
# Software Packaging



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Better Scientific Software tutorial @ NOAA Global Systems Laboratory

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# License, Citation and Acknowledgements

## License and Citation



- **The requested citation the overall tutorial is:** David E. Bernholdt, Anshu Dubey, and Patricia A. Grubel, Better Scientific Software tutorial, in NOAA Global Systems Laboratory, Boulder, Colorado, 2023. DOI: 10.6084/m9.figshare.23796606.
- Individual modules may be cited as *Speaker, Module Title*, in *Tutorial Title*, …

## Acknowledgements


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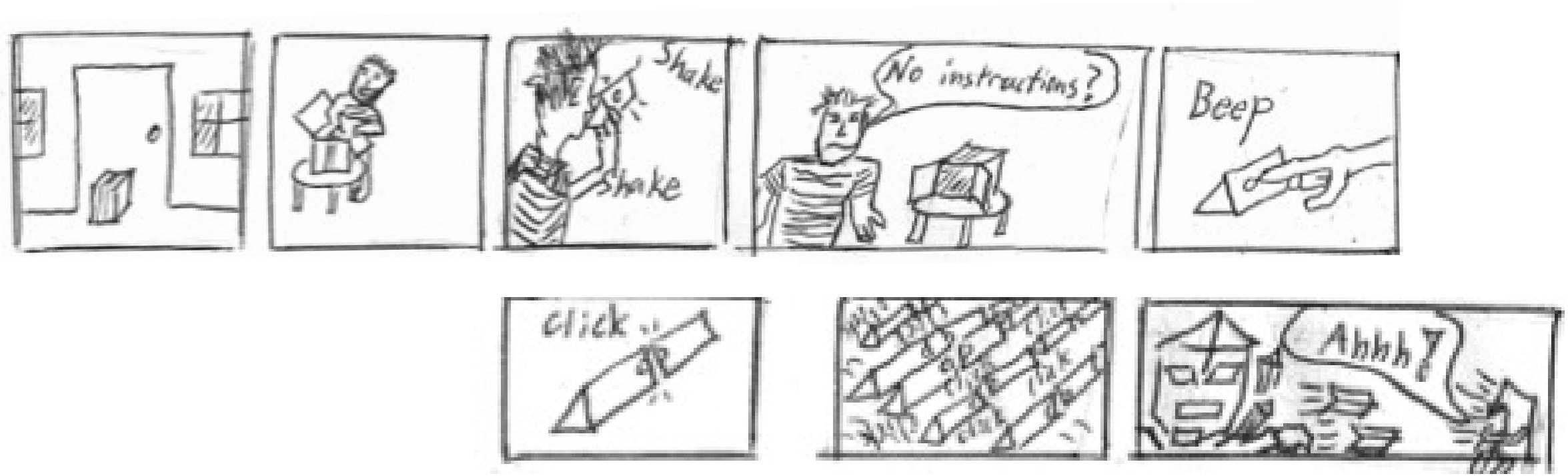
# Outline

- 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

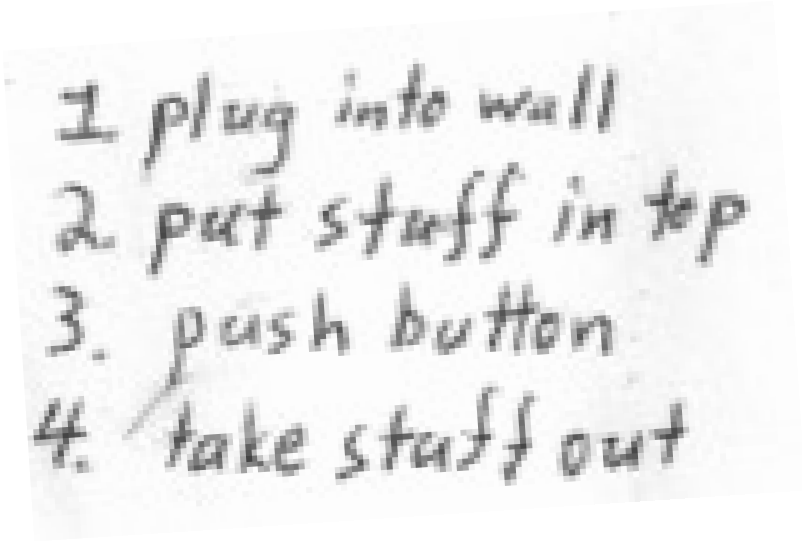
# Why Package?




