff sqm xray xtalutil

-- **NOT Building Tools:**

-- **tcpb-cpp - BUILD\_TCPB is not enabled**

-- **tcpb-cpp/pytcpb - BUILD\_TCPB is not enabled**

-- **reaxff\_puremd - BUILD\_REAXFF\_PUREMD is not enabled**

-- **gpu\_utils - Requires CUDA**

-- **packmol\_memgen - Disabled by user**

-- **moft - Disabled by user**

-- **\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\***

-- Environment resource files are provided to set the proper environment

-- variables to use AMBER and AmberTools. This is required to run any Python

-- programs (like MMPBSA.py, ParmEd, MCPB.py, and pytraj)

--

-- If you use a Bourne shell (e.g., bash, sh, zsh, etc.), source the

-- /Users/indahlangit/downloads/amber24//amber.sh file in your shell. Consider adding the line

-- test -f /Users/indahlangit/downloads/amber24//amber.sh && source /Users/indahlangit/downloads/amber24//amber.sh

-- to your startup file (e.g., ~/.bashrc)

--

-- If you use a C shell (e.g., csh, tcsh), source the

-- /Users/indahlangit/downloads/amber24//amber.csh file in your shell. Consider adding the line

-- test -f /Users/indahlangit/downloads/amber24//amber.csh && source /Users/indahlangit/downloads/amber24//amber.csh

-- to your startup file (e.g., ~/.cshrc)

--

-- NOTE: MacOS users might need to source it in ~/.bash\_profile file

-- Amber will be installed to /Users/indahlangit/downloads/amber24/

-- Configuring done (54.6s)

-- Generating done (1.1s)

-- Build files have been written to: /Users/indahlangit/downloads/amber24\_src/build

1. **Make install (failed at 96%)**

[ 96%] Building Fortran object src/pmemd/src/CMakeFiles/pmemd.decomp.dir/axis\_optimize.F90.o

[ 96%] Building Fortran object src/pmemd/src/CMakeFiles/pmemd.decomp.dir/fft1d.F90.o

[ 96%] Building Fortran object src/pmemd/src/CMakeFiles/pmemd.decomp.dir/mdin\_ewald\_dat.F90.o

[ 96%] Building Fortran object src/pmemd/src/CMakeFiles/pmemd.decomp.dir/random.F90.o

[ 96%] Building Fortran object src/pmemd/src/CMakeFiles/pmemd.decomp.dir/reservoir.F90.o

**/Users/indahlangit/downloads/amber24\_src/src/pmemd/src/reservoir.F90:167:24:**

167 | Netcdf reservoir or use Sander'

| **1**

**Warning:** Missing '**&**' in continued character constant at **(1)** [**-Wampersand**]

**/Users/indahlangit/downloads/amber24\_src/src/pmemd/src/reservoir.F90:177:19:**

177 | reservoir structure energies')

| **1**

**Warning:** Missing '**&**' in continued character constant at **(1)** [**-Wampersand**]

**/Users/indahlangit/downloads/amber24\_src/src/pmemd/src/reservoir.F90:175:8:**

175 | if (alloc\_failed .ne. 0) &

| **^**

**Warning:** '**alloc\_failed**' may be used uninitialized [**-Wmaybe-uninitialized**]

**/Users/indahlangit/downloads/amber24\_src/src/pmemd/src/reservoir.F90:121:40:**

121 | integer :: alloc\_failed

| **^**

**note:** '**alloc\_failed**' was declared here

[ 96%] Building Fortran object src/pmemd/src/CMakeFiles/pmemd.decomp.dir/state\_info.F90.o

[ 96%] Building Fortran object src/pmemd/src/CMakeFiles/pmemd.decomp.dir/ti.F90.o

**/Users/indahlangit/downloads/amber24\_src/src/pmemd/src/ti.F90:1480:21:**

1480 | sc\_deg\_lcl = 3.0d0 \* sc\_atm\_cnt

| **1**

**Warning:** Possible change of value in conversion from REAL(8) to INTEGER(4) at **(1)** [**-Wconversion**]

[ 96%] Building Fortran object src/pmemd/src/CMakeFiles/pmemd.decomp.dir/dihedrals.F90.o

**/Users/indahlangit/downloads/amber24\_src/src/pmemd/src/dihedrals.i:2:7:**

2 | use ti\_decomp\_mod

| **1**

**Fatal Error:** Cannot open module file '**ti\_decomp\_mod.mod**' for reading at **(1)**: No such file or directory

compilation terminated.

make[2]: \*\*\* [src/pmemd/src/CMakeFiles/pmemd.decomp.dir/dihedrals.F90.o] Error 1

make[1]: \*\*\* [src/pmemd/src/CMakeFiles/pmemd.decomp.dir/all] Error 2

make: \*\*\* [all] Error 2