PSI4: THEN AND NOW

ANDREW C. SIMMONETT
JUSTIN M. TURNEY
LORI A. BURNS

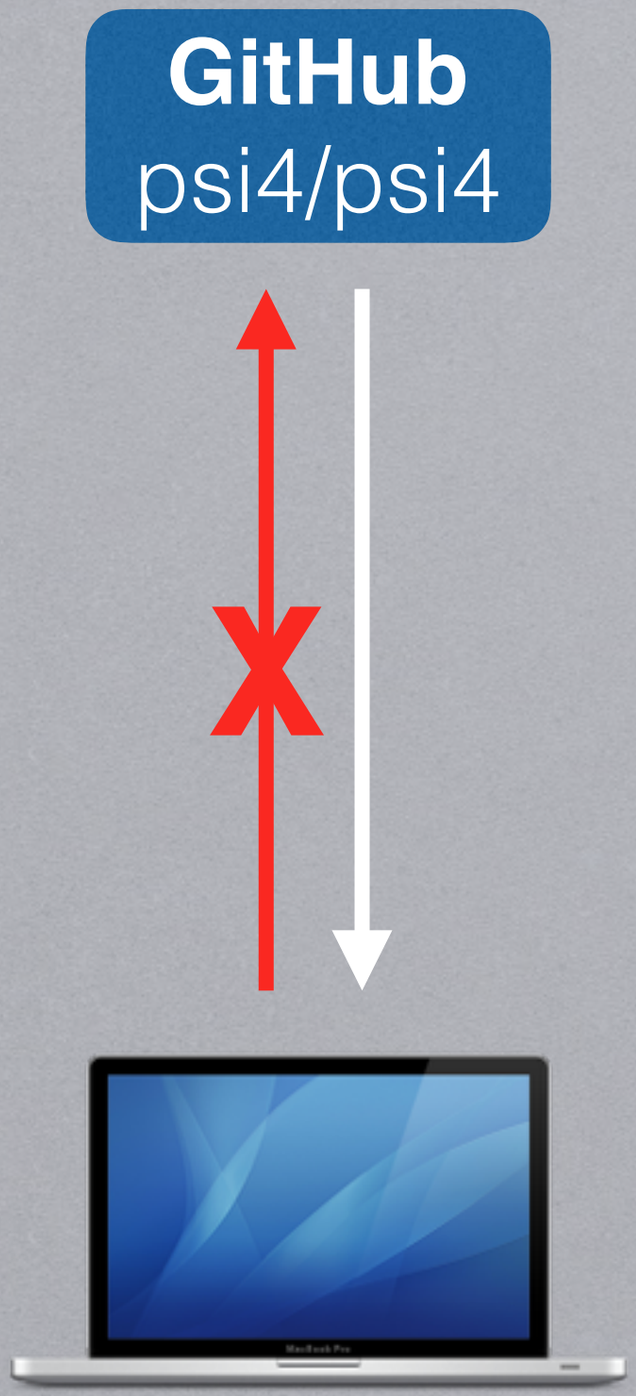
DEVELOPERS MEETING, UGA
4 NOVEMBER 2016

PART I: CONTRIBUTING TO PSI4

ANDY C. SIMMONETT

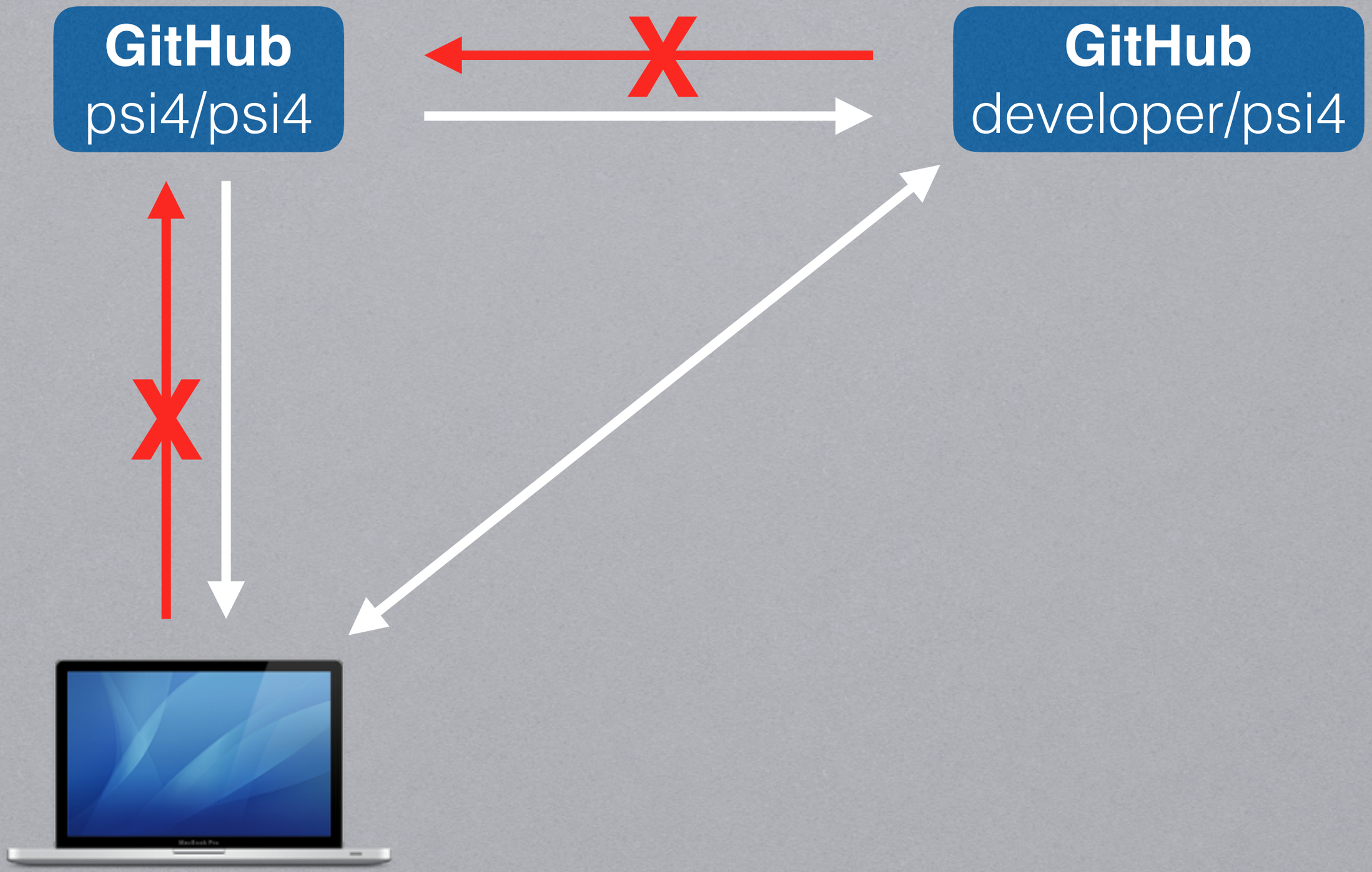
USING GITHUB'S PULL REQUESTS

DIRECT PUSHES TO MASTER NO LONGER ALLOWED



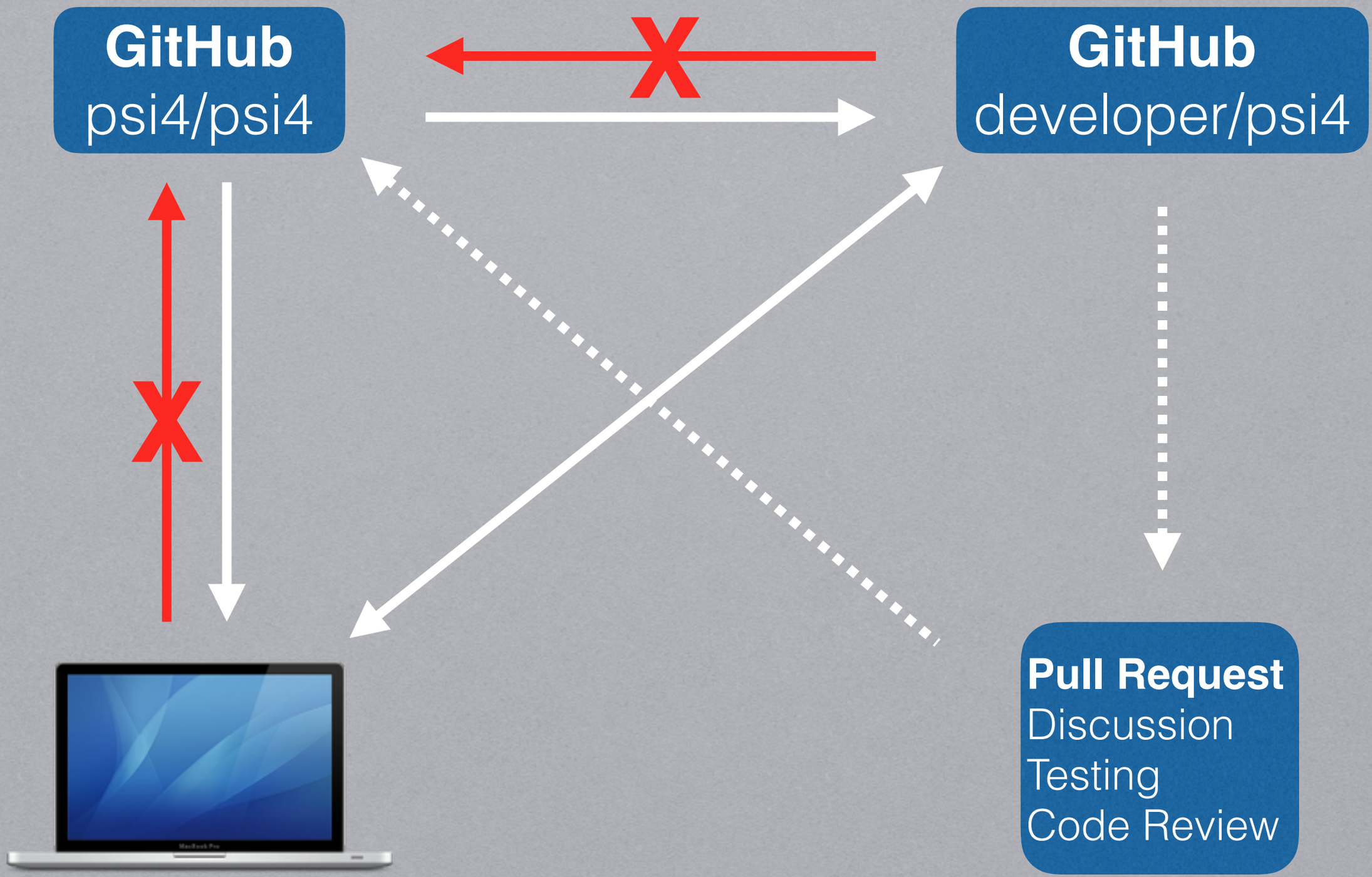
USING GITHUB'S PULL REQUESTS

DIRECT PUSHES TO MASTER NO LONGER ALLOWED

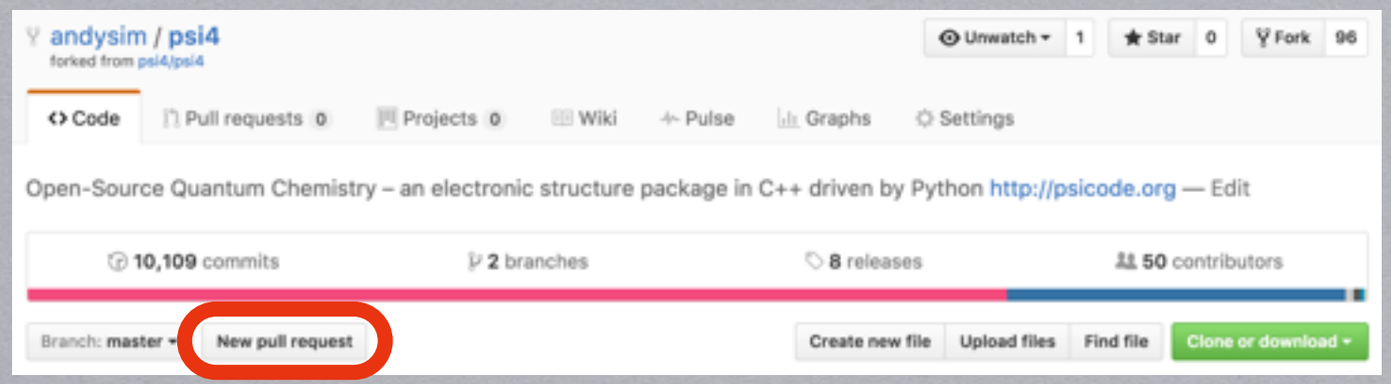


USING GITHUB'S PULL REQUESTS

DIRECT PUSHES TO MASTER NO LONGER ALLOWED