- 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

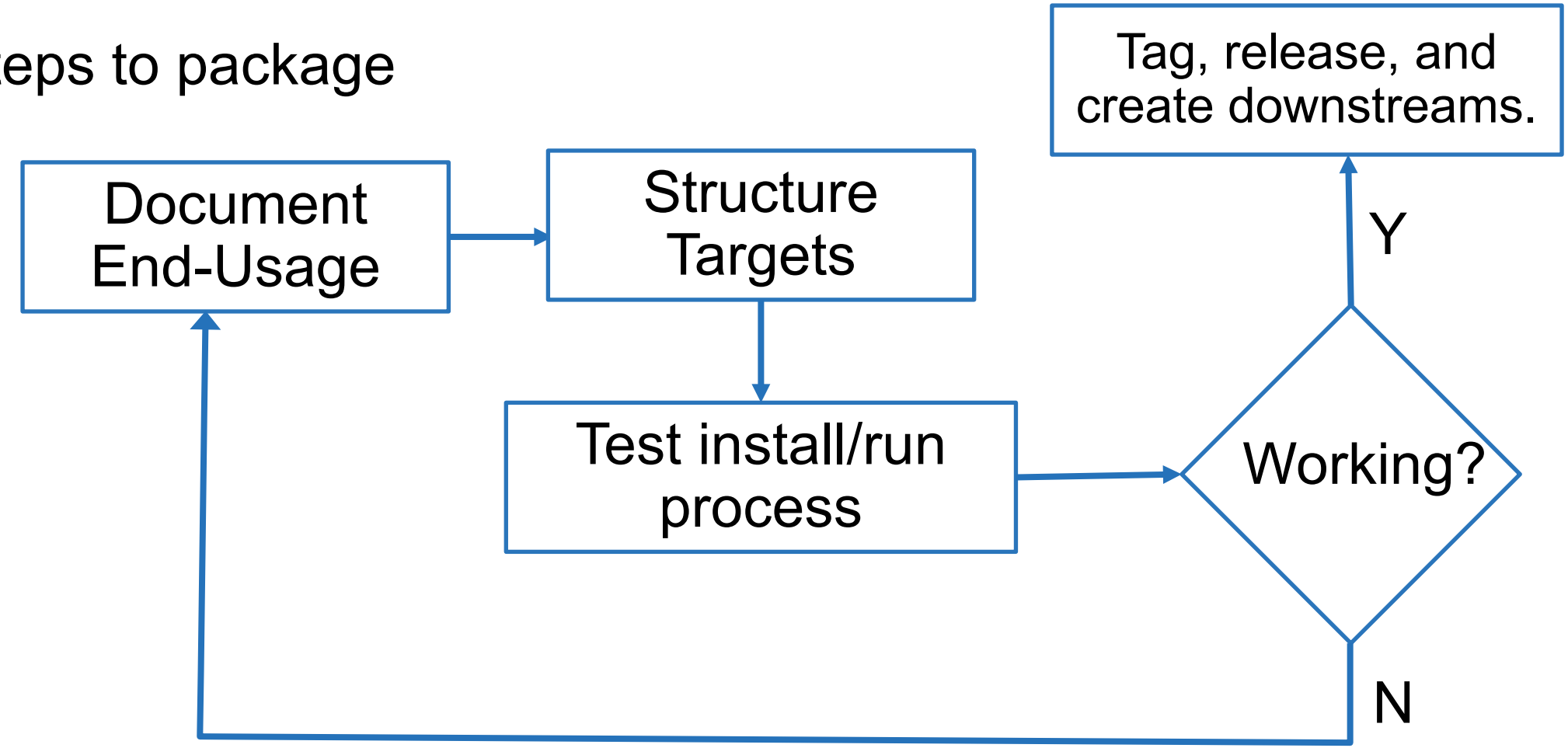
```
$PREFIX/lib/$PROJ
        libheat.so
        libheat.a
```

Front-lines: Documentation!

