Software Packaging

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Better Software for Reproducible Science tutorial @ SC23

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License and Citation

- **The requested citation the overall tutorial is:** David E. Bernholdt, Patricia A. Grubel, David M. Rogers, and Gregory R. Watson, Better Software for Reproducible Science tutorial, in The International Conference for High-Performance Computing, Networking, Storage, and Analysis (SC23), Denver, Colorado, 2023. DOI: 10.6084/m9.figshare.24226105.
- 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.

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Outline

- Why package?
- General Guidelines & Themes
- Simple Walk-Throughs
  - python package
  - Fortran – cmake exports
  - C++ – cmake exports
  - Spack
- Containers
- Performance portability concerns?
- Real-World Examples
  - DCA++: cuda2hip compatibility layer
  - ZFP: scikit-build for cython
  - Cabana: Kokkos with spack

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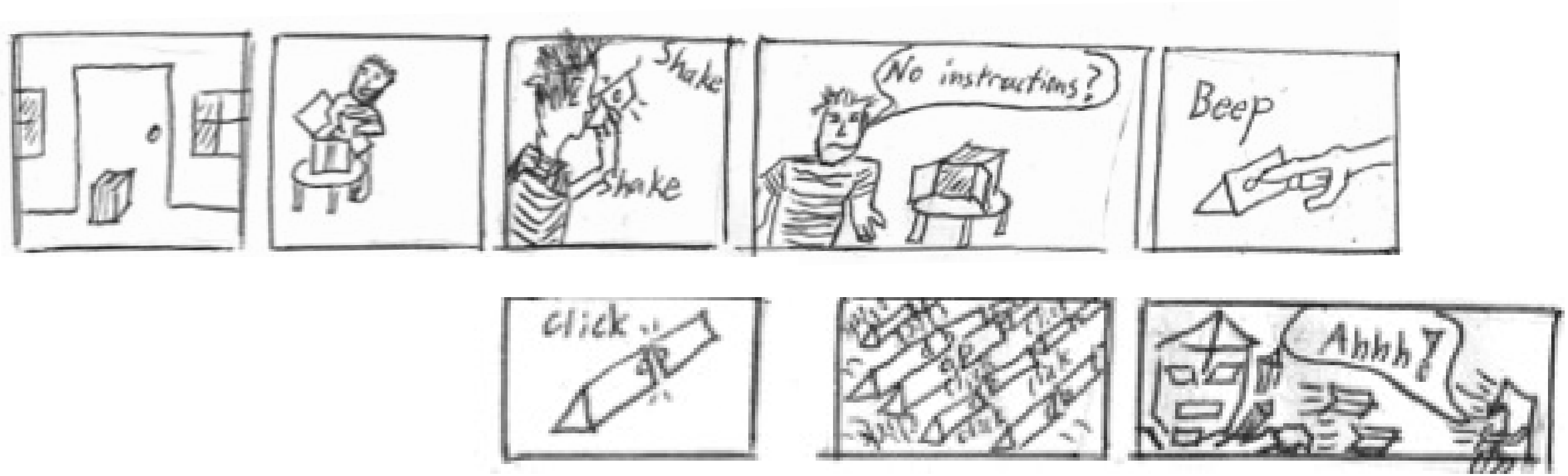
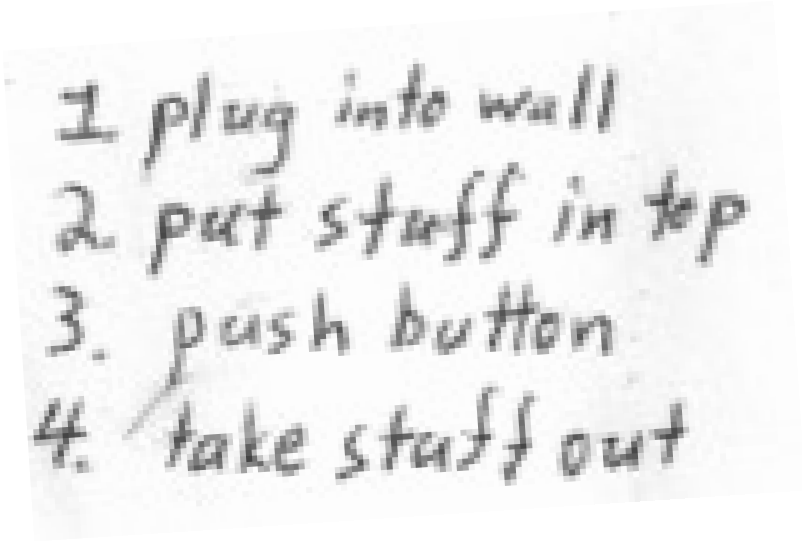
Why Package?