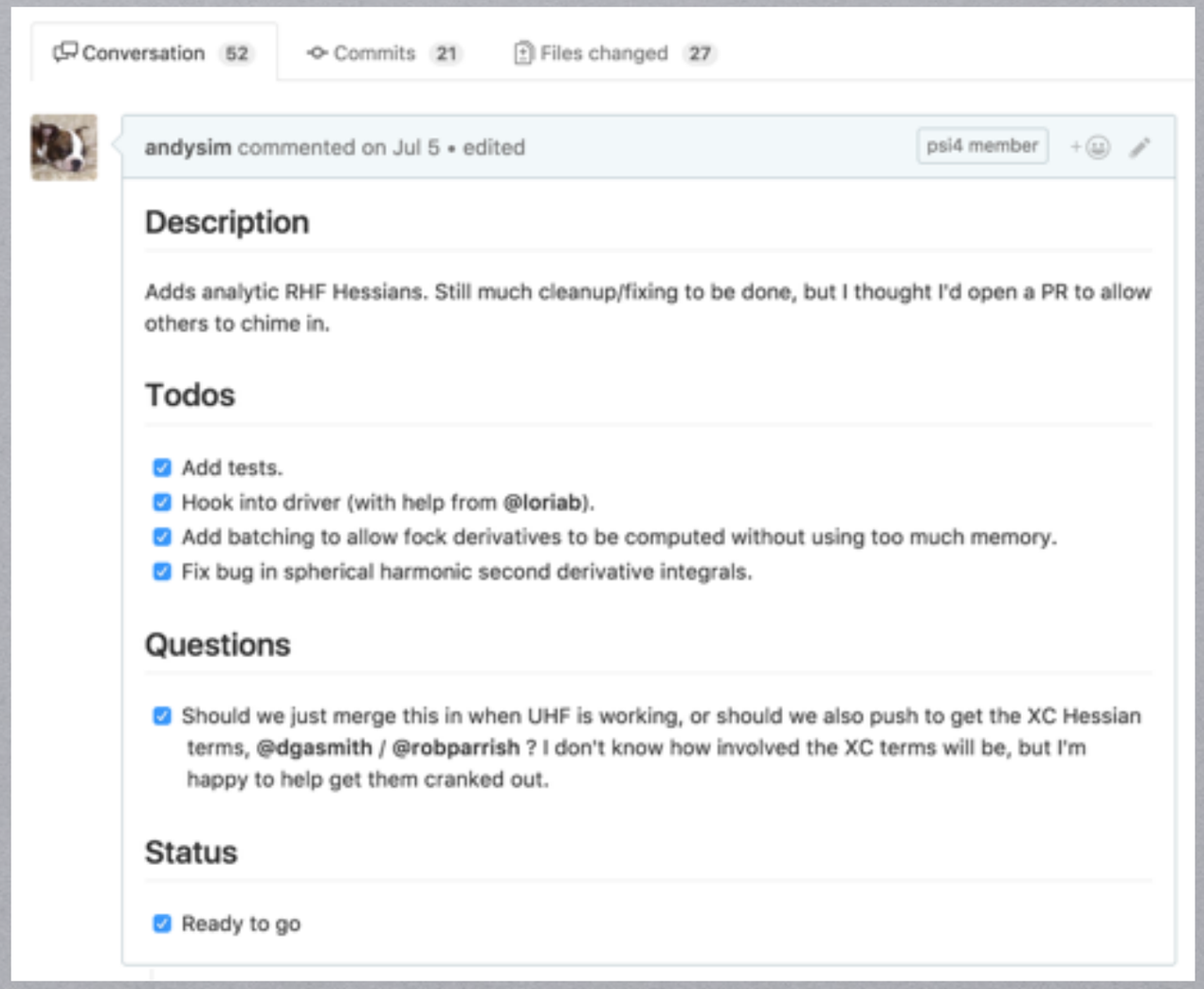


ISSUING A PULL REQUEST
FROM YOUR PERSONAL GITHUB HOMEPAGE

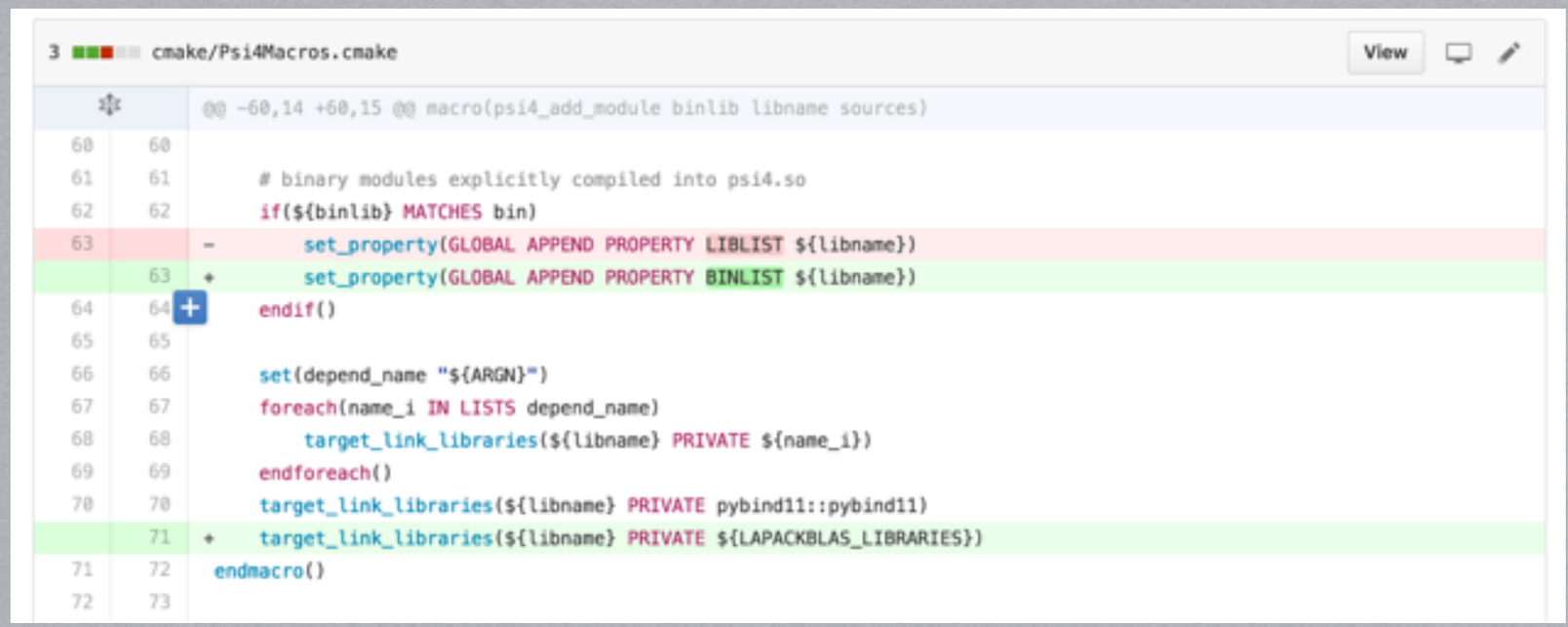


Launching a PR

The PR info screen



INTERACTIVITY OF PULL REQUESTS
GETTING FEEDBACK FROM OTHER DEVELOPERS


3 cmake/Psi4Macros.cmake

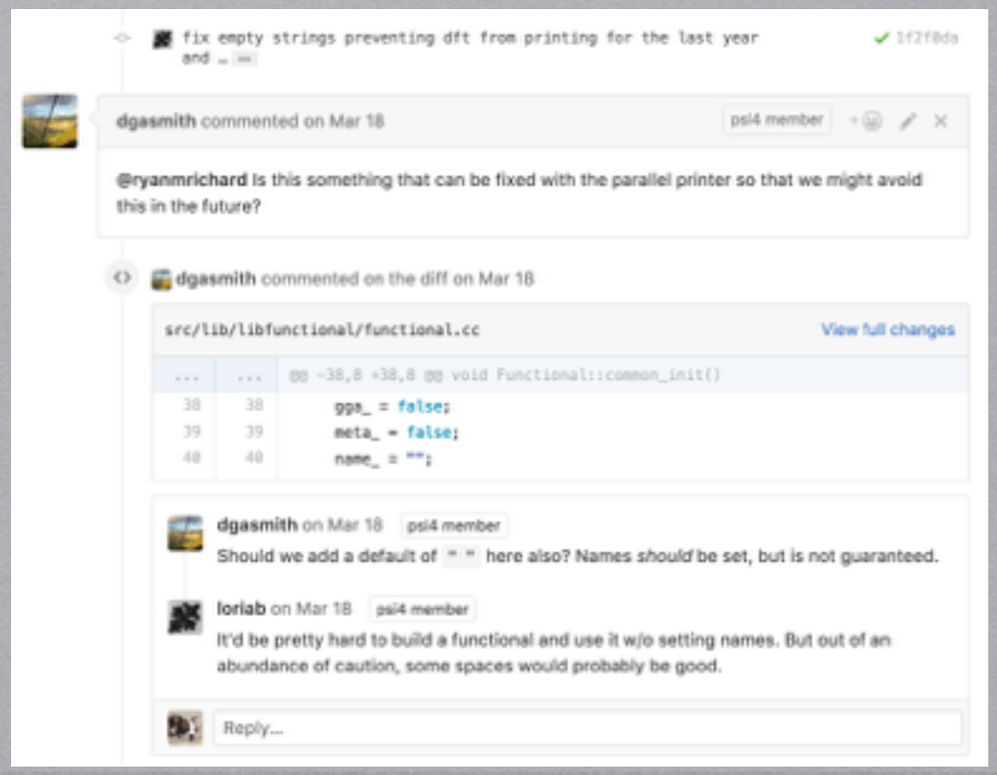
View

@@ -60,14 +60,15 @@ macro(psi4_add_module binlib libname sources)

```
60  60
61  61      # binary modules explicitly compiled into psi4.so
62  62      if(${binlib} MATCHES bin)
63      -       set_property(GLOBAL APPEND PROPERTY LIBLIST ${libname})
    63  +       set_property(GLOBAL APPEND PROPERTY BINLIST ${libname})
64  64      endif()
65  65
66  66      set(depend_name "${ARGN}")
67  67      foreach(name_i IN LISTS depend_name)
68  68          target_link_libraries(${libname} PRIVATE ${name_i})
69  69      endforeach()
70  70      target_link_libraries(${libname} PRIVATE pybind11::pybind11)
    71  +   target_link_libraries(${libname} PRIVATE ${LAPACKBLAS_LIBRARIES})
71  72  endmacro()
72  73
```

The review screen

The conversation screen


fix empty strings preventing dft from printing for the last year and … — 1f2f0da

dgasmith commented on Mar 18 — psi4 member

@ryanmrichard Is this something that can be fixed with the parallel printer so that we might avoid this in the future?

dgasmith commented on the diff on Mar 18

src/lib/libfunctional/functional.cc — View full changes

```
...  ...  @@ -38,8 +38,8 @@ void Functional::common_init()
38   38      gga_ = false;
39   39      meta_ = false;
40   40      name_ = "";
```

dgasmith on Mar 18 — psi4 member

Should we add a default of `" "` here also? Names *should* be set, but is not guaranteed.