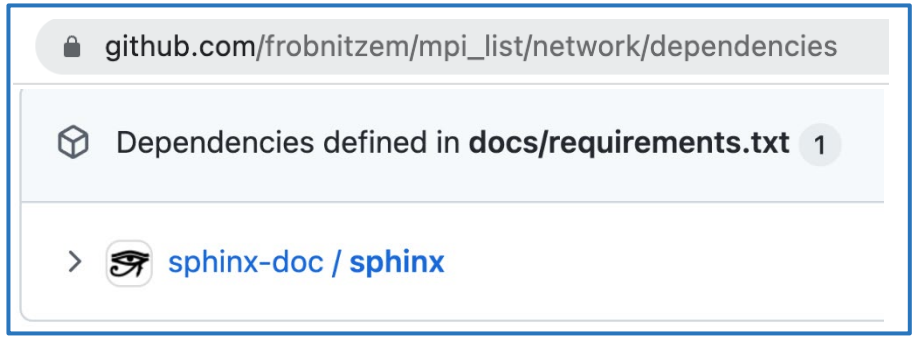
* what's expected to work?
* where / how do I configure it?

# 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

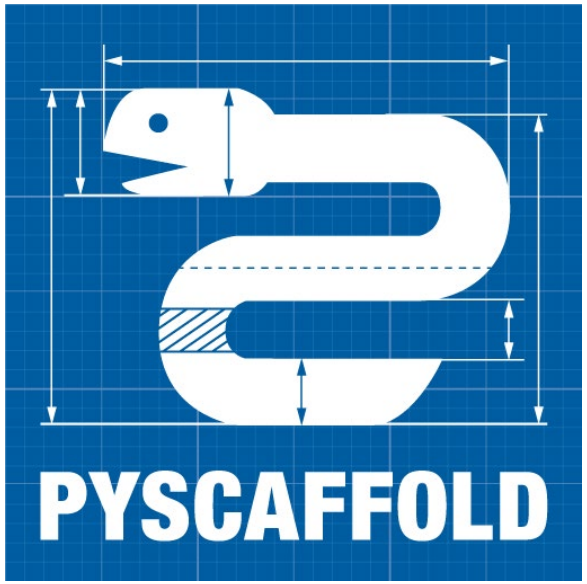
```
$ pip3 install pyscaffold
$ pip3 install tox
$ putup heateq
