

L3: Building, Testing and Debugging Scientific Software

P. de Oliveira Castro, M. Jam
September 30, 2025

Master Calcul Haute Performance et Simulation - GLHPC | UVSQ

1. Building, Testing and Debugging Scientific Software
2. Makefiles
3. CMake
4. Debugging Tools
5. Software Testing
6. Unity Test Framework

Building, Testing and Debugging Scientific Software

- Build systems: Advanced Makefiles, introduction to CMake for managing multi-file and multi-platform projects.
- Debugging: GDB, Valgrind for detecting memory errors and leaks.
- Software testing:
 - Principles: Unit testing, integration testing.
 - Test frameworks in C (e.g., Unity).
 - Importance of testing for regression prevention and validation.
- Code documentation: Doxygen.

Makefiles

Dependency Management

- How to determine which files have changed?



Figure 1: makefile-dependencies

- dependencies: `main.o` depends on changes in `lib.h`

- A `Makefile` uses a declarative language to describe targets and their dependencies.
- It is executed by the `make` command, which allows building different targets.
 - `make` uses timestamps to determine which files have changed.
 - `make` evaluates rules recursively to satisfy dependencies.

```
prog: main.c lib.c lib.h
    clang -o prog main.c lib.c -lm

target: dependencies
\t  command to build the target from the dependencies
```


Separate Compilation

```
prog: main.o lib.o
    clang -o prog main.o lib.o -lm

main.o: main.c lib.h
    clang -c -o main.o main.c

lib.o: lib.c lib.h
    clang -c -o lib.o lib.c
```

If `lib.c` is modified, which commands will be executed?

You can add targets that do not correspond to a produced file. For example, it is useful to add a `clean` target to clean the project.

```
clean:
    rm -f *.o prog
.PHONY: clean
```

`.PHONY` specifies that the `clean` rule should always be executed. Declaring all phony targets ensures they are always called (even if a file with the same name is created).

```
make clean  
make prog  
make
```

- If `make` is called with a rule, that rule is built.
- If `make` is called without arguments, the first rule is built. It is customary to include a default `all:` rule as the first rule.

```
all: prog  
  
prog: ...
```

Variables

```
CC=clang
CFLAGS=-O2
LDFLAGS=-lm

prog: main.o lib.o
    $(CC) -o prog main.o lib.o $(LDFLAGS)

main.o: main.c lib.h
    $(CC) $(CFLAGS) -c -o main.o main.c

lib.o: lib.c lib.h
    $(CC) $(CFLAGS) -c -o lib.o lib.c
```

Variables can be overridden when calling make, e.g.,

```
make CC=gcc
```

Special Variables

<code>\$@</code>	target name
<code>\$^</code>	all dependencies
<code>\$<</code>	first dependency

```
prog: main.o lib.o
    $(CC) -o $@ $^ $(LDFLAGS)

main.o: main.c lib.h
    $(CC) $(CFLAGS) -c -o $@ $<

lib.o: lib.c lib.h
    $(CC) $(CFLAGS) -c -o $@ $<
```

The last two rules are very similar...

Before

```
main.o: main.c lib.h
    $(CC) $(CFLAGS) -c -o $@ $<

lib.o: lib.c lib.h
    $(CC) $(CFLAGS) -c -o $@ $<
```

With Implicit Rule

```
%.o: %.c
    $(CC) $(CFLAGS) -c -o $@ $<

main.o: lib.h
lib.o: lib.h
```

- `automake / autoconf`: automatic generation of complex makefiles and management of system-specific configurations.
- `cmake`, `scons`: successors to Makefile, offering more elegant syntax and new features.

CMake

- **Advantages of Makefiles:**
 - Simplicity and transparency.
 - No additional tools required.
 - Direct control over the build process.
- **Advantages of CMake:**
 - Cross-platform support (Linux, Windows, macOS).
 - Generates build files for multiple build systems (Make, Ninja, etc.).
 - Modular and target-based design.
 - Built-in support for testing, installation, and packaging.