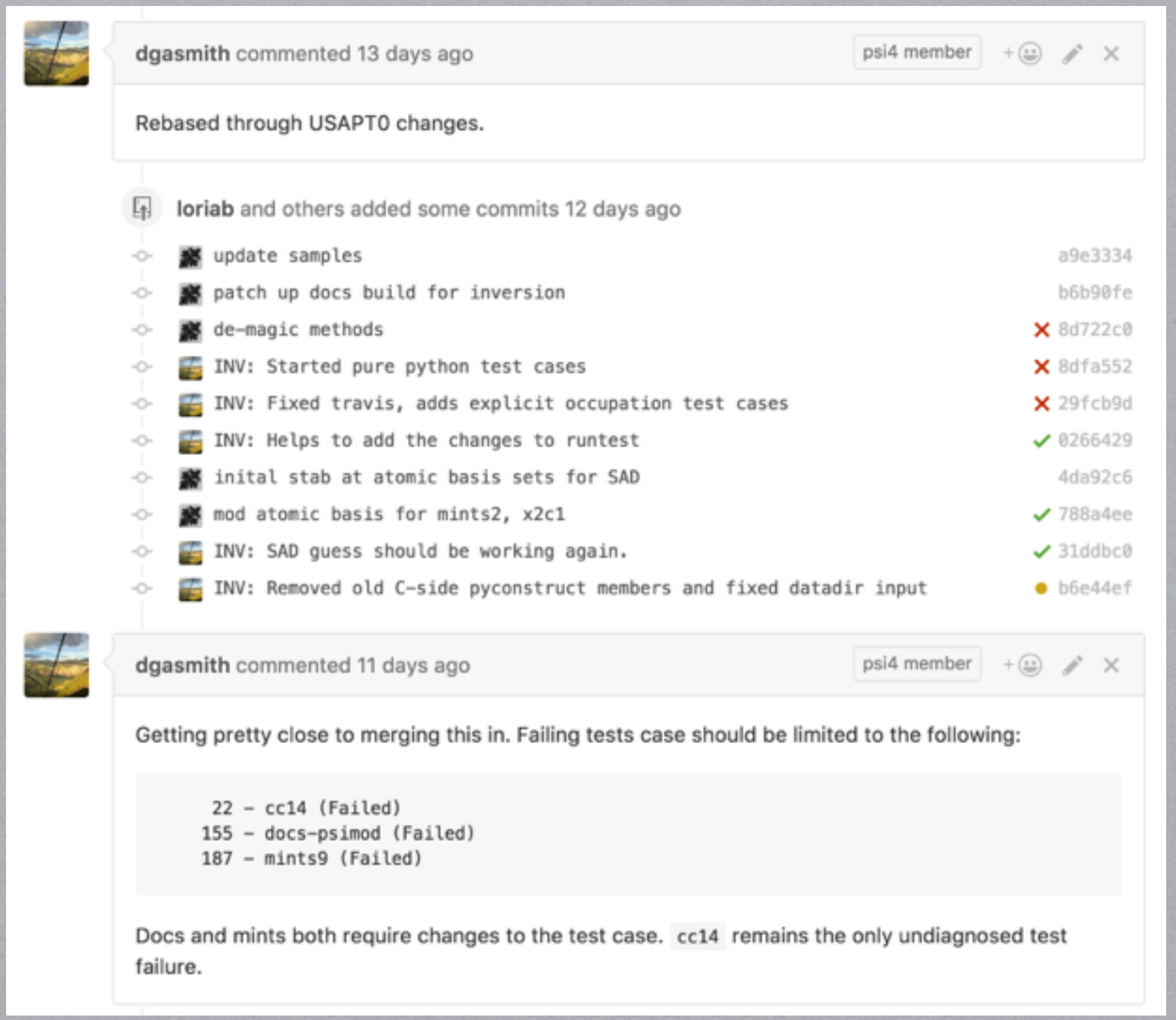
loriab on Mar 18 — psi4 member

It'd be pretty hard to build a functional and use it w/o setting names. But out of an abundance of caution, some spaces would probably be good.