$ cd heateq # tests in tests/ subdir.
$ tox
```

```
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

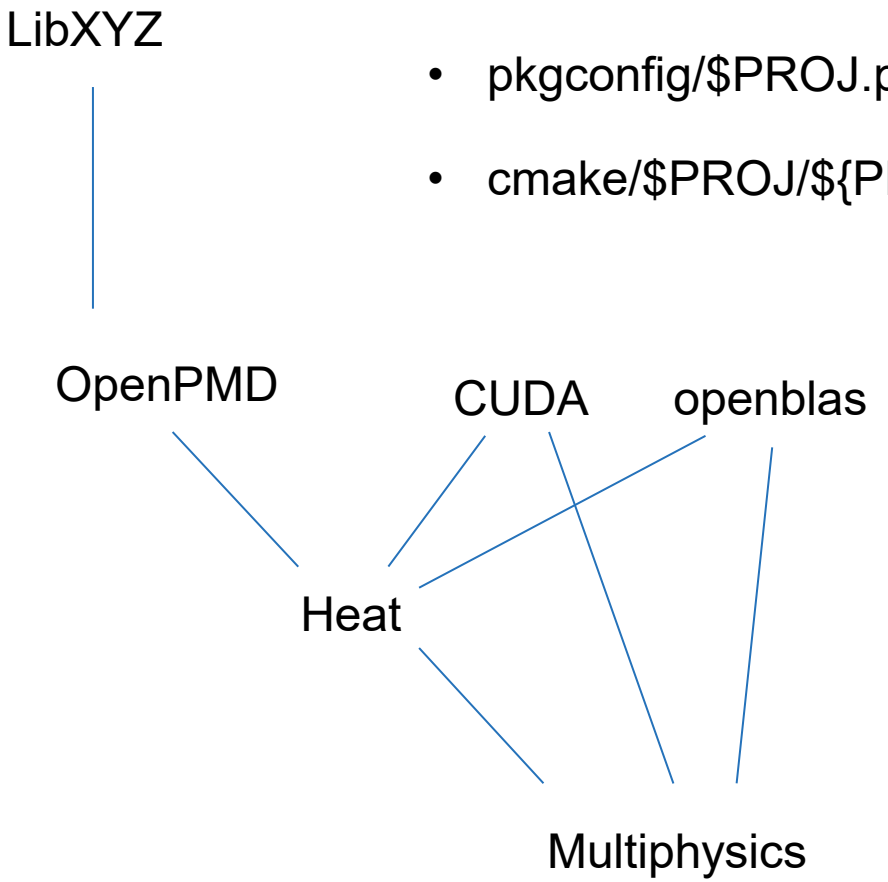
Requires referencing correctly

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> ...

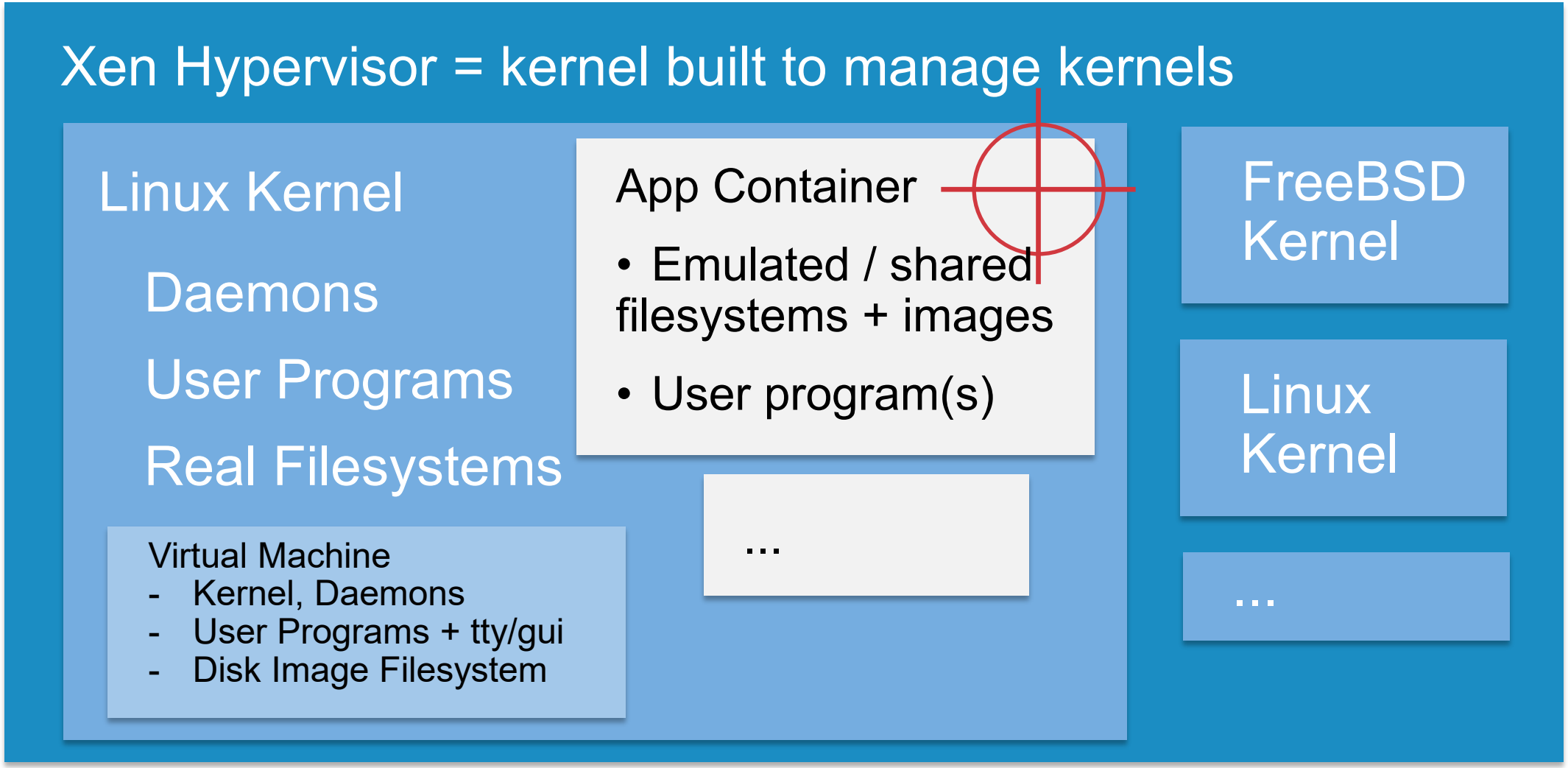
