Software Packaging – Condensed Version

David M. Rogers (he/him)
Oak Ridge National Laboratory

Better Scientific Software tutorial @ ISC23

Contributors: David M. Rogers (ORNL), IDEAS-ECP Team

License, Citation and Acknowledgements

License and Citation

- **The requested citation the overall tutorial is:** Anshu Dubey and David M. Rogers, Better Scientific Software tutorial, in ISC High Performance, Hamburg, Germany and online, 2023. DOI: 10.6084/m9.figshare.22790762.
- Individual modules may be cited as *Speaker, Module Title*, in *Tutorial Title*, …

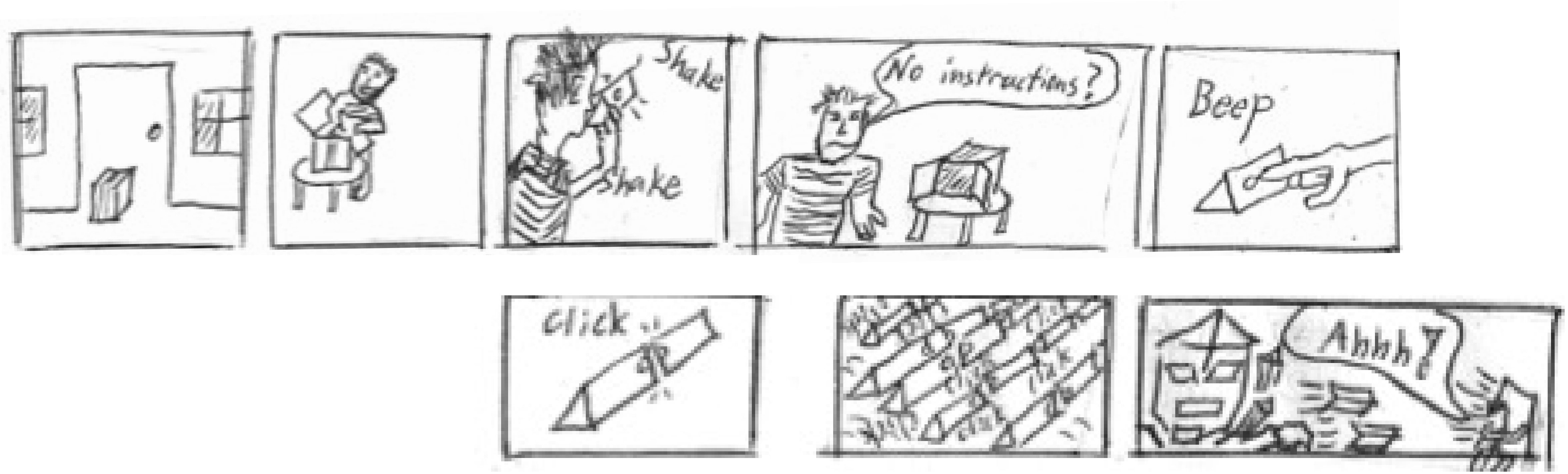
Acknowledgements

- This work was supported by the U.S. Department of Energy Office of Science, Office of Advanced Scientific Computing Research (ASCR), and by the Exascale Computing Project (17-SC-20-SC), a collaborative effort of the U.S. Department of Energy Office of Science and the National Nuclear Security Administration.
- This work was performed in part at the Argonne National Laboratory, which is managed by UChicago Argonne, LLC for the U.S. Department of Energy under Contract No. DE-AC02-06CH11357.
- This work was performed in part at the Lawrence Livermore National Laboratory, which is managed by Lawrence Livermore National Security, LLC for the U.S. Department of Energy under Contract No. DE-AC52-07NA27344.
- This work was performed in part at the Los Alamos National Laboratory, which is managed by Triad National Security, LLC for the U.S. Department of Energy under Contract No.89233218CNA000001
- This work was performed in part at the Oak Ridge National Laboratory, which is managed by UT-Battelle, LLC for the U.S. Department of Energy under Contract No. DE-AC05-00OR22725.
- This work was performed in part at Sandia National Laboratories. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Outline

- Why package?
- General Guidelines & Themes
- Running Walk-Through
  - ~~python package~~
  - C++ code – cmake exports
  - ~~Fortran – cmake exports~~
  - ~~Spack~~
- Containers

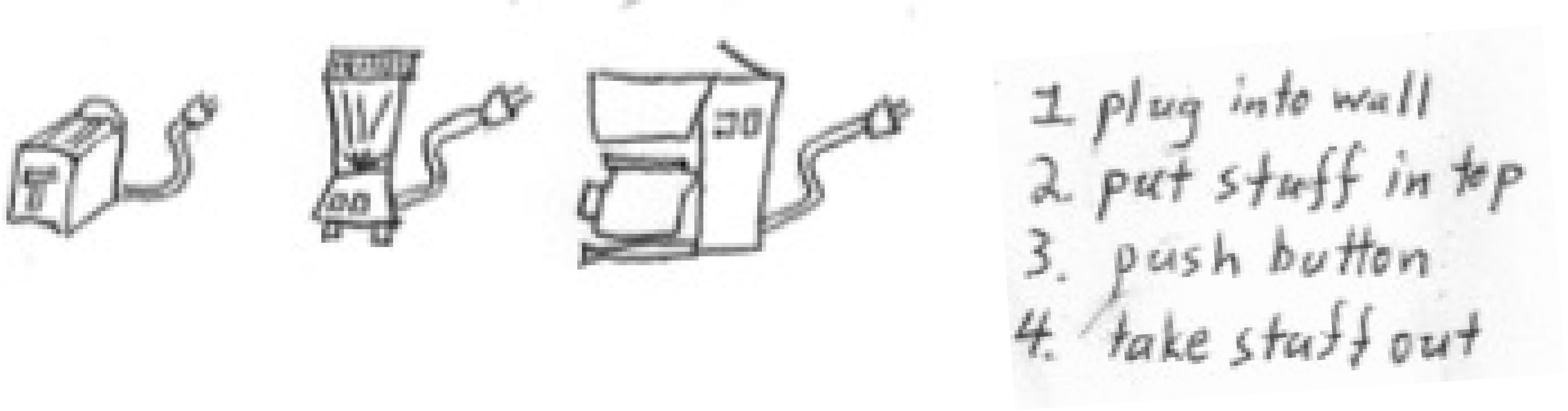
Why Package?