- 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



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.

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)?

Simple Walk-Throughs

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

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
```

executable

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

headers

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

libraries

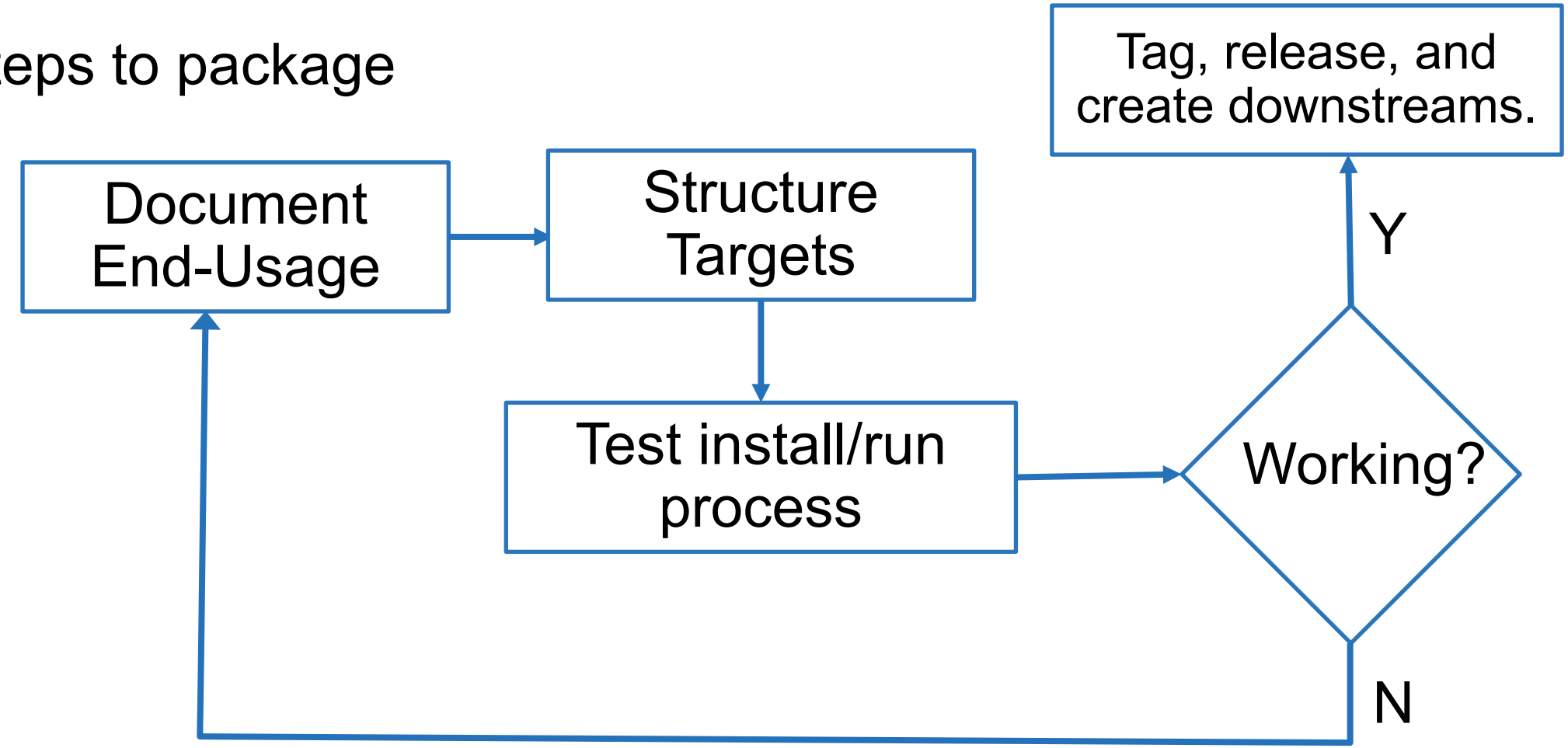
```
$PREFIX/lib/$PROJ
        libheat.so
        libheat.a
```

Front-lines: Documentation!

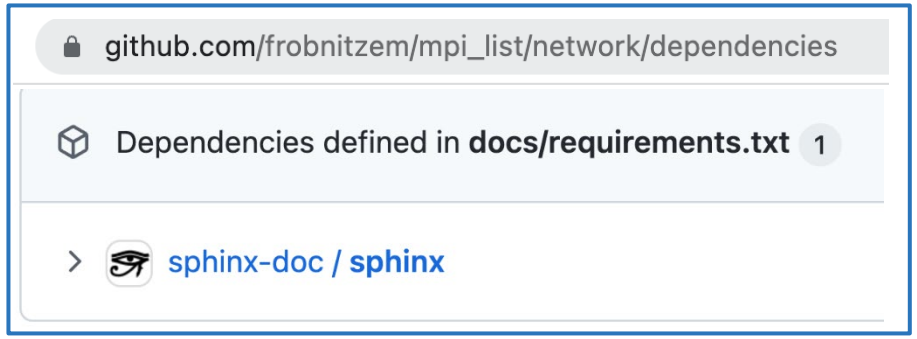
* what's expected to work?
* where / how do I configure it?

Hello Numerical World Example (heat equation)

- Steps to package



Importing a Python Package



basic

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