https://spack.readthedocs.io/en/latest/packaging_guide.html#dependency-specs

# "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)

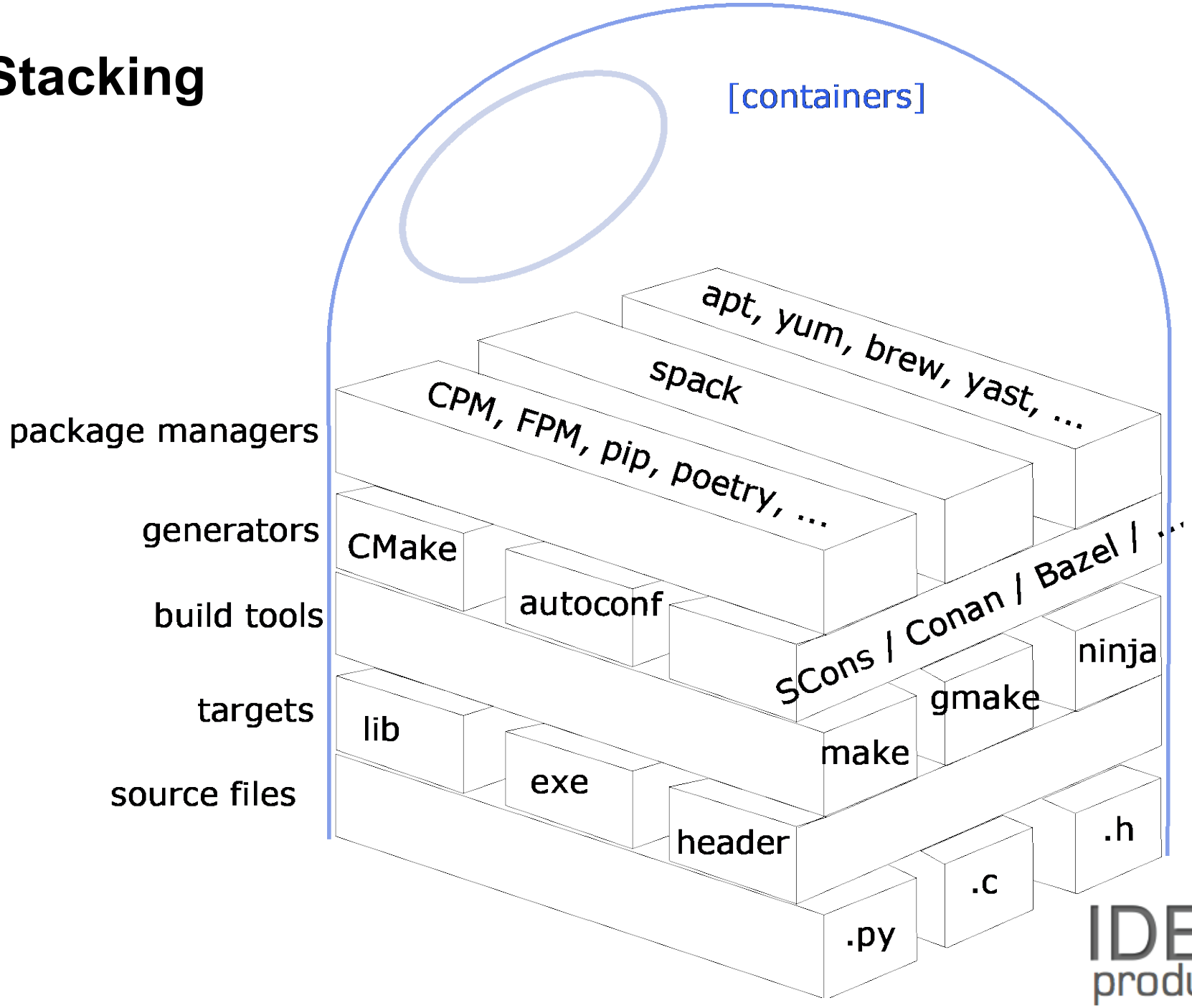
## Containers [Docker, Apptainer, Charlie-Cloud, ...]