- What does it do?
- How do I set it up?
- Automation *can* be good...
  - but requires really great documentation!

Why Package?

- Standards and conventions save everyone time



Hello Numerical World Example (heat equation)

github.com/bssw-tutorial/simple-heateq

```
33  COPYING
56  README
36  CMakeLists.txt
20  Makefile
13  build.sh
--> src/
    143    src/pheat.py
    192    src/cheat.cc
    269    src/fheat.f90
```

- Minimal working code for each language: parameter class, energy/integrator class, and main function
- Time to build up the developer and user interfaces!

Guidelines & Themes

- Start from a portable build system
- Keep source and documentation together
  - So changes are synced
  - YMMV: LAMMPS does this, pyscf does not
- Keep source and tests together
  - Note: some projects maintain separate "reference artifact" repositories
- Split (and separately package) projects that become large
  - Especially true for "optional" components and abstraction layers (aka. "glue-code")

Guidelines & Themes

- Do: Have a CI-level integration test (simulate an external user)
- Do: document manual install process – *what steps do you actually run?*
  - Many projects do this even for dependencies (especially difficult ones)
  - Example: PIConGPU documents how to install Boost (great – since boost has many options)
  - Example: DFT-FE documents how to install Deal.II (great - since Deal.II is complex)
  - Example: lots more inside .github/workflows folders
- Don't: assume everyone will have access to apt-get / docker / VM for getting dependencies

---- as a package consumer ---

- Do: Complain (politely) when something doesn't compile / install / run as documented
  - These are vital fixes and the devs will (should) thank you.
- Do: submit issues / PRs for docs for upstreams
  - Great way to make friends & forge collaborations.

What and Where to File Bugs? Issues? Doc. Requests?

- Doesn't compile / install / run as documented? No documentation?
  - These are vital fixes and the devs will (*should*) thank you.
  - But *first* check HPC site facilities / colleagues.
  - Then complain (politely) to maintainers when something doesn't work.
  - "standard" contribution policy: If it isn't obvious to someone, it should be documented.
- Got it working?
  - Document in your own project (will help onboarding, and you later).
  - Reply to same people anyway. (can increase your project's visibility)
- Submit issues / PRs for docs to upstreams.
  - Great way to make friends & forge collaborations.
- Send self-contained, full examples (reference existing docs).

Hello Numerical World Example (heat equation)

- How will other projects use this work?

```
33  COPYING
56  README
36  CMakeLists.txt
20  Makefile
13  build.sh
--> src/
    143    src/pheat.py
    192    src/cheat.cc
    269    src/fheat.f90
```

<u>Front-lines: Documentation!</u>

* what's expected to work?
* where / how do I configure it?

executable

```
$PREFIX/bin/
        artifact-tools
        run-parallel
        run-serial
```

headers

```
$PREFIX/include/$PROJ
        config.h
        heat.h
        heat.mod
```

libraries

```
$PREFIX/lib/$PROJ
        libheat.so
        libheat.a
```

Using the package stack during/with development

- C++:
  - Maintain a "env.sh" file loading appropriate modules
  - Install all packages you build up into a common "/usr/local" prefix
  - Do development there, but be aware that env changes machine to machine
- Python:
  - Create a poetry project to use for its virtual environment
    - cd <project>; poetry shell
  - Keep working scripts / gist-s there
- Spack:
  - Create a spack environment (spack env create; spack env activate; spack install; spack load)
  - Note also: spack build-env <project name> bash (sets CXXFLAGS, etc.)
  - These will load up the environment variables for accessing your installed software

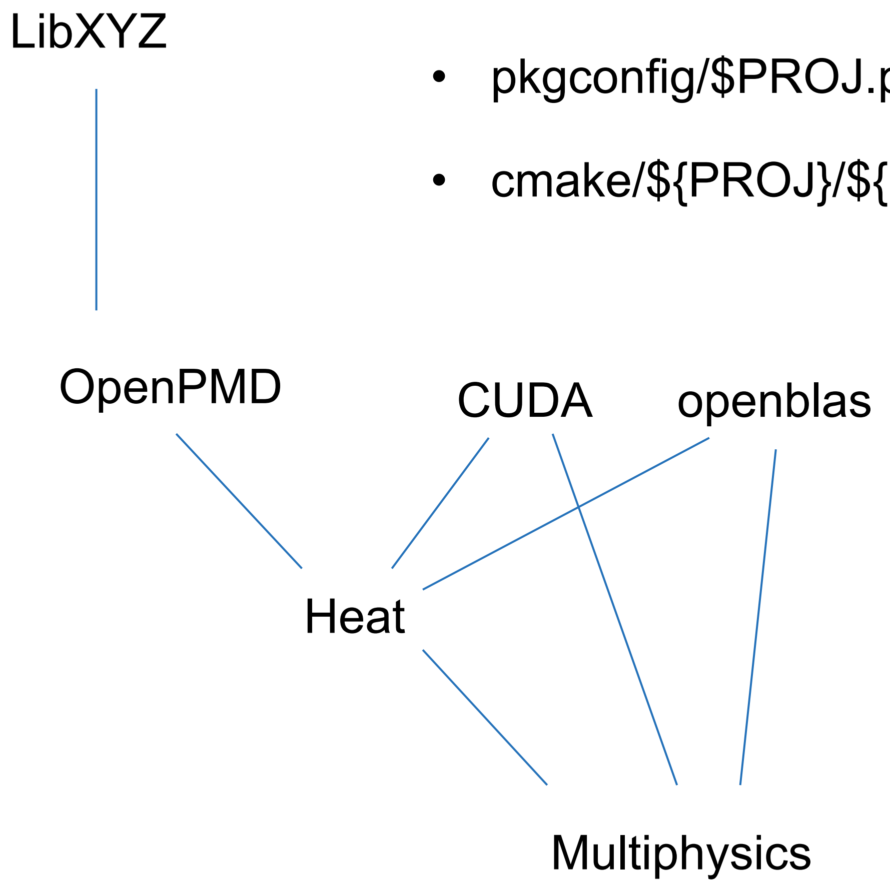
Main complication: working on multiple packages at once – usu. Special specs exist for sourcing filesystem paths / github repos directly

Complications: Software Supply Chain Stability / Security

- Packaging systems may install vulnerable software
- Regularly test your dependencies – check for CVE-s on dependencies?
- Add GPG-signatures to releases
  - Ensures the code has not been tampered with
  - Places responsibility on developer for ensuring software stack trustworthiness
- Lockfiles – npm package-lock.json / Gemfile.lock / poetry.lock / Spack.lock (kind of) / etc.
  - Allows auditing of exact versions for all installed dependencies

Complications: Transitive Build / Link Requirements

- Header include paths
- Library search paths
- Compiler features
  - e.g. C++11/14/17/20
  - Compiler-dependent runtimes (GCC OpenMP vs. Clang)
- Linking features
  - Fat-binary formatted coprocessor objects.