```
$ pip install –r requirements.txt
# or
$ 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
(venv) $ pip install -e .
(venv) $ python3
>>> import app
>>>
```

```
# app.py

from heateq.pheat import Params
```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Python Library Structure

<prefix>/lib/python3.x/site-packages/

- src/pheat.py

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

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

  |
  v

Inside the heateq package:
 from .pheat import simulate

Outside the package:
 from heateq.pheat import simulate

Packaging with pyscaffold

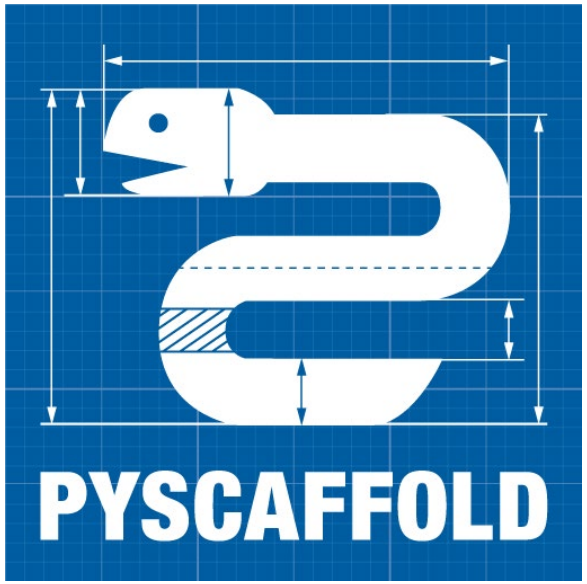
```
$ pip3 install pyscaffold
$ pip3 install tox
$ putup heateq
$ cd heateq # tests in tests/ subdir.
$ tox
```

```
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 Fortran Package

basic

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

```
/* app.f90 */
program app
  use ArgParser
  use EnergyField

...
```

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::fheateq)
endif()
```

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

#cmakedefine ENABLE_HEATEQ
```

Fortran Library Structure

- src/fheat.f90

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

module EnergyField ------> include/heateq/energyfield.mod
use ArgParser
------> lib/libfheateq.a