- 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)

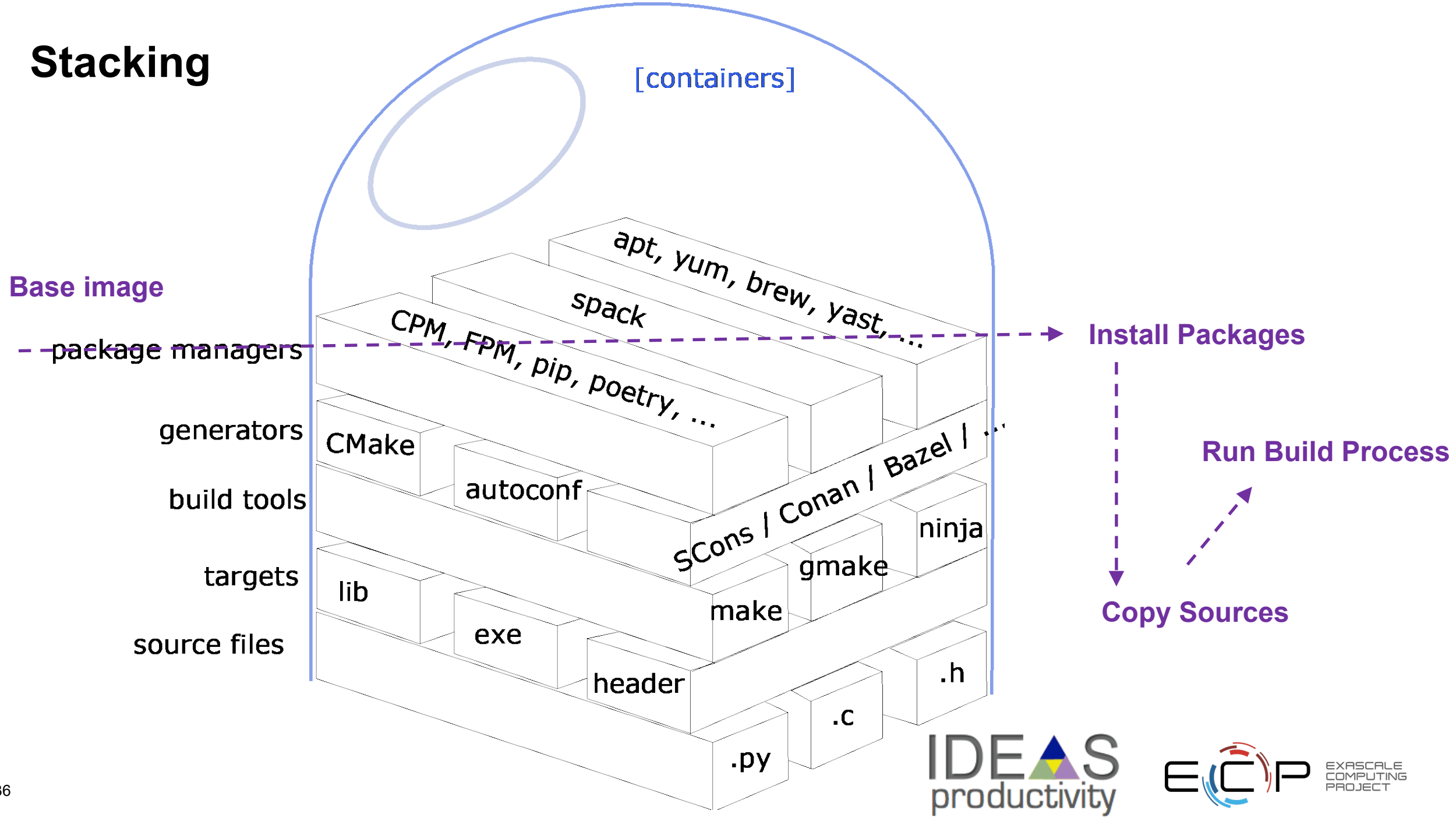
**Both:**

**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

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  - 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
```