Intended to be solved by (pick one)

- pkgconfig/$PROJ.pc
- cmake/${PROJ}/${PROJ}Config.cmake

Installing a library with CMake

```
# CMakeLists.txt
...
install(TARGETS ${installable_libs}
      DESTINATION lib
      EXPORT HeatEqTargets)
install(EXPORT HeatEqTargets
  FILE HeatEqTargets.cmake
  NAMESPACE HeatEq::
  DESTINATION lib/cmake/HeatEq
)
... # 15 more lines of cmake cruft
```

```
# Config.cmake.in

@PACKAGE_INIT@

include (
"${CMAKE_CURRENT_LIST_DIR}/HeateqTargets.cmake" )

include(CMakeFindDependencyMacro)
find_dependency(MPI 2.0 REQUIRED)

check_required_components(<package name>)
```

- References:
  - github.com/frobnitzem/lib0
  - https://code.ornl.gov/99R/mpi-test
  - https://cmake.org/cmake/help/git-stage/manual/cmake-packages.7.html#creating-packages

Package Publication Steps – C++ with cmake

- After editing CMakeLists.txt:
- Check and run tests with cmake; make && ctest
- Update ChangeLog, documentation
- git tag -m "Bug fixes to v1.1.1" v1.1.2
- git push
- Change public facing websites, modules, spack versions, links, etc. to point to new version
  – For spack <package name>/package.py, use "spack checksum <package name>"
- ** Users should find and use new versions **
  – This highlights the need for testing deployments using both simultaneous versions and update-in-place strategies. Did you document that?

Net result

```
33  COPYING
56  README
36  CMakeLists.txt
20  Makefile
13  build.sh
--> src/
     143     src/pheat.py
     192     src/cheat.cc
     269     src/fheat.f90
```

```
33  COPYING
80  README
29  ChangeLog
50  CMakeLists.txt
20  Makefile
13  build.sh
--> tests/
      30     test_heat.sh
--> src/
     143     pheat.py
     192     cheat.cc
     269     fheat.f90
```

- CMakeLists.txt: added library export and a test (calling test_heat.sh)
- README: note "find_package" and "ctest" commands
- ChangeLog: document your success!

"Progression" of Packaging

- Build System
  - Automake / scons / cmake / mesonbuild.com
- Package Management
  - Pkg-config / CMake Package Manager / spack
- Containerization
  - Singularity / charliecloud + docker-compose

- References
  - https://supercontainers.github.io/sc20-tutorial/
  - https://fluid-run.readthedocs.io/en/latest/HowTo/setup_your_repo.html

Containerization

Xen Hypervisor = kernel built to manage kernels

Linux Kernel

Daemons

User Programs

Real Filesystems

Virtual Machine
- Kernel, Daemons
- User Programs + tty/gui
- Disk Image Filesystem

App Container

- Emulated / shared filesystems + images
- User program(s)

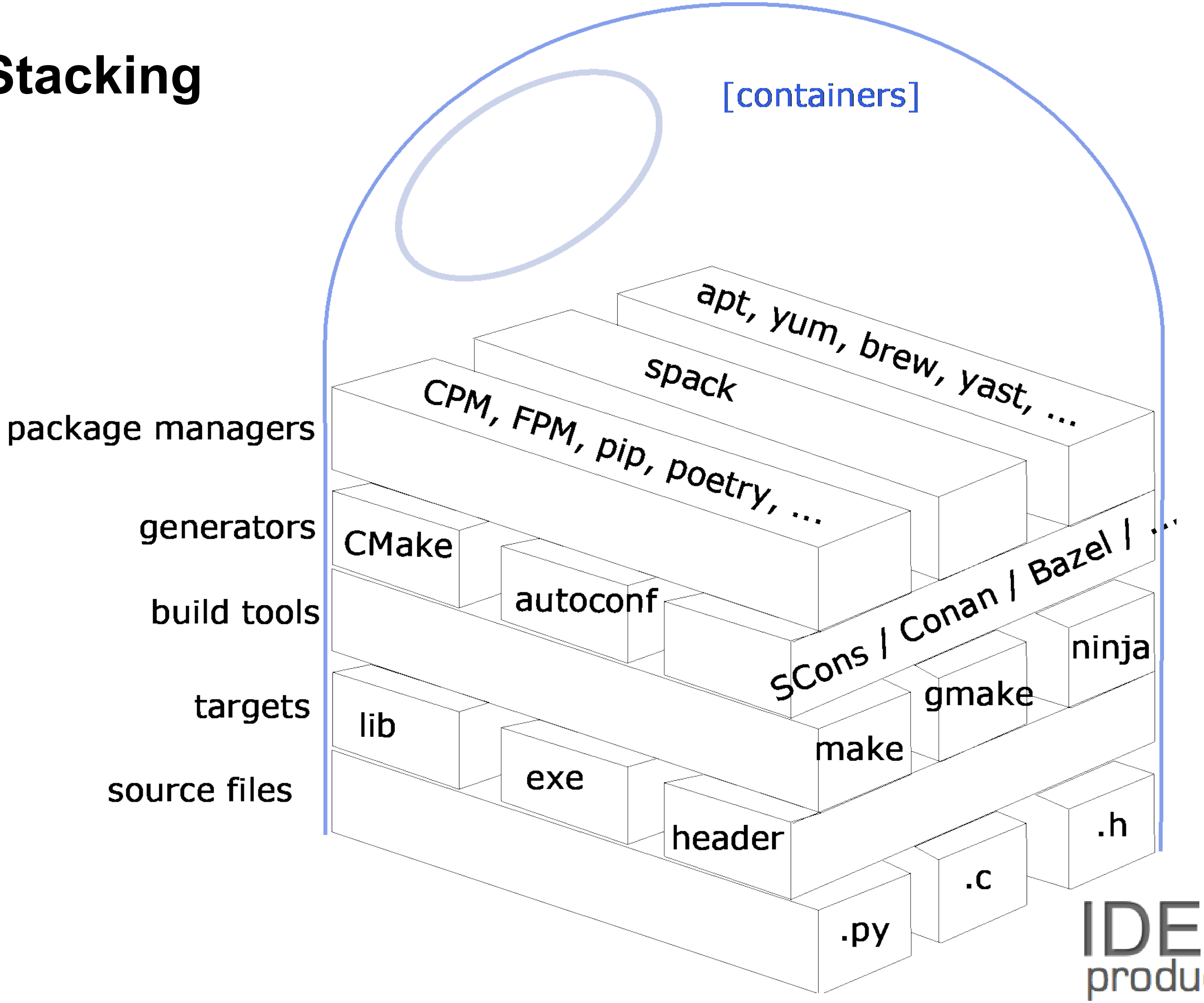
...