Reply…

AUTOMATIC CODE TESTING

SEEING WHICH COMMITS BREAK THE TESTS



CONTINUOUS INTEGRATION TOOLS

TRAVIS / DISTELLI / CONDA-BUILD

psi4 / psi4 build passing

Current Branches Build History Pull Requests Build #581 More options

✓ Merge pull request #479 from jgonthier/USAPT

Open-shell SAPT0

Commit f23b5f1

Compare 7ed9a5f..f23b5f1

DS Daniel Smith authored G GitHub committed

#581 passed

Restart build

Elapsed time 50 min 50 sec

Total time 2 hrs 58 min 21 sec

13 days ago

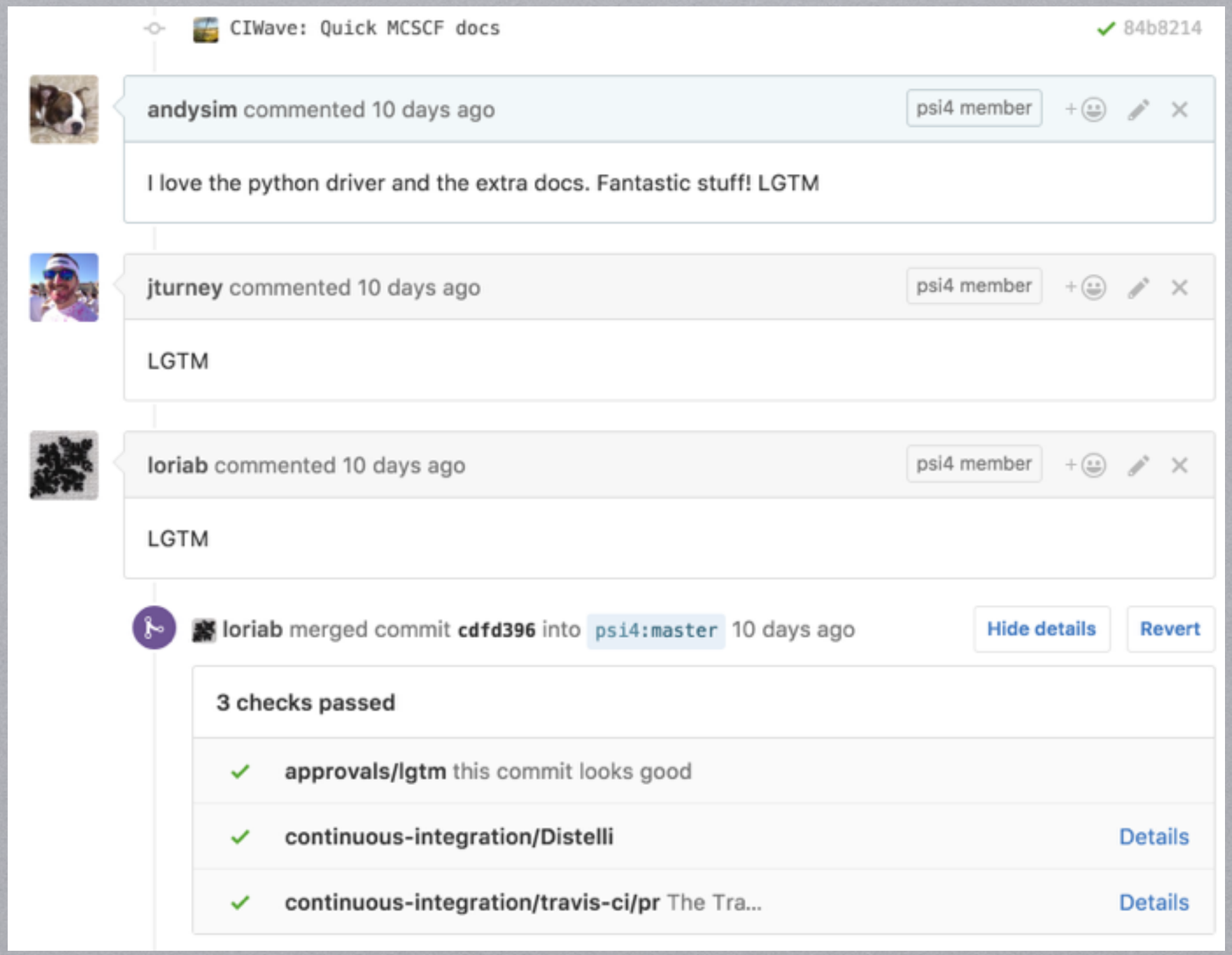
Build Jobs

✓	#581.1	Compiler: clang C++	CXX_COMPILER='clang++-3.6' C_COMPILER='cla	35 min 40 sec
✓	#581.3	Compiler: gcc C++	CXX_COMPILER='g++-4.9' C_COMPILER='gcc-4.9'	43 min 20 sec
✓	#581.4	Compiler: gcc C++	CXX_COMPILER='g++-6' C_COMPILER='gcc-6' For	50 min 48 sec
✓	#581.5	Compiler: gcc C++	CXX_COMPILER='g++-6' C_COMPILER='gcc-6' For	47 min 57 sec

Allowed Failures ?