- **CMake as a Meta-Build System:**
 - Generates build files for different generators (e.g., Make, Ninja).
 - Abstracts platform-specific details.
- **Workflow:**
 1. Write `CMakeLists.txt` to define the project.
 2. Configure the project:

```
cmake -B build
```

3. Build the project:

```
cmake --build build  
# or when using Make as backend  
make -C build
```

Out-of-source builds are recommended to keep source directories clean.

```
cmake_minimum_required(VERSION 3.15)
project(MyProject LANGUAGES C)

set(CMAKE_C_STANDARD 11)
```

- `cmake_minimum_required`: Specifies the minimum version of CMake required.
- `project`: Defines the project name and the programming language(s) used.
- `set`: Sets variables, e.g., C standard version.

Adding an Executable

```
add_executable(my_executable src/main.c)
```

- Creates an executable named `my_executable`.

Adding a Shared Library

```
add_library(my_library SHARED src/library.c)
```

- Creates a shared library named `libmy_library.so` (on Linux).

Linking Libraries to Executables

```
add_library(my_library SHARED src/library.c)
add_executable(my_executable src/main.c)
target_link_libraries(my_executable PRIVATE my_library)
```

- `add_library`: Creates a shared library.
- `add_executable`: Creates an executable.
- `target_link_libraries`: Links the library to the executable.

`PRIVATE` means that `my_executable` uses `my_library`, but `my_library` does not need to be linked when other targets link to `my_executable`.

Library dependency transitivity

```
add_library(libA SHARED src/libA.c)
add_library(libB SHARED src/libB.c)
target_link_libraries(libB PUBLIC libA)
add_executable(my_executable src/main.c)
target_link_libraries(my_executable PRIVATE libB)
```

- `my_executable` is linked to `libB` and also to `libA` because `libB` links to `libA` with `PUBLIC`.
- If `libB` linked to `libA` with `PRIVATE`, `my_executable` would not be linked to `libA`.
- If `libB` linked to `libA` with `INTERFACE`, `my_executable` would be linked to `libA` but not `libB`.
- See this reference for more details.

```
include_directories(include)
```

- Adds the `include` directory globally for all targets.
- **Limitation:** Can lead to conflicts in larger projects.

Target-Specific Include Directories

```
target_include_directories(my_library  
    PUBLIC include  
)
```

- **PUBLIC:** Include directory is needed when building and using the library.
- **PRIVATE:** Include directory is needed only when building the library.
- **INTERFACE:** Include directory is needed only when using the library.

Porting our minimal Makefile example to CMake

```
cmake_minimum_required(VERSION 3.15)
project(MyProject LANGUAGES C)

# Add the executable target
add_executable(prog main.c lib.c)

# Specify include directories for the target
target_include_directories(prog
    PRIVATE ${CMAKE_CURRENT_SOURCE_DIR})

# Add compile options
target_compile_options(prog PRIVATE ${CFLAGS})

# Link libraries if needed
target_link_libraries(prog PRIVATE m)
```

- **Debug Build:**
 - Includes debug symbols for debugging.
 - Example flags: `-g`, `-O0`.
- **Release Build:**
 - Optimized for performance.
 - Example flags: `-O3`, `-DNDEBUG`.

Setting Build Types in CMake

```
if(NOT CMAKE_BUILD_TYPE)
  set(CMAKE_BUILD_TYPE RelWithDebInfo CACHE STRING "Build type"
      FORCE)
endif()
```

- Build types: Debug, Release, RelWithDebInfo, MinSizeRel.
 - CACHE: Makes the variable persistent across CMake runs. In out-of-source builds `CMakeLists.txt` is not re-evaluated on subsequent runs.
 - FORCE: Overrides any previous value.
 - STRING: "Build type" provides a description in CMake GUI.

```
target_compile_options(my_library PRIVATE
    $$<CONFIG:Debug>:-g -Wall>
    $$<CONFIG:Release>:-O3 -DNDEBUG>
)
```

- **Generator Expressions:** `$<CONFIG:Debug>` applies flags only for Debug builds.

```
install(TARGETS my_library
  LIBRARY DESTINATION lib
  PUBLIC_HEADER DESTINATION include
)
```

- Installs the shared library to the `lib` directory.
- Installs public headers to the `include` directory.

```
include(GNUInstallDirs)

install(TARGETS my_library
  LIBRARY DESTINATION ${CMAKE_INSTALL_LIBDIR}
  PUBLIC_HEADER DESTINATION ${CMAKE_INSTALL_INCLUDEDIR}
)
```

- Defines standard GNU library and include directories paths.