FreeBSD Kernel

Linux Kernel

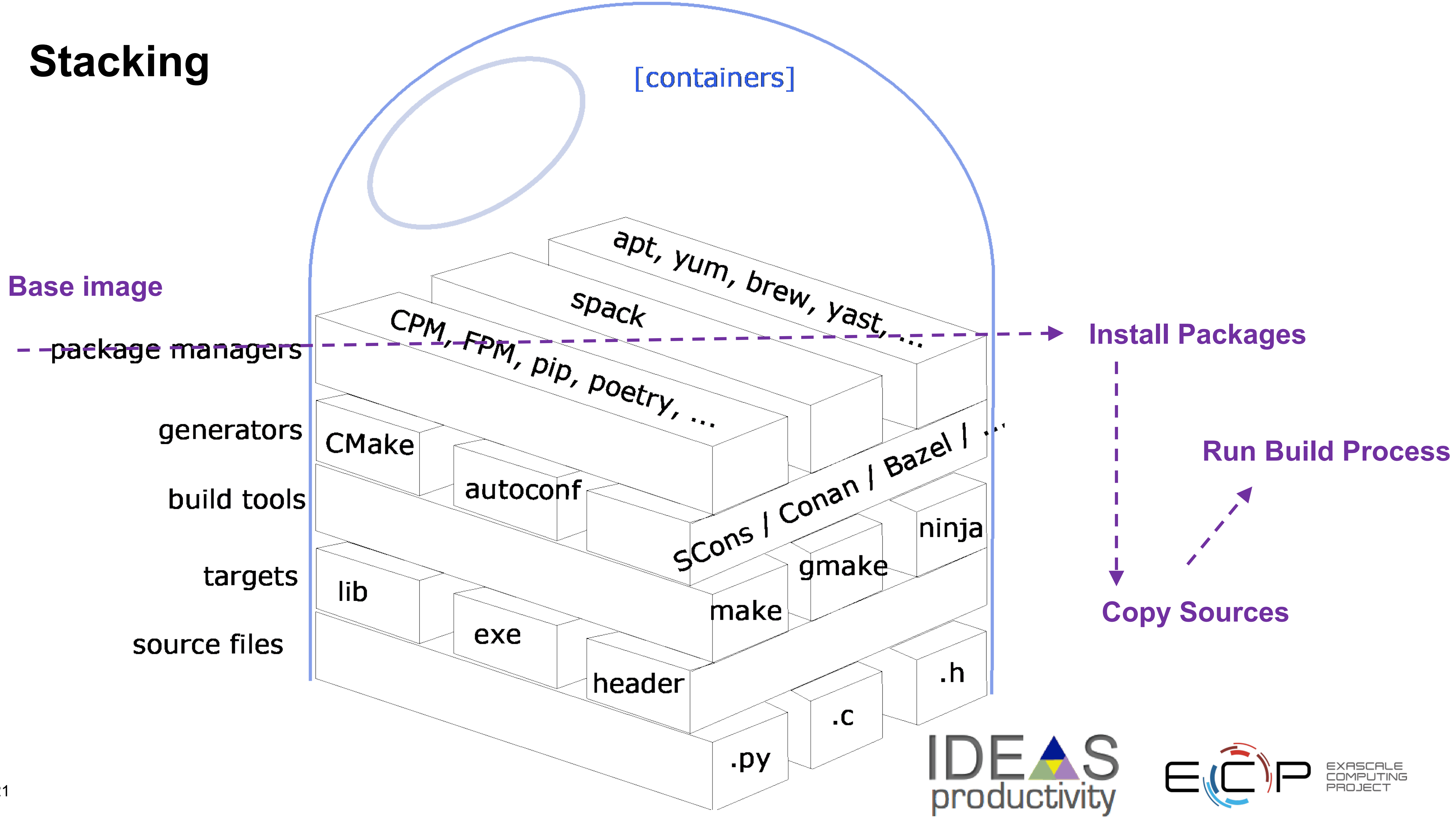
...

Stacking



[containers]
package managers
generators
build tools
targets
source files
apt, yum, brew, yast, ...
spack
CPM, FPM, pip, poetry, ...
CMake
autoconf
SCons / Conan / Bazel / ...
ninja
gmake
make
lib
exe
header
.h
.c
.py

Stacking



[containers]
Base image
package managers
generators
build tools
targets
source files
apt, yum, brew, yast, ...
spack
CPM, FPM, pip, poetry, ...
CMake
autoconf
SCons / Conan / Bazel / ...
ninja
gmake
make
lib
exe
header
.h
.c
.py
Install Packages
Run Build Process
Copy Sources

Container Build Examples

User documentation

```
BootStrap: localimage
From: heateq.sif

%files
   ./app.py /app/app.py

%post
   pip install aiohttp pygit2 mpi-list

%runscript
   /app/app.py

%help
   Simulate heat equation and post to REST API.
```

Container Build File

```
BootStrap: docker
From: python:3.9

%files
   ./heateq /build/heateq

%post
   apt-get -y update
   apt-get -y install openblas cmake build-essential
   pip install numpy scipy
   mkdir /build/heateq/build && cd /build/heateq/build
   cmake ..; make -j4 install

%help
   Installs heateq library
```

```
#!/bin/sh

singularity build --remote heateq.sif heateq.def
```

https://fastapi.tiangolo.com/deployment/docker/#build-a-docker-image-for-fastapi
https://supercontainers.github.io/sc20-tutorial/02.docker/index.html
https://cloud.sylabs.io/builder