|
v

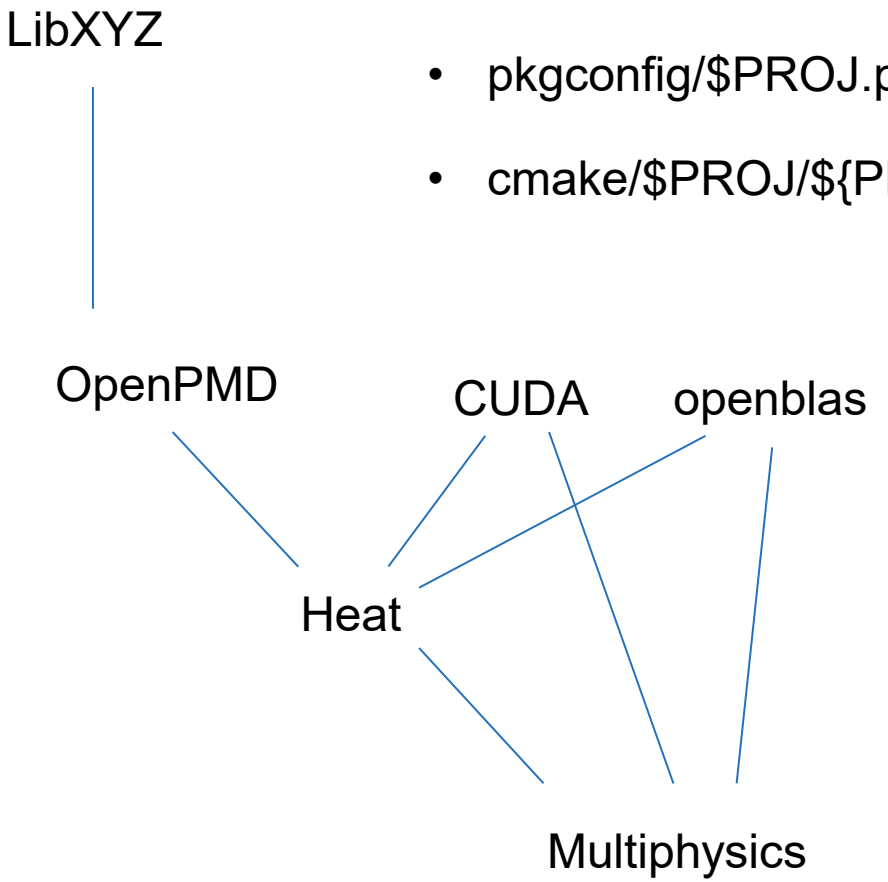
Requires referencing correctly

use EnergyField

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

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 Fortran library with CMake

```
# CMakeLists.txt
...
add_library(fheateq
    src/argparser.f90
    src/energyfield.f90)
install(TARGETS fheateq
        DESTINATION lib
        EXPORT heateqTargets)
install(EXPORT heateqTargets
  FILE heateqTargets.cmake
  NAMESPACE heateq::
  DESTINATION lib/cmake/heateq
)
... # 15 more lines of cmake cruft
```

```
# heateq.cmake.in

@PACKAGE_INIT@

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

include(CMakeFindDependencyMacro)
find_dependency(MPI 2.0 REQUIRED)

check_required_components(heateq)
```

Installs to <prefix>/lib/cmake/heateq/heateq.cmake

- References:
  - github.com/bssw-tutorial/simple-heateq (pkg branch)
  - Note: the cruft is done for you in "cmake/install.cmake: install_libs()"

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
```

- fheateq.cmake/pc.in – see examples
- README: note how downstreams should use "find_package(<package name>)" and target_link_libraries()
- example -- simple downstream consumer of this library
- ChangeLog: document your success!

```
 33  COPYING
 86  README
 29  ChangeLog
 50  CMakeLists.txt
  8  fheateq.cmake.in
  9  fheateq.pc.in
--> cmake/
     65    install.cmake
     23    rpath.cmake
 20  Makefile
--> example/
      9    CMakeLists.txt
     18    test.sh
 13  build.sh
--> src/
     143    pheat.py
     192    cheat.cc
     125    fheat.f90
      44    ArgParser.f90
      98    EnergyField.f90
```

Importing a C++ Package

basic

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

```
/* app.cpp */

#include <heateq/heat.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::cheateq)
endif()
```

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

#cmakedefine ENABLE_HEATEQ
```

C++ Library Structure

- include/heateq/heat.hpp
  - struct Params {}
  - struct Energy {}
- src/cheat.cpp
  - struct Params {}
  - struct Energy {}

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

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

|
|
|
v

#include <heateq/heat.hpp>

Requires referencing correctly

```
g++ –I$inst/include              \
   –L$inst/lib                   \
   -Wl,-rpath,$inst/lib –lcheateq   \
   -o app app.cpp
```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Installing a C++ library with CMake

```
# CMakeLists.txt
...
add_library(cheateq src/cheateq.cpp)
install(TARGETS cheateq
        DESTINATION lib
        EXPORT cheateqTargets)
install(EXPORT cheateqTargets
  FILE cheateqTargets.cmake
  NAMESPACE cheateq::
  DESTINATION lib/cmake/cheateq
)
... # 15 more lines of cmake cruft
```

```
# cheateq.cmake.in

@PACKAGE_INIT@

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

include(CMakeFindDependencyMacro)
find_dependency(MPI 2.0 REQUIRED)

check_required_components(cheateq)
```

- 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
  - Can also create a cheateq.pc.in for pkg-config (see *pkg* branch)

Package Publication Steps – C++/Fortran 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?