Generating and Building the Project

1. Configure the Project:

```
cmake -B build
```

- Generates build files in the build directory.

2. Build the Project:

```
cmake --build build  
# or when using Make as backend  
make -C build
```

3. Run the Program:

```
./build/my_executable
```


- **Use Target-Based Commands:**
 - Prefer `target_include_directories` over `include_directories`.
 - Prefer `target_link_libraries` over global linking.
- **Organize `CMakeLists.txt`:**
 - Group related targets together.
 - Use comments to explain sections.
- **Use Modern CMake Features:**
 - Generator expressions for conditional configurations.
 - `FetchContent` for managing external dependencies.

Debugging Tools

Buggy program example

```
/* Linked list of n = 5 nodes
```

```
head -> [ val = 4 | next --|--> [ val = 3 | next --|--> ... -> [ val = 0 | next = NULL | ] ] ]
```

```
*/
```

```
#include <stdlib.h>
```

```
#include <assert.h>
```

```
struct Node
```

```
{  
    int val;  
    struct Node *next;  
};
```

```
int main()
```

```
{  
    int n = 5;  
  
    struct Node *head = init_list(n);  
    // ... do something with the list ...  
    delete(head);  
  
    return 0;  
}
```

Linked List Initialization and Deletion

```
struct Node *init_list(int n)
{
    struct Node *head = NULL;
    for (int i = 0; i < n; ++i)
    {
        struct Node *p = malloc(sizeof *p);
        assert(p != NULL);
        p->val = i;
        p->next = head;
        head = p;
    }
    return head;
}

void delete(struct Node *head)
{
    while (head)
    {
        struct Node *next = head->next;
        free(head);
        head = next;
    }
}
```

Running the program...

```
$ gcc -g -O0 -o buggy buggy.c  
$ ./buggy  
Segmentation fault (core dumped)
```

GDB: GNU Debugger

- Inspect the state of a program at the moment it crashes.
- Step through the code line by line.
- Inspect variables and memory.
- Set breakpoints to pause execution at specific lines.

(Live demonstration)

```
$ gdb ./buggy
Program received signal SIGSEGV, Segmentation fault.
0x000055555555522b in delete (head=0xa45d97b66d0683e8) at buggy.c:28
28      struct Node *next = head->next;
(gdb) x head
0xa45d97b66d0683e8:      Cannot access memory at address 0
                        xa45d97b66d0683e8
```

Valgrind: memory debugging and leak detection

- Detects memory leaks, invalid memory access, and uninitialized memory usage.
- Runs the code in a virtual sandbox that monitors every memory operation.

(Live demonstration)

```
$ valgrind --leak-check=full ./buggy
==537945== Invalid read of size 8
==537945==    at 0x109243: delete (buggy.c:30)
==537945==    by 0x109282: main (buggy.c:40)
==537945== Address 0x4a94188 is 8 bytes inside a block of size
    16 free'd
==537945==    at 0x484988F: free (in /usr/libexec/valgrind/
    vgpreload_memcheck-amd64-linux.so)
==537945==    by 0x10923E: delete (buggy.c:29)
==537945==    by 0x109282: main (buggy.c:40)
==537945== Block was alloc'd at
==537945==    at 0x4846828: malloc (in /usr/libexec/valgrind/
    vgpreload_memcheck-amd64-linux.so)
==537945==    by 0x1091B2: init_list (buggy.c:15)
==537945==    by 0x109272: main (buggy.c:38)
```

Other tools: ASAN, UBSAN

- **AddressSanitizer (ASAN):** Detects memory errors such as buffer overflows and use-after-free.
- **UndefinedBehaviorSanitizer (UBSAN):** Detects undefined behavior in C/C++ programs.
- Works on threaded programs and has lower overhead than Valgrind.