After containerization

```
 33  COPYING
120  README
 29  ChangeLog
 50  CMakeLists.txt
 20  Makefile
 15  heateq.def
  3  build-singularity.sh

 --> tests/
       30    test_heat.sh
 --> src/
      143    pheat.py
      192    cheat.cc
      269    fheat.f90
```

Conclusion

- Documentation is the beginning and end of packaging
  - Makefiles, dependency lists, and scripts are no substitute for explanations
- Lots of standards & tools to choose from!
  - Make / CMake / autotools
  - py-scaffold / poetry
  - setup,py/"make-ext", scikit-build+cython
  - spack
- Packaging helps you...
  - Interact with your users
  - Improve your developing experience (lower cognitive load)
  - More easily test
  - Deploy faster

Acknowledgments

- IDEAS-ECP Team:
  - David Bernholdt
  - Patricia Grubel
  - Mark Miller
  - Axel Huebl
- PIConGPU Team:
  - Sunita Chandrasekaran
  - Rene Widera
  - Klaus Steiniger
  - Alexander Debus
- DFT-FE Team:
  - Vikram Gavini
  - Sambit Das
  - Phani Motamarri
- DCA++ Team:
  - Peter Doak
  - Thomas Maier
- ZFP Team:
  - Peter Lindstrom
- OLCF/HPE/Spack Teams:
  - Matt Belhorn
  - Luke Roskop
  - Massimiliano Culpo
  - Todd Gamblin

Article on CI team practices:

https://bssw.io/blog_posts/bright-spots-team-experiences-implementing-continuous-integration

IDEAS productivity EXASCALE COMPUTING PROJECT

fin

Simple Walk-Throughs

- Python - pyscaffold
- C++ - CMake Library Export
- Fortran – CMake Library Export
- C++ – spack

Package Publication Checklist

pre-flight checks

- Is this something I am going to re-use?
- Is the documentation good enough that another developer can quickly get it working?
- Can I hold development of new features while I package up what's here?
  - "pausing" a good idea is nontrivial
- Have I tested it in practice? – start from a clean copy, follow the directions / tests
- Am I ready to support users of this software? (or write a disclaimer)
- Have I picked a license and figured out what copyright assignment & internal reviews need to happen.
- Have I documented my git workflow (what do branches / tags represent)?

Hello Numerical World Example (heat equation)

github.com/bssw-tutorial/simple-heateq

```
33  COPYING
56  README
36  CMakeLists.txt
20  Makefile
13  build.sh
--> src/
    143    src/pheat.py
    192    src/cheat.cc
    269    src/fheat.f90
```

- Minimal working code for each language: parameter class, energy/integrator class, and main function
- Time to build up the developer and user interfaces!

Hello Numerical World Example (heat equation)

- How will other projects use this work?

```
33  COPYING
56  README
36  CMakeLists.txt
20  Makefile
13  build.sh
--> src/
    143    src/pheat.py
    192    src/cheat.cc
    269    src/fheat.f90
```

<u>Front-lines: Documentation!</u>

* what's expected to work?
* where / how do I configure it?

executable

```
$PREFIX/bin/
        artifact-tools
        run-parallel
        run-serial
```

headers

```
$PREFIX/include/$PROJ
        config.h
        heat.h
        heat.mod
```

libraries

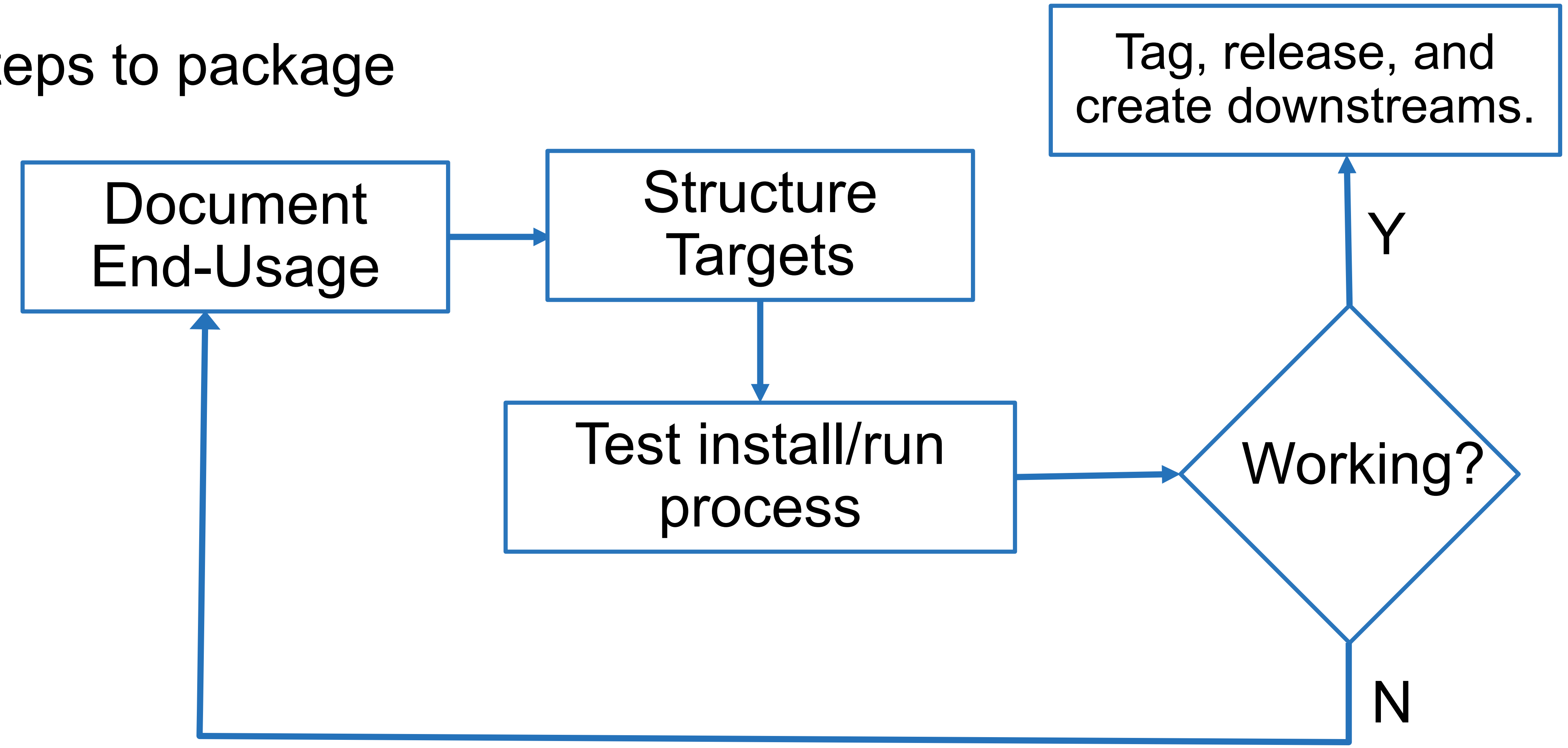
```
$PREFIX/lib/$PROJ
        libheat.so
        libheat.a
```