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Going further – additional notes and resources

- We've generated test scripts – add them to CI
  - This lets you easily try multiple different build environments (OS, compiler, etc.)
  - You will notice quickly when a new (upstream) dependency release breaks your code.
  - This will naturally lead you to put dependency compatibility versions in build files and docs.
- Some good examples for Fortran package structure:
  - Well documented: https://github.com/leonfoks/coretran
  - Namespace conventions: https://selalib.github.io/
  - Fortran standard lib (using fypp meta-programming): https://github.com/fortran-lang/stdlib
  - Fortran Package Index: https://fortran-lang.org/, https://www.archaeologic.codes/software
  - Fortran Package Manager: https://fpm.fortran-lang.org/
    - Alternative / complementary approach to cmake that works well within the Fortran ecosystem

Package Publication Steps – C++ with cmake +

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
```

```
# 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

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Anatomy of a Spack Dependency "spec"

```
193     - e4s_22.02_gpu_specs:
194       # Minimal diff from v21.11
195       - amrex@22.02 +rocm~cuda amdgpu_target=gfx90a
196       - kokkos@3.5.00 +rocm~cuda~wrapper~openmp amdgpu_target=gfx90a
197       - strumpack@6.3.0 ~slate+rocm~cuda amdgpu_target=gfx90a
198       - 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> ...

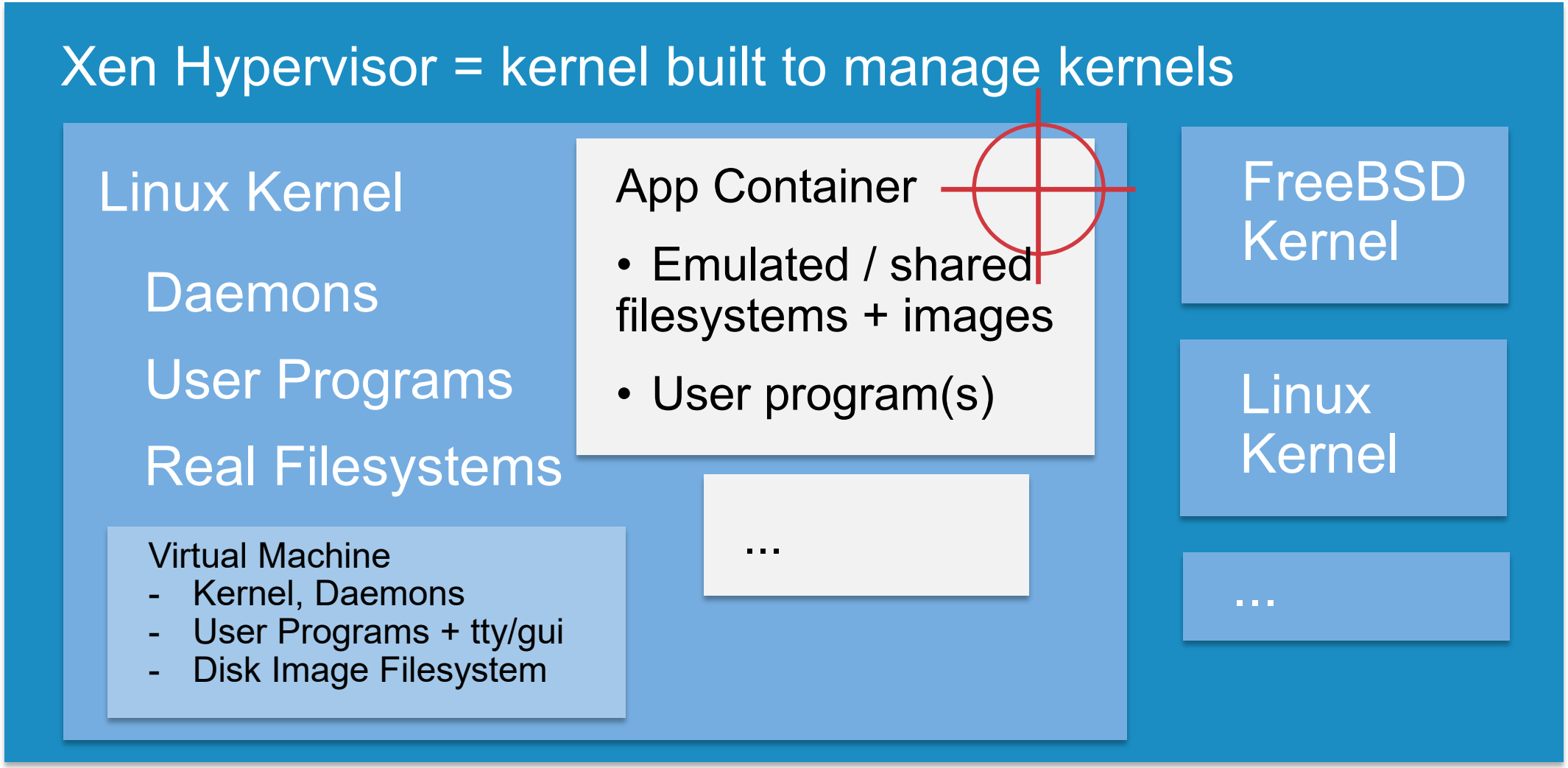
https://spack.readthedocs.io/en/latest/packaging_guide.html#dependency-specs

"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



