Installation Guide for M3SYM v1.0

Papoian Lab, University of Maryland

Contents

1	Unp	packing M3SYM		
2	Set	etting up the Makefile		
	2.1	Compilers and libraries needed		
	2.2	Editing the Makefile		
		2.2.1 Compiler and library choices		
		2.2.2 Optimization flags		
	2.3	Command line compilation macros		
		Dependency file		
	2.5	Compilation		
3	Rur	nning the M3SYM executable		

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. The macros available for user editing are:

Macro	Description
CHEMISTRY	Enable system chemistry
MECHANICS	Enable system mechanics
	Enable dynamic rate changing. This macro
DYNAMICRATES	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
TRACK_DEPENDENTS	Track reaction dependents in system
TRACK_ZERO_COPY_N	For activation of reactions
TRACK_UPPER_COPY_N	For activation of reactions
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.