IDEAS productivity

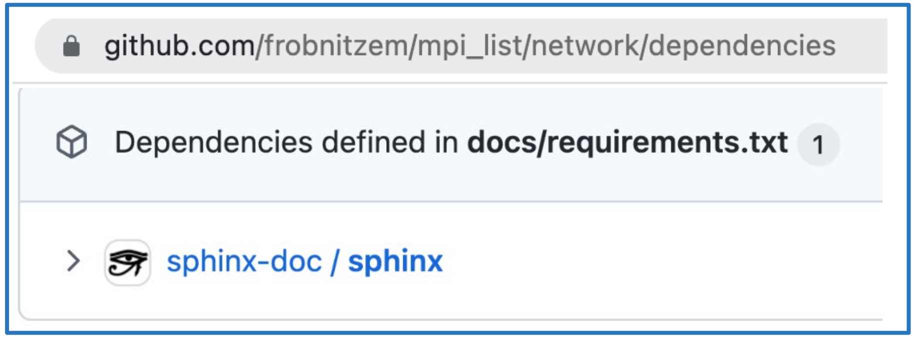
ECP EXASCALE COMPUTING PROJECT

Hello Numerical World Example (heat equation)

- Steps to package



Importing a Python Package



basic

```
# requirements.txt
heateq >= 0.1
```

```
pip install –r requirements.txt
export PYTHONPATH=/path/to/heateq
python3 app.py
```

```
# app.py

import heateq
```

advanced

```
# setup.cfg

install_requires =
    heateq >= 0.1
```

```
python –m venv venv
source venv/bin/activate
pip install -e .
python3
>>> import app
>>>
```

```
# app.py

from heateq.pheat import Params
```

Python Library Structure

- src/pheat.py

class Params
class Energy -copy--> heateq/pheat.py (copy)
def simulate(p)

- __init__.py

(can be empty) -copy--> heateq/__init__.py

|
v

Inside the heateq package:
  from .pheat import Params

Outside the package:
  from heateq.pheat import simulate

Packaging with pyscaffold

```
pip3 install pyscaffold
pip3 install tox
putup heateq
cd heateq # tests in tests/ subdir.
tox
```

```
default run-test: commands[0] | pytest
======================= test session starts ========================
platform darwin -- Python 3.9.0, pytest-6.2.2, py-1.10.0, pluggy-0.13.1 -- plugins:
cov-2.11.1
collected 2 items

tests/test_skeleton.py::test_fib PASSED                    [ 50%]
tests/test_skeleton.py::test_main PASSED                   [100%]

---------- coverage: platform darwin, python 3.9.0-final-0 -----------
Name                    Stmts   Miss Branch BrPart  Cover   Missing
------------------------------------------------------------------------
src/heateq/__init__.py      6      0      0      0   100%
src/heateq/skeleton.py     32      1      2      0    97%   135
------------------------------------------------------------------------
TOTAL                      38      1      2      0    98%

======================== 2 passed in 0.07s =========================
  default: commands succeeded
  congratulations :)
```

pyscaffold.org

Net result

```
33  COPYING
56  README
36  CMakeLists.txt
20  Makefile
13  build.sh
--> src/
     143     src/pheat.py
     192     src/cheat.cc
     269     src/fheat.f90
```

```
 33  COPYING.rst
 80  README.rst
  5  AUTHORS.rst
 13  CHANGELOG.rst
  8  pyproject.toml
 68  tox.ini
 21  setup.py
100  setup.cfg
     docs/
     tests/
 36  CMakeLists.txt
 20  Makefile
 13  build.sh
 --> src/
      143     heateq/pheat.py
      192     cheat.cc
      269     fheat.f90
```

- setup.cfg: editable list of project data & dependencies
- pyproject.toml, tox.ini, setup.py: auto-generated boilerplate
- README: note "pip -e install ." command

Importing a C++ Package

basic

```
g++  –I$inst/include/heateq        \
    –L$inst/lib                    \
    -Wl,-rpath,$inst/lib –lheat    \
    -o app app.cpp
```

```
/* app.cpp */

#include <heateq.hpp>

…
```

advanced

```
# CMakeLists.txt
option(ENABLE_HEATEQ "Use heateq library." ON)

if(ENABLE_HEATEQ)
   find_package(HeatEq 1.0 REQUIRED)
   target_link_libraries(app PRIVATE HeatEq::heat)
endif()
```

```
/* app.hpp.in */

#cmakedefine ENABLE_HEATEQ
```

C++ Library Structure

- src/cheat.cpp

  struct Params {}
  struct Energy {}

- include/heat.hpp

  struct Params {}
  struct Energy {}

--(g++ -shared)--> lib/heat.so

------(copy)-----> include/heat.hpp

|
|
|
v

#include <heat.hpp>

Fortran Library Structure

- src/fheat.f90

```
        ---- gfortran –shared --->
module ArgParser       ------>   include/argparser.mod

module EnergyField     ------>   include/energyfield.mod
  use ArgParser
                ------>   lib/heat.so
```

```
     |
     v
```

Requires referencing correctly

```
use EnergyField
```

```
gfortran –I$inst/include/heateq        \
        –L$inst/lib                    \
        -Wl,-rpath,$inst/lib –lheat    \
        -o app app.f90
```

Package Publication Steps – Fortran with cmake

- Adding cmake target + tests – same as for C++.
- Structure your package following a good example!