Virtualization vs. Containerization

Virtual Machines [VirtualBox, KVM+QEMU, ...]

- Act at the OS-level, run their own kernel
- Disk image filesystem (lots of space)
- Some support processor emulation
- Must be self-contained (think network-level connectivity like NFS-mounts)

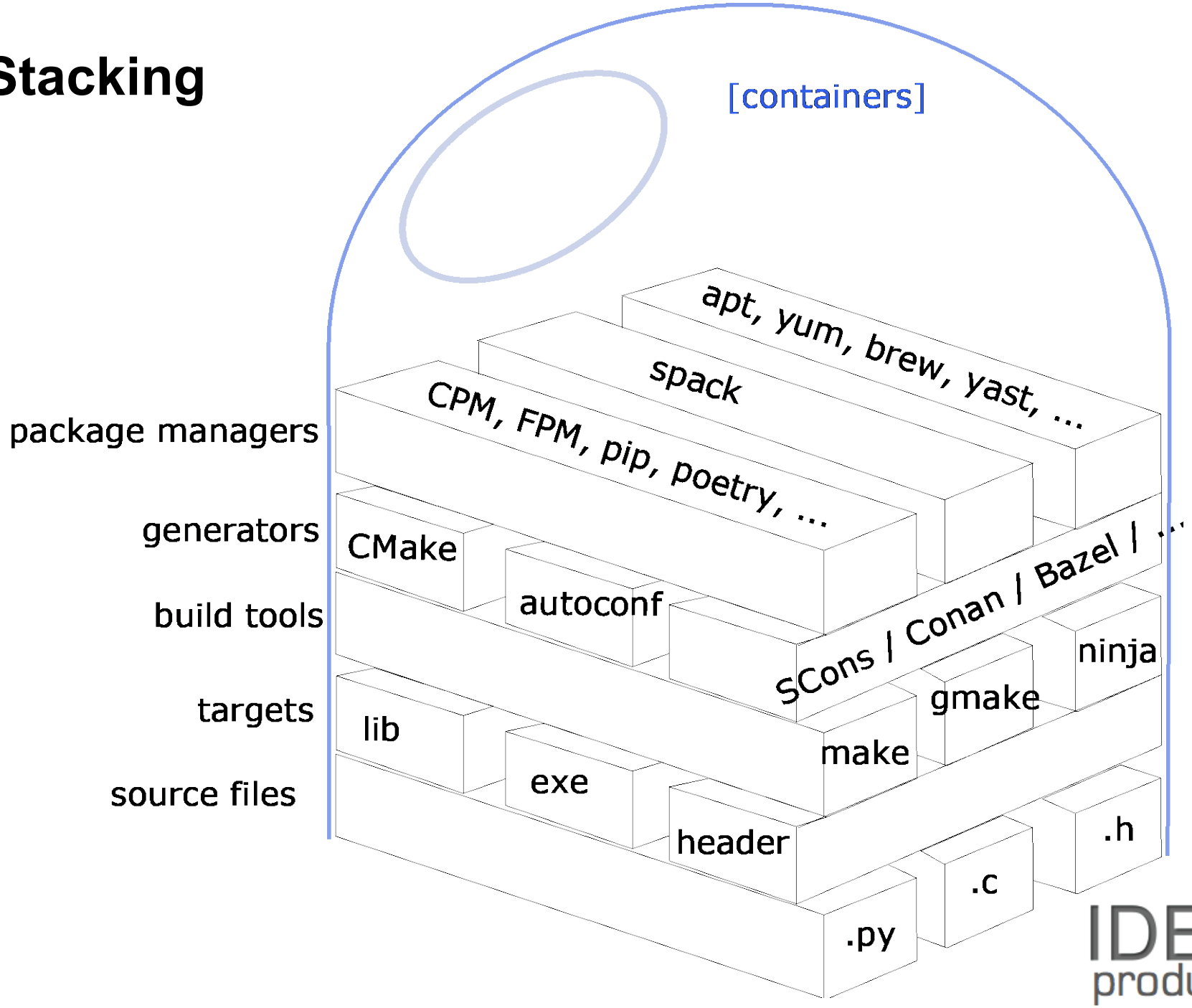
Containers [Docker, Apptainer, Charlie-Cloud, ...]

- Act at the application-level, and share the same OS
- Virtual filesystems = fully custom system libraries, SW stack, and tools
- Can still mount/map libraries and system facilities from host
- Distinguish "image" (stored container) from "container" (running container)

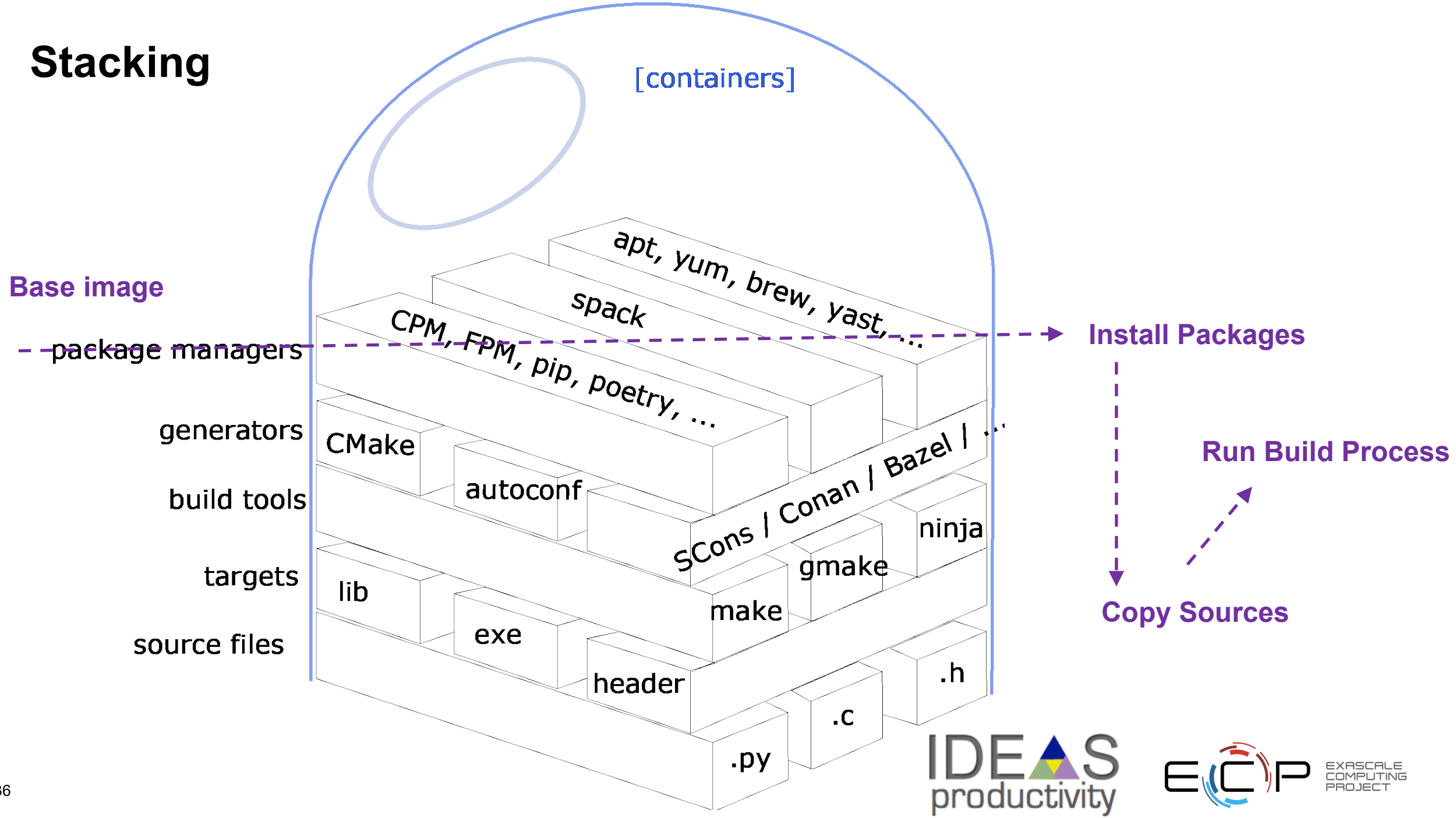
Both:

allow checkpoint / restart

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

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