(live demonstration)

```
$ gcc -fsanitize=address -g -O0 -o buggy_asan buggy.c
$ ./buggy_asan
=====
==538335==ERROR: AddressSanitizer: heap-use-after-free on address
    0x502000000098 at pc 0x5bec7c7343e9 bp 0x7ffdf3015150 sp 0
    x7ffdf3015140
READ of size 8 at 0x502000000098 thread T0
    #0 0x5bec7c7343e8 in delete /home/poliveira/test-gdb/buggy.c
    :30
    #1 0x5bec7c73442c in main /home/poliveira/test-gdb/buggy.c:40
```


Software Testing

Importance of Software Testing

- 1996: Ariane-5 self-destructed due to an unhandled floating-point exception, resulting in a \$500M loss.
- 1998: Mars Climate Orbiter lost due to navigation data expressed in imperial units, resulting in a \$327.6M loss.
- 1988-1994: FAA Advanced Automation System project abandoned due to management issues and overly ambitious specifications, resulting in a \$2.6B loss.
- 1985-1987: Therac-25 medical accelerator malfunctioned due to a thread concurrency issue, causing five deaths and numerous injuries.

Technical Debt



Figure 2: Software Costs (Applied Soft. Measurement, Capers Jones)

Development Costs

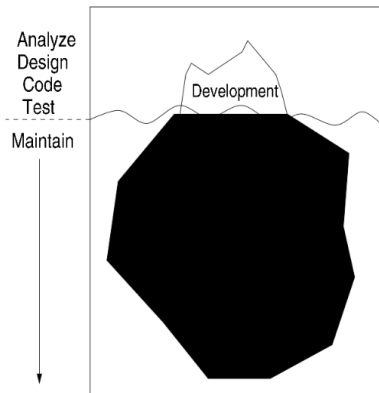


1/3 planning

1/6 coding

1/4 component test

1/4 system test



Development costs are only the tip of the iceberg.

Figure 3: Software Costs (Nancy Leveson)

- **Validation:** Does the software meet the client's needs?
 - "Are we building the right product?"
- **Verification:** Does the software work correctly?
 - "Are we building the product right?"

- Formal methods
- Modeling and simulations
- Code reviews
- Testing

Testing Process



V Cycle Model

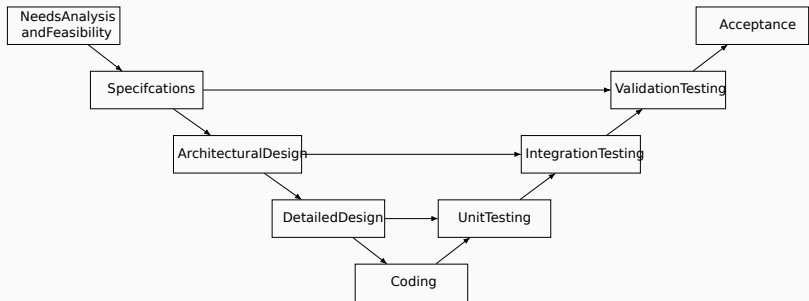


Figure 5: V-Model: Validation followed by Verification

Different Types of Tests

- **Unit Tests:**
 - Test individual functions in isolation.
 - Test-driven development (TDD): Focus on writing maintainable, simple, and decoupled code.
- **Integration Tests:**
 - Test the correct behavior when combining modules.
 - Validate only functional correctness.
- **Validation Tests:**
 - Test compliance with specifications.
 - Test other characteristics: performance, security, etc.
- **Acceptance Tests:**
 - Validate requirements with the client.
- **Regression Tests:**
 - Ensure that fixed bugs do not reappear.

Black-Box and White-Box Testing

Black-Box Testing (Functional)

- Tests are generated from specifications.
- Uses assumptions different from the programmer's.
- Tests are independent of implementation.
- Difficult to find programming defects.

White-Box Testing (Structural)

- Tests are generated from source code.
- Maximizes coverage by testing all code branches.
- Difficult to find omission or specification errors.

Both approaches are complementary.

What to Test?

- Running the program on all possible inputs is too costly.
- Choose a subset of inputs:
 - Partition inputs into equivalence classes to maximize coverage.
 - Test all code branches.
 - Test edge cases.
 - Test invalid cases.
 - Test combinations (experimental design).