!	#581.2	Compiler: clang C++	CXX_COMPILER='clang++-3.9' C_COMPILER='cla	36 sec

ACCEPTING/MERGING A PR
AFTER TEAM APPROVAL



WORKFLOW FOR CONTRIBUTING

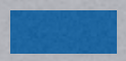
MAKING THE CHANGES/SETTING UP THE PR

upstream

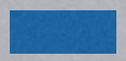
origin

local

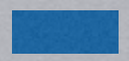
master



master



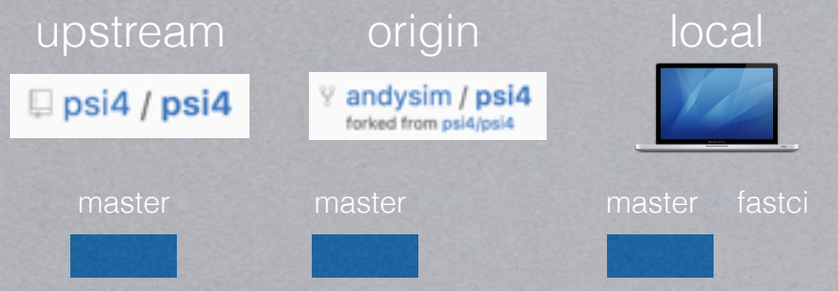
master



1)
```
git clone git@github.com:andysim/psi4
git remote add upstream git@github.com:psi4/psi4
```

WORKFLOW FOR CONTRIBUTING

MAKING THE CHANGES/SETTING UP THE PR

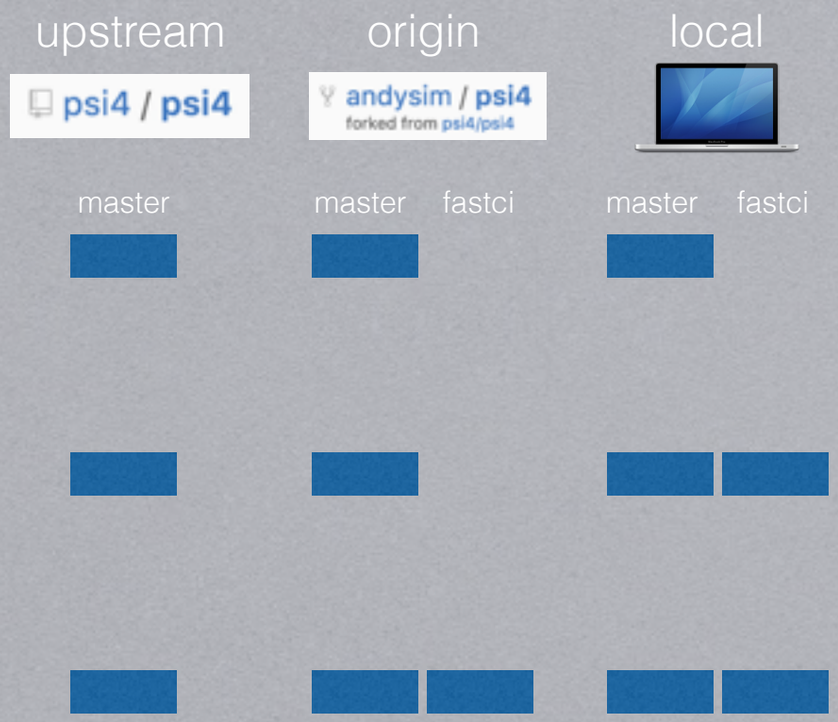


1) `git clone git@github.com:andysim/psi4`
`git remote add upstream git@github.com:psi4/psi4`

2) `git checkout -b fastci`

WORKFLOW FOR CONTRIBUTING

MAKING THE CHANGES/SETTING UP THE PR



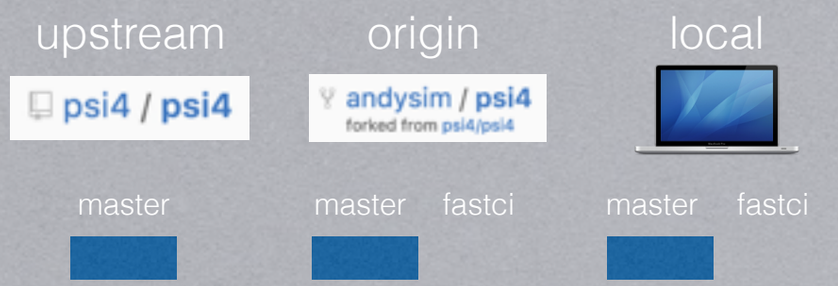
1) `git clone git@github.com:andysim/psi4`
`git remote add upstream git@github.com:psi4/psi4`