- Refs:
  - Well documented example: https://github.com/leonfoks/coretran
  - Modern conventions example: https://selalib.github.io/
  - Fortran Package Index: https://fortran-lang.org/, https://www.archaeologic.codes/software
  - Fortran Package Manager: https://fpm.fortran-lang.org/

Package Publication Steps – C++ with cmake + Spack

spack.readthedocs.io

```python
# heateq/package.py

from spack import *

class HeatEq(CMakePackage):
    "HeatEq: heat conduction kernels"
    homepage = "https://..."

    variant('openmp', default=True)
    depends_on("py-pybind11@2.6.2")
    depends_on('llvm-openmp', when='%apple-clang +openmp')

    def cmake_args(self):
        spec = self.spec
        args = [ "-DMY_BUILD_TESTS=YES"
                 "-DENABLE_OPENMP=%s" % ("+openmp" in spec) ]
        return args
```

productivity

EXASCALE COMPUTING PROJECT

Package Publication Steps – C++ with cmake + Spack

spack.readthedocs.io

- Spack replaces "build.sh" with a spec

```
33  COPYING
84  README
29  ChangeLog
50  CMakeLists.txt
20  Makefile
~~13  build.sh~~
--> tests/
     30    test_heat.sh
--> src/
     143    pheat.py
     192    cheat.cc
     269    fheat.f90
```

```python
# heateq/package.py

from spack import *

class HeatEq(CMakePackage):
    "HeatEq: heat conduction kernels"
    homepage = "https://..."
    maintainers = ["github-id"]
    def cmake_args(self):
        mpi = self.spec["mpi"]
        return [ "-DMPI_HOME={0}"
                 .format(mpi.prefix) ]
```

- README: now references "spack install heateq"
- Eventually: package.py knows how to compile your package's variants and historical versions

IDEAS productivity

ECP EXASCALE COMPUTING PROJECT

Anatomy of a Spack Dependency "spec"

```
  - e4s_22.02_gpu_specs:
    # Minimal diff from v21.11
    - amrex@22.02 +rocm~cuda amdgpu_target=gfx90a
    - kokkos@3.5.00 +rocm~cuda~wrapper~openmp amdgpu_target=gfx90a
    - strumpack@6.3.0 ~slate+rocm~cuda amdgpu_target=gfx90a
    - sundials@6.1.1 +rocm~cuda amdgpu_target=gfx90a
```

https://github.com/mpbelhorn/olcf-spack-environments/blob/develop/hosts/frontier/envs/base/spack.yaml

<package name>@<version>

+<enabled option> ~<disabled option>

% <compiler>@<compiler version>

^<dependency1> ^<dependency2> ...

https://spack.readthedocs.io/en/latest/packaging_guide.html#dependency-specs

Anatomy of a Spack Dependency "spec"

<package name>@<version>

+<enabled option> ~<disabled option>

% <compiler>@<compiler version>

^<dependency1> ^<dependency2> ...

Advanced Examples:
spack edit gcc

- compile-time options to your package:
  - variant('option-name', default=False, description='help text')
- dependency for your package:
  - depends_on("spec string", when="string-to-test-against-my-spec") #, type='build'
- package idiom:

```
def cmake_args(self):
    spec = self.spec
    if spec.satisfies("+myoption"): ...
```

https://spack.readthedocs.io/en/latest/packaging_guide.html#dependency-specs

HPC: modules and Spack Development Environments

- Logically, provide a "load package" command
- Spack vs. modules:
  - Spack can create TCL or lmod modules
  - Spack can provide its own "environment views" outside of modules
- All these boil down to setting environment variables

Intermediate Example: C++ with spack

- https://github.com/qcscine/sparrow - semi-empirical quantum chemistry
- git clone https://github.com/spack/spack; source spack/share/spack/setup-env.sh; spack compiler find
- spack create https://github.com/qcscine/sparrow/archive/refs/tags/3.0.0.tar.gz
  - creates spack/var/spack/repos/builtin/packages/sparrow/package.py
- spack list cereal; spack info boost ~> depends_on("boost@1.65.0:")

Helpful commands:

```
  spack dev-build <package>  # skip download & build from the current source directory
  spack install -u cmake         # download the package & run cmake
  spack cd <package>             # change to the directory where spack is working
  spack build-env <package> bash # run a shell with env setup to build (and develop)
  spack clean                    # clears spack's download/build cache
```

https://spack-tutorial.readthedocs.io/en/latest/tutorial_packaging.html

Spack package.py

- spec = self.spec
- spec['mpi'].prefix, spec['mpi'].libs, spec['mpi'].headers

- https://spack.readthedocs.io/en/latest/spack.util.html#module-spack.util.prefix

https://spack.readthedocs.io/en/latest/packaging_guide.html#accessing-dependencies

State of Practice – Packaging for Portability

Portability (kernels)

Kokkos
Raja
Alpaka
DPC++ / SYCL
... Thrust
std::execution::par_unseq

Real-World Example: DCA++

- Dynamic Cluster Approximation
  - Electron correlation involving many tensor contractions (matrix multiplies)
  - C++ code
  - Implements own matrix math library, adding HIP backend
- Challenge
  - Minimal additions to existing CUDA build method
  - Several types of link helpers – runtime, blas, kernel
- Solution
  - Use cmake to include a header-translation layer and change link options – minimal changes to source code.

Real-World Example: DCA++

```
// src/linalg/util/info_gpu.cpp

// This file implements gpu info functions.

#include "dca/config/haves_defines.hpp"
#if defined(DCA_HAVE_CUDA)
#include "dca/linalg/util/error_cuda.hpp"
#elif defined(DCA_HAVE_HIP)
#include "dca/linalg/util/error_hip.hpp"
#include "dca/util/cuda2hip.h"
#endif
```

- References:
  - https://github.com/CompFUSE/DCA
  - https://github.com/twhite-cray/quip
  - https://code.ornl.gov/99R/mpi-test/-/tree/gpu_support

Real-World Example: pyscf extension template

- Python Atomic Orbital Code – HF, DFT, some CC
  - Modular python design
  - Kernels implemented in C for efficiency
  - Extended functionality as plugins (e.g. analysis helpers, MPI parallelization)
- Challenge
  - Enable pyscf to "import" its plugins
  - Allow plugins to incorporate compiled C libraries
- Solution
  - Standardize package layout and provide a templated "setup.py" file.

