

Installation Guide for M3SYM v1.0

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1 Unpacking M3SYM

To unpack the M3SYM tar file, run the following command in your terminal shell:

```
> tar -xvf M3SYM.tar -C <InstallDirectory>
```

Once this is complete, all source code and other files will be in the chosen directory.

2 Setting up the Makefile

The Makefile for compilation of M3SYM will be in `InstallDirectory/M3SYM`, along with all source code that is needed for compilation.

2.1 Compilers and libraries needed

M3SYM is a C++ program that can be compiled with the following C++11 compilers:

- GCC 4.7 and above (Full C++11 support)
- Clang 3.3 and above (Also full C++11 support, default Apple compiler)

Compiling with incomplete C++11 compatibility may result in compilation errors.

M3SYM uses the following math and utility libraries:

- Boost libraries 1.49 or above
- GSL library

2.2 Editing the Makefile

2.2.1 Compiler and library choices

The Makefile can be edited to include a compiler or library in a non-default directory by changing the `CXX`, `CPPFLAGS`, and `LDLIBS` variables within the Makefile.

2.2.2 Optimization flags

The code can be compiled with either `DEBUG` flags, which specifies the default debugging flags for compatibility with GDB and other debugger tools. For optimal performance, compile with the `FAST` flag, which gives a number of optimization flags. This can be edited for the system specifications.

2.3 Command line compilation macros

The command line macros can be edited in the Makefile to turn on or off certain code capabilities. See the Usage guide for more details on these macros and their implications. *While these macros are customizable, we highly recommend the default usage as previously defined in the original Makefile for full capability.* The macros available for user editing are:

| Macro | Description |
|--------------------|---|
| CHEMISTRY | Enable system chemistry. |
| MECHANICS | Enable system mechanics. |
| DYNAMICRATES | Enable dynamic rate changing. This macro can only be specified if both CHEMISTRY and MECHANICS are enabled. |
| BOOST_MEM_POOL | Enable boost memory pool optimizations. |
| BOOL_POOL_NSIZE | Set boost memory pool size. Default value is 65536. |
| TRACK_DEPENDENTS | Track reaction dependents in system. |
| TRACK_ZERO_COPY_N | For activation of reactions based on copy number. |
| TRACK_UPPER_COPY_N | For activation of reactions based on copy number. |
| REACTION_SIGNALING | Enable reaction callback signaling. |
| RSPECIES_SIGNALING | Enable species callback signaling. |

2.4 Dependency file

An optional dependency file can be generated by running the command `make Makefile.dep`. This command will automatically be performed when the typical make function is executed.

2.5 Compilation

The code can be compiled into an executable file `M3SYM` by running `make` at the command line. `make clean` will erase all object files as well as the executable in the local directory.

3 Running the M3SYM executable

To run the executable, put the following command into the terminal shell:

```
> ./M3SYM -s <SystemFile> -i <InputDirectory> -o <OutputDirectory>
```

More details on the system input file and directories can be found in the Usage guide.