Example of Partitioning (1/3)

Specification

```
/* compare returns:  
 * 0 if a is equal to b  
 * 1 if a is strictly greater than b  
 * -1 if a is strictly less than b  
 */  
int compare (int a, int b);
```

What inputs should be tested?

Equivalence Classes (2/3)

Variable	Possible Values
a	{positive, negative, zero}
b	{positive, negative, zero}
result	{0, 1, -1}

Example Test Cases

a	b	result
10	10	0
20	5	1
3	7	-1
-30	-30	0
-5	-10	1
...

It is possible to select a subset of classes!

a	b	result
-2147483648	-1	-1

- Automatic test generation.
- Test coverage calculation.
- Mutation testing.
- Fuzzing.
- Importance of using automated testing tools.
- Importance of using continuous integration tools.

Unity Test Framework



Figure 6: Unity Logo

Unity Test Framework

- Lightweight and simple unit testing framework for C.
- Designed for embedded systems but can be used in any C project.
- Provides a set of macros and functions to define and run tests.

- Separate Unity tests into a separate directory, e.g., `tests/`.
- Include the Unity header in your test files:

```
#include "unity.h"
```

- Requires linking against the Unity library
- We will link against a static library `libunity.a`, since Unity uses CMake, we will use `FetchContent` to add it to our projects.

- test_functions use TEST macros provided by Unity to assert conditions.

```
void test_function_name(void) {  
    ...  
    TEST_ASSERT_EQUAL_INT(expected, actual);  
    TEST_ASSERT_NOT_NULL(pointer);  
    TEST_ASSERT_TRUE(condition);  
    ...  
}
```

- Reference for all assertions: [Unity Assertions](#)

Example: testing our linked list

```
#include "unity.h"
#include "buggy.h"
void test_delete_single_node(void) {
    struct Node *head = init_list(1);
    TEST_ASSERT_NOT_NULL(head); // head should not be NULL
    TEST_ASSERT_EQUAL_INT(0, head->val); // head should be 0
    delete(head); // should not crash
    TEST_ASSERT_NULL(head); // head should be NULL after deletion
}
void test_delete_multiple_nodes(void) {
    struct Node *head = init_list(5);
    TEST_ASSERT_EQUAL_INT(4, head->val); // head should be 4
    TEST_ASSERT_EQUAL_INT(3, head->next->val);
    delete(head); // should not crash
    TEST_ASSERT_NULL(head); // head should be NULL after deletion
}
```

- Create a test runner function to execute all tests:

```
int main(void) ## Boundary Tests{  
    UNITY_BEGIN();  
    RUN_TEST(test_function_name);  
    ...  
    return UNITY_END();  
}
```

- SetUp and TearDown functions can be defined to run before and after each test.

```
void setUp(void) {  
    // Code to run before each test  
}  
  
void tearDown(void) {  
    // Code to run after each test  
}
```

Code Coverage with unit tests

- Use `gcov` or `llvm-cov` to measure code coverage of your tests.
- Compile your code with coverage flags:

```
gcc --coverage -g -O0 -o test_runner test_runner.c my_code.c -lunity
```

- `gcov` instruments the basic blocks of code to record what is executed during tests.
- `gcovr` generate HTML reports showing which parts of the code were covered by tests.

Documentation with Doxygen

- Doxygen is a documentation generator for C, C++, and other languages.
- It extracts comments from the source code and generates documentation in various formats (HTML, LaTeX, etc.).
- Use special comment blocks to document functions, parameters, return values, and more.
- Example of a documented function:

```
/**  
 * @brief Initializes a linked list with n nodes.  
 * @param n Number of nodes to create.  
 * @return Pointer to the head of the linked list  
 * @return NULL if memory allocation fails.  
 */  
struct Node *init_list(int n);
```

- Generate documentation using the `doxygen` command with a configuration file (`Doxyfile`).

- Course “Automated Software Testing,” Sébastien Bardin.
- CMake Tutorial
- CMake Best Practices
- Unity Test Framework
- Valgrind
- GDB
- ASAN/UBSAN
- Doxygen