New article on CI team practices:

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

Bonus Material

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

Package Publication Steps – C++ with cmake +

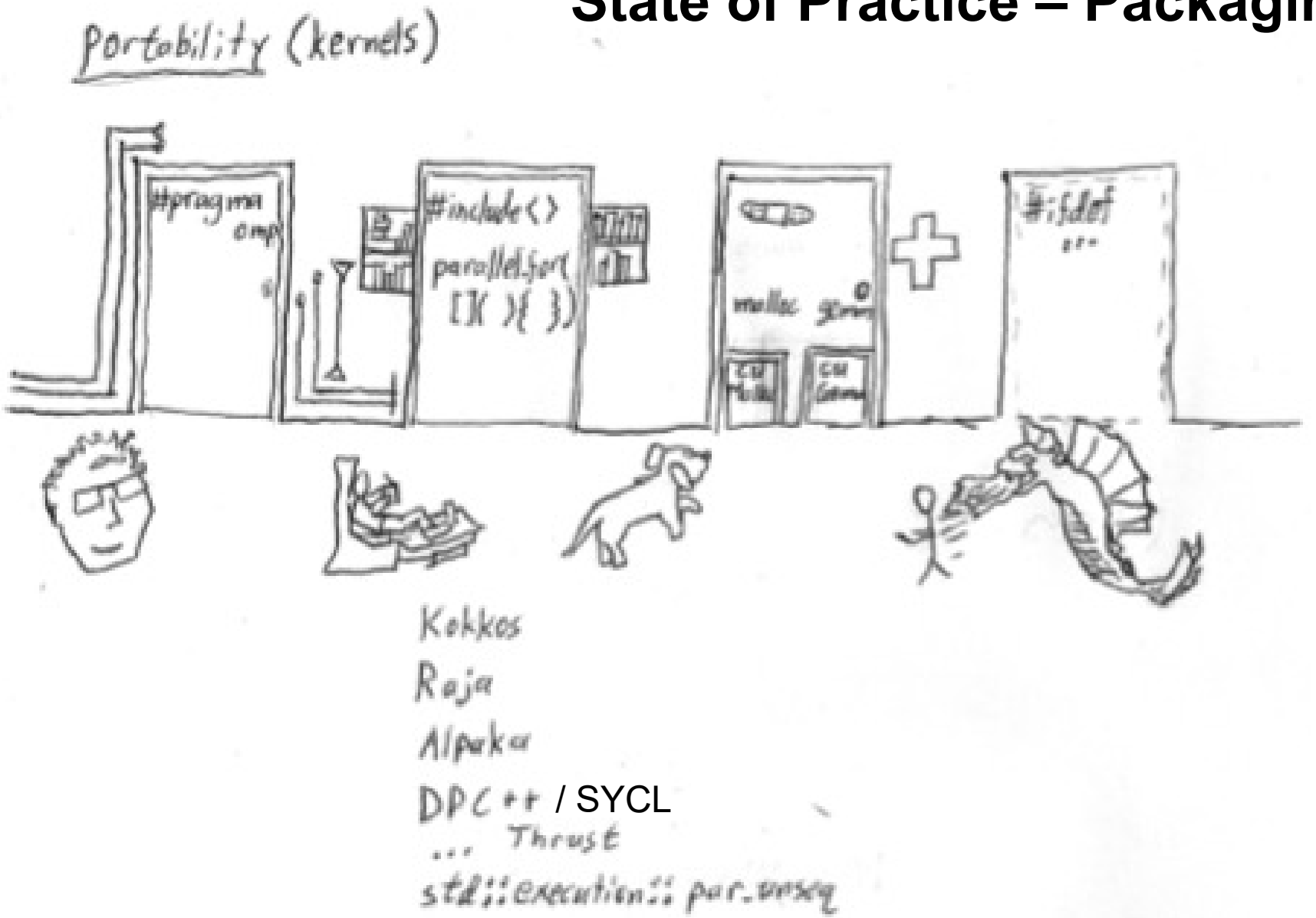
spack.readthedocs.io

```
# 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

State of Practice – Packaging for Portability



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))
```

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

Hacking the package stack

- C++:
  - Maintain a "env.sh" file loading appropriate modules
  - 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 ...)
  - Note also: spack build-env <project name> bash (sets CXXFLAGS, etc.)
  - These will load up the environment variables for accessing your installed software.

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