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Better Scientific Software tutorial, ISC, June 2021





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- The requested citation the overall tutorial is: David E. Bernholdt, Anshu Dubey, Patricia A. Grubel, Rinku K. Gupta, and David M. Rogers, Better Scientific Software tutorial, in ISC High Performance, online, 2021. DOI: 10.6084/m9.figshare.14642520
- Individual modules may be cited as *Speaker, Module Title*, in Better Scientific Software tutorial...

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### Hello Numerical World Example (heat equation)

github.com/bssw-tutorials/hello-numerical-world

```
$ wc *.C

125    494    4161 args.C    # parse arguments

220    718    5667 heat.C    # main() – stores all vars

151    498    3888 utils.C    # I2_norm, write, copy, init

26    119    820 ftcs.C    # standard, centered stencil

27    123    833 upwind15.C # alternate integration schemes

94    344    2134 crankn.C

43    190    1299 exact.C    # comparison solution
```

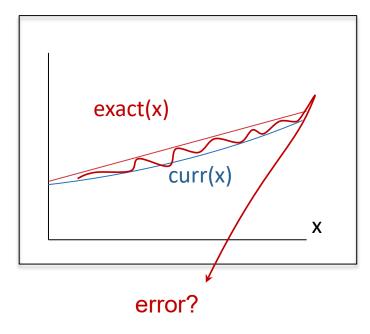
- Lots of setup code prepares problem for kernel calls
- Isolated, swappable kernel calls
  - Imagine adding kernels to larger, multi-physics application.
- How can we support testing all these kernel configurations

### What to Test?

github.com/bssw-tutorials/hello-numerical-world

### Types of Tests:

- code coverage ensure options parse, bad cases detected, utilities fuction, etc.
- steady-state (should be straight line)
  - external script can test file write() as well
- solution time-dependence vs. reference
  - $(d/dx)^2 \sin(ax) = -a^2 \sin(ax)$
- integration between codes?
- test compile/run in multiple precisions?
  - combinatorial problems listing tests in for() or matrix...

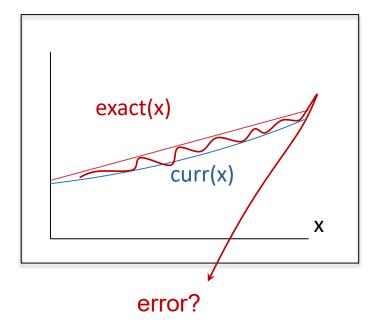




### Running Tests via makefile

github.com/bssw-tutorials/hello-numerical-world

```
$ make check all
   c++ -c -linclude -DHEAT_VERSION_MAJOR=0 -
   DHEAT VERSION MINOR=5 args.C -o args.o
   c++ -o heat heat.o utils.o args.o exact.o ftcs.o upwind15.o
   crankn.o -lm
    ./heat runame=check outi=0 maxt=-5e-8 ic="rand(0,0.2,2)"
     runame="check"
   Stopped after 001490 iterations for threshold 2.46636e-15
   cat check/check soln final.curve
   # Temperature
    ./check.sh check/check soln final.curve 0
make completes: commands succeeded
```



steady-state test (should be straight line)



### TODO – try out new build tools and add tests to them

- Replace makefile with CMakeLists.txt
  - replaces rules with targets (tied to a list of source files)
  - targets have attributes
    - target\_link\_libraries (e.g. MPI::MPI\_CXX)
    - target\_include\_directories (many already inferred from link libraries)
    - target\_compile\_features (e.g. cxx\_std11)
  - provides find\_package command
  - targets can be installed
- Replace "make check all" with ctest
  - reduces glue code
  - different interface for adding tests
- End Result: contrast two methods of testing.





## existing makefile

#### makefile

```
# Implicit rule for object files
%.o: %.C
$(CXX) -c $(CXXFLAGS) $(CPPFLAGS) $< -o $@

# Linking the final heat app
heat: $(OBJ)
$(CXX) -o heat $(OBJ) $(LDFLAGS) -lm
```

Standard makefile – user selects compile flags.

- but flags and features are compiler and system-specific
- enter automake and cmake -> generate makefiles



### **Conversion to cmake (entire file)**

cmake.org/cmake/help/latest/command/add\_test.html

#### CMakeLists.txt

```
cmake_minimum_required(VERSION 3.8)
project(heat VERSION 0.5 LANGUAGES CXX)
# can change boolean variable with "-DCMAKE BUILD TESTS=OFF"
option(BUILD_TESTS "Build the tests accompanying this program." ON)
# pass cmake options (e.g. version) into a header
configure file(include/version.H.in include/version.H)
add executable(heat args.C crankn.C ...) # list sources
# feature – lets cmake adjust flags for compiler --std=c++11 vs –c11
target compile features(heat cxx std 11)
# include directories for all files in this target:
target_include_directories(heat ${PROJECT_BINARY_DIR}/include)
if(BUILD_TESTS) add_subdirectory(tests) endif() # subdir for tests
install(TARGETS heat DESTINATION bin) # "make install" target
```

## existing tests

makefile include (tests.mk)

#### Create a test driver to:

- 1. run executable
- 2. check result
- 3. clean up outputs



### Addition to CMakeLists.txt

tests/CMakeLists.txt

Lots of potential for programmatically creating tests!

Try and keep it simple – complex cmake code is bad form.



### Bonus: swap out test driver (perl -> awk)

tests/testDriver.sh

```
#!/bin/bash
set –e # exit immediately on error
errbnd=1e-7
alg="$2"
$1 alg=$alg runame=check $alg outi=0 maxt=-5e-8 ic="rand(0,0.2,2)"
# absolute error check (deviation from straight line)
err=\frac{awk 'function abs(x){return ((x < 0.0) ? -x : x)}; BEGIN {err=1e10;} ! /#/ {err1=abs($2-$1); if(err1)}; if(err1)}
< err) err = err1;} END {print err;}' check_$alg/check_${alg}_soln_final.curve)</pre>
echo "Error = $err"
rm -fr check $alg # delete directory to test is re-runnable
awk "BEGIN {exit($err >= $errbnd);}" # final return code
```

# **Running**

cmake ..
make -j
cd tests && ctest

```
Test project hello-numerical-world/build/tests
  Start 1: ftcs
1/3 Test #1: ftcs ...... Passed 0.02 sec
  Start 2: crankn
2/3 Test #2: crankn ...... Passed 0.02 sec
  Start 3: upwind15
3/3 Test #3: upwind15 ...... Passed 0.03 sec
100% tests passed, 0 tests failed out of 3
Total Test time (real) = 0.08 sec
```

## Conclusion – C, kernels, makefiles, CMakeLists, coverage, etc.

- Start your projects small, stay organized
  - makefiles provide fast development path
  - add tests before complexity grows!
  - simple to do with a "make check" target
- cmake (like autoconf) helps make portable builds
  - find\_package
  - programmatic build options
  - set target properties -> cmake looks up compiler flags for you
- good testing strategies exist for both
  - directly run the executable with all options
  - create shell-script "test driver"
  - build stand-alone executables loading a library