- References:
  - https://github.com/pyscf/extension-template

Real-World Example: pyscf extension template

```
# setup.py
...
def make_ext(pkg_name, srcs,
          libraries=[], library_dirs=[pyscf_lib_dir],
          include_dirs=[], extra_compile_flags=[],
          extra_link_flags=[], **kwargs):
    return Extension(pkg_name, srcs,
                libraries = libraries,
                library_dirs = library_dirs,
                include_dirs = include_dirs + library_dirs,
                extra_compile_args = extra_compile_flags,
                extra_link_args = extra_link_flags,
                runtime_library_dirs = runtime_library_dirs, **kwargs)

if 'SO_EXTENSIONS' in metadata:
    settings['ext_modules'] = [make_ext(k, v) for k, v in SO_EXTENSIONS.items()]
```

- References:
  - https://github.com/pyscf/extension-template

Real-World Example: ZFP

- Scientific Data Compression Library
  - C++ code
  - Focus is on multidimensional arrays
- Challenge
  - Export all functionality to python with minimal effort
  - C++ code contains non-trivial data structures and link dependencies
- Solution
  - Adopt scikit-build process using cython C++ wrappers

- References:
  - https://github.com/LLNL/zfp
  - https://scikit-build.readthedocs.io

Real-World Example: ZFP

```
# python/zfpy.pyx
...
cpdef bytes compress_numpy(
    np.ndarray arr,
    double tolerance = -1,
    double rate = -1,
    int precision = -1,
    write_header=True
):
  ...

  # Setup zfp structs to begin compression
  cdef zfp_field* field =
         _init_field(arr)
  cdef zfp_stream* stream =
         zfp_stream_open(NULL)
```

```
# python/CMakeLists.txt

...
add_cython_target(zfpy zfpy.pyx C)
```

```
# python/zfpy.pxd

import cython
cimport libc.stdint as stdint

cdef extern from "bitstream.h":
    cdef struct bitstream:
        pass
    bitstream* stream_open(void* data, size_t)
    void stream_close(bitstream* stream)

...
```

- References:
  - https://github.com/LLNL/zfp
  - https://scikit-build.readthedocs.io

Real-World Example: Cabana

https://github.com/ECP-copa/Cabana

- Molecular Dynamics (Particle) simulation library
  - C++ code using Kokkos performance portability library
  - Focus is on flexible data layouts for particles
- Challenge
  - Provide a spack compile recipe correctly targeting Kokkos library
  - Allow user-selection of kokkos backends and features to be visible from library
  - Connect to library consumers (MD applications)
- Solution
  - Careful documentation of spack options required from its Kokkos dependency

Real-World Example: Cabana

https://github.com/ECP-copa/Cabana

```
# spack edit cabana

from spack.pkg.builtin.kokkos import Kokkos

...
    _versions = {
        ":0.2.0": "-legacy",
        "0.3.0": "@3.1:",
        "0.4.0": "@3.2:"
    }
    for _version, _kk_version in _versions.items():
        for _backend in _kokkos_backends:
            if (_kk_version == "-legacy" and _backend == 'pthread'):
                _kk_spec = 'kokkos-legacy+pthreads'
            elif (_kk_version == "-legacy" and
                  _backend not in ['serial', 'openmp', 'cuda']):
                continue
            else:
                _kk_spec = 'kokkos{0}+{1}'.format(_kk_version, _backend)
            depends_on(_kk_spec, when='@{0}+{1}'.format(_version, _backend))
```


productivity

PROJECT

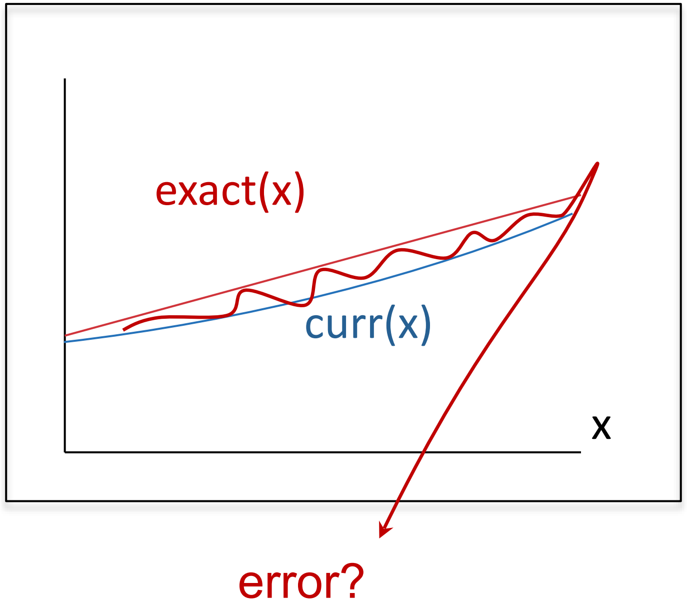
Makefile Recommendations

- 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

Running Tests via makefile

```
$ make check_all
    c++ -c  -Iinclude -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)

CMakeLists.txt

https://cmake.org/cmake/help/latest/guide/tutorial/index.html

```
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)

```
...
check_crankn/check_crankn_soln_final.curve:
	./heat alg=crankn runame=check_crankn outi=0 maxt=-5e-8 ic="rand(0,0.2,2)"
check_crankn: heat check_crankn/check_crankn_soln_final.curve
	cat check_crankn/check_crankn_soln_final.curve
	./check.sh check_crankn/check_crankn_soln_final.curve

check_upwind15/check_upwind15_soln_final.curve:
	./heat alg=upwind15 ...
```

Create a test driver to:

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

Addition to CMakeLists.txt

https://cmake.org/cmake/help/latest/command/add_test.html

tests/CMakeLists.txt

```
enable_testing()

add_test(NAME heat_help
      COMMAND $<TARGET_FILE:heat> help)

add_test(NAME crankn
      COMMAND testDriver.sh $<TARGET_FILE:heat> crankn)

# functions/for/if/adding tests
```

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=$(awk 'function abs(x){return ((x < 0.0) ? -x : x)}; BEGIN {err=1e10;} ! /#/ {err1=abs($2-$1); if(err1 < err) err = err1;} END {print err;}' check_$alg/check_${alg}_soln_final.curve)

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
```

Going Further

- Reproduce these testing strategies on another repository
  - github.com/frobnitzem/simple-heateq (same problem, different design)
- Brainstorm some simple tests you could add to your own project
  - checks you've run manually
  - difficult-to-setup and reproduce cases that could be automated
- Add some "blank tests" to your project
  - reduces the barrier to increased testing
  - What would make reporting on your build / run status better/simpler/more accessible?

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