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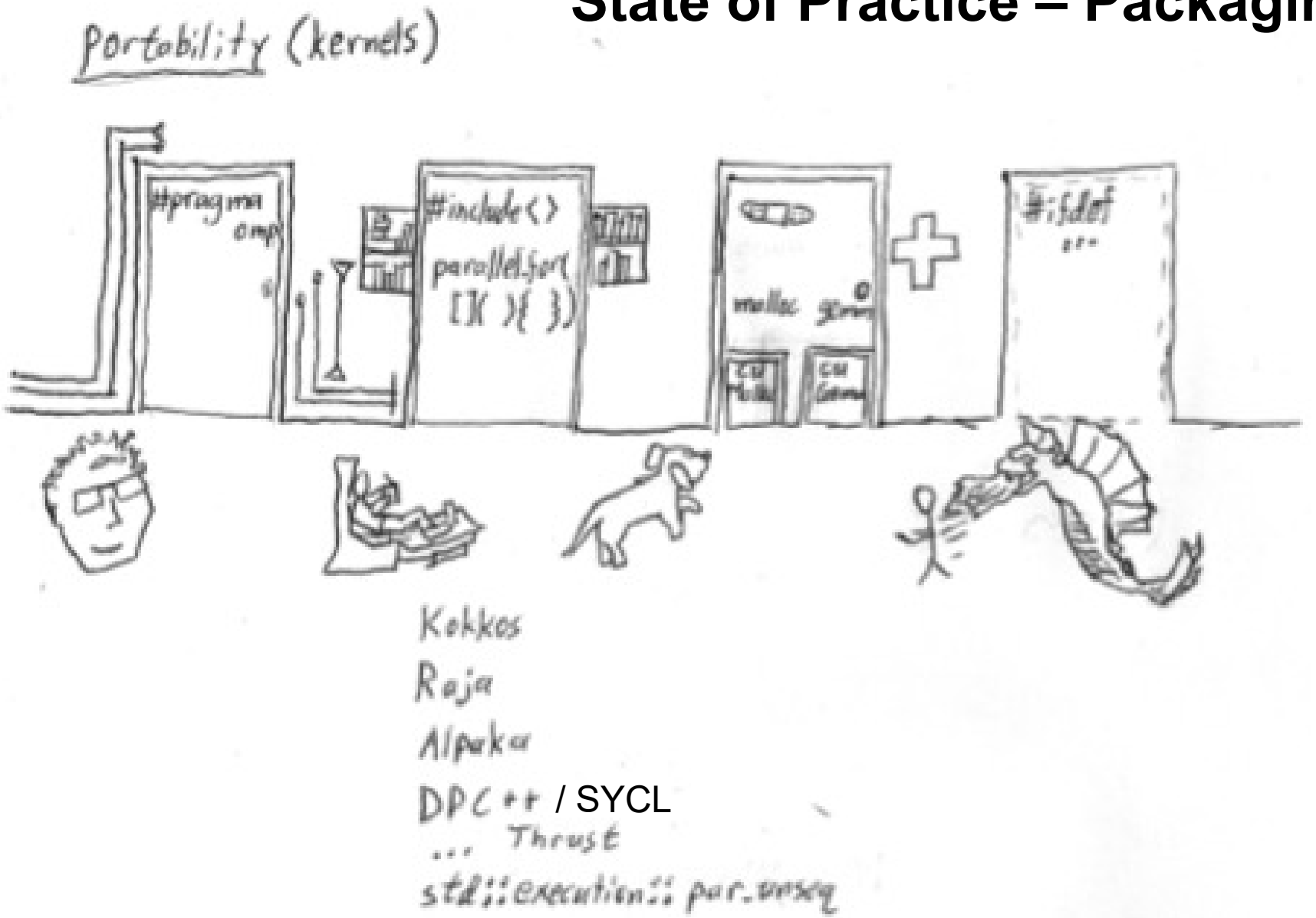
EXASCALE COMPUTING PROJECT

# 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