2) `git checkout -b fastci`

3) `git push origin fastci`

WORKFLOW FOR CONTRIBUTING

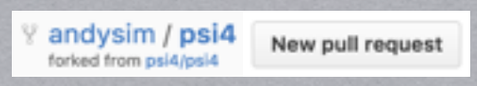
MAKING THE CHANGES/SETTING UP THE PR



1) `git clone git@github.com:andysim/psi4`
`git remote add upstream git@github.com:psi4/psi4`

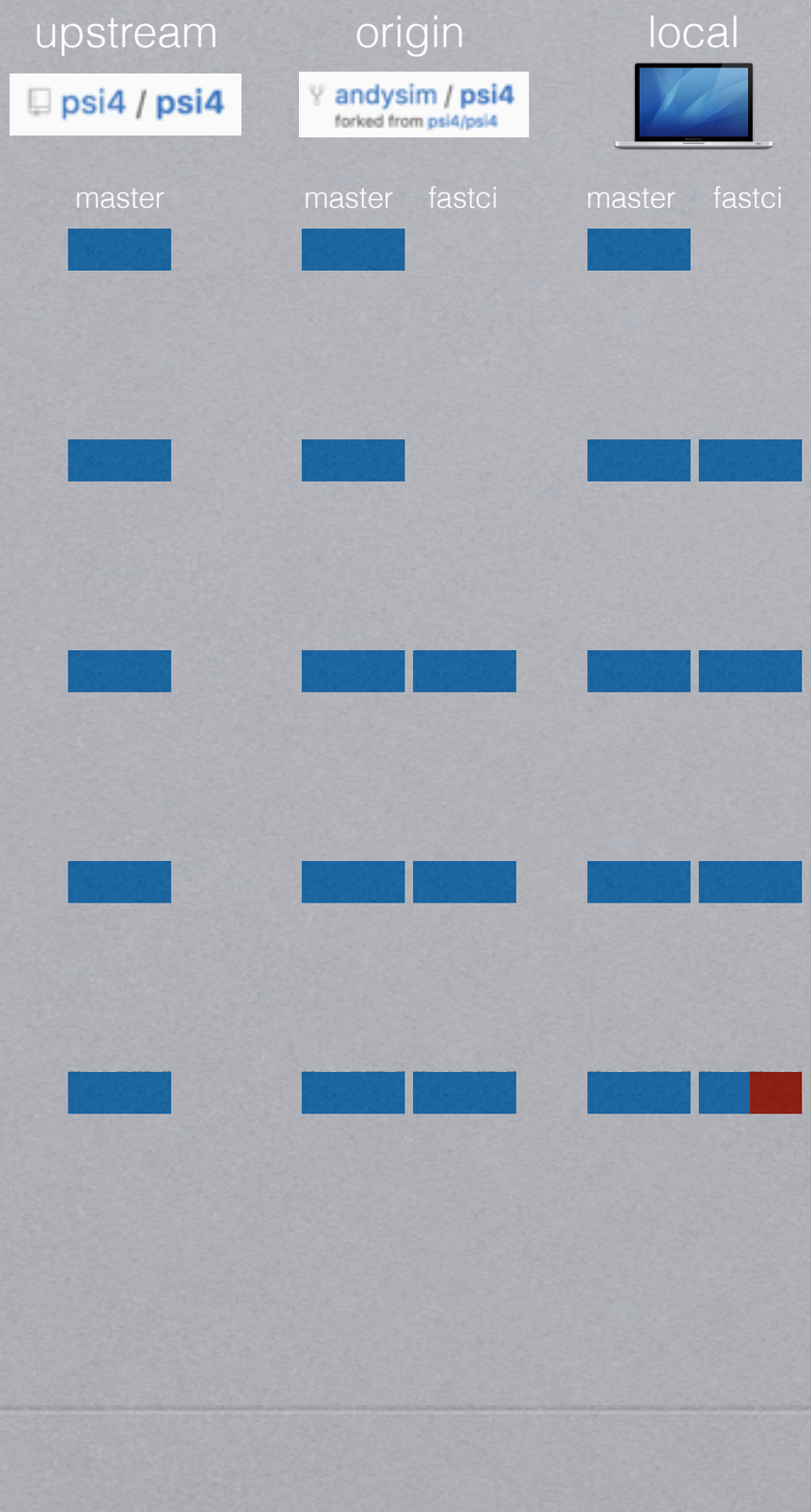
2) `git checkout -b fastci`

3) `git push origin fastci`

4) 

WORKFLOW FOR CONTRIBUTING

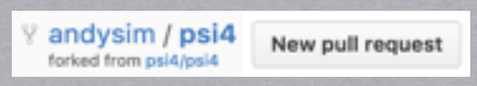
MAKING THE CHANGES/SETTING UP THE PR



1) `git clone git@github.com:andysim/psi4`
`git remote add upstream git@github.com:psi4/psi4`

2) `git checkout -b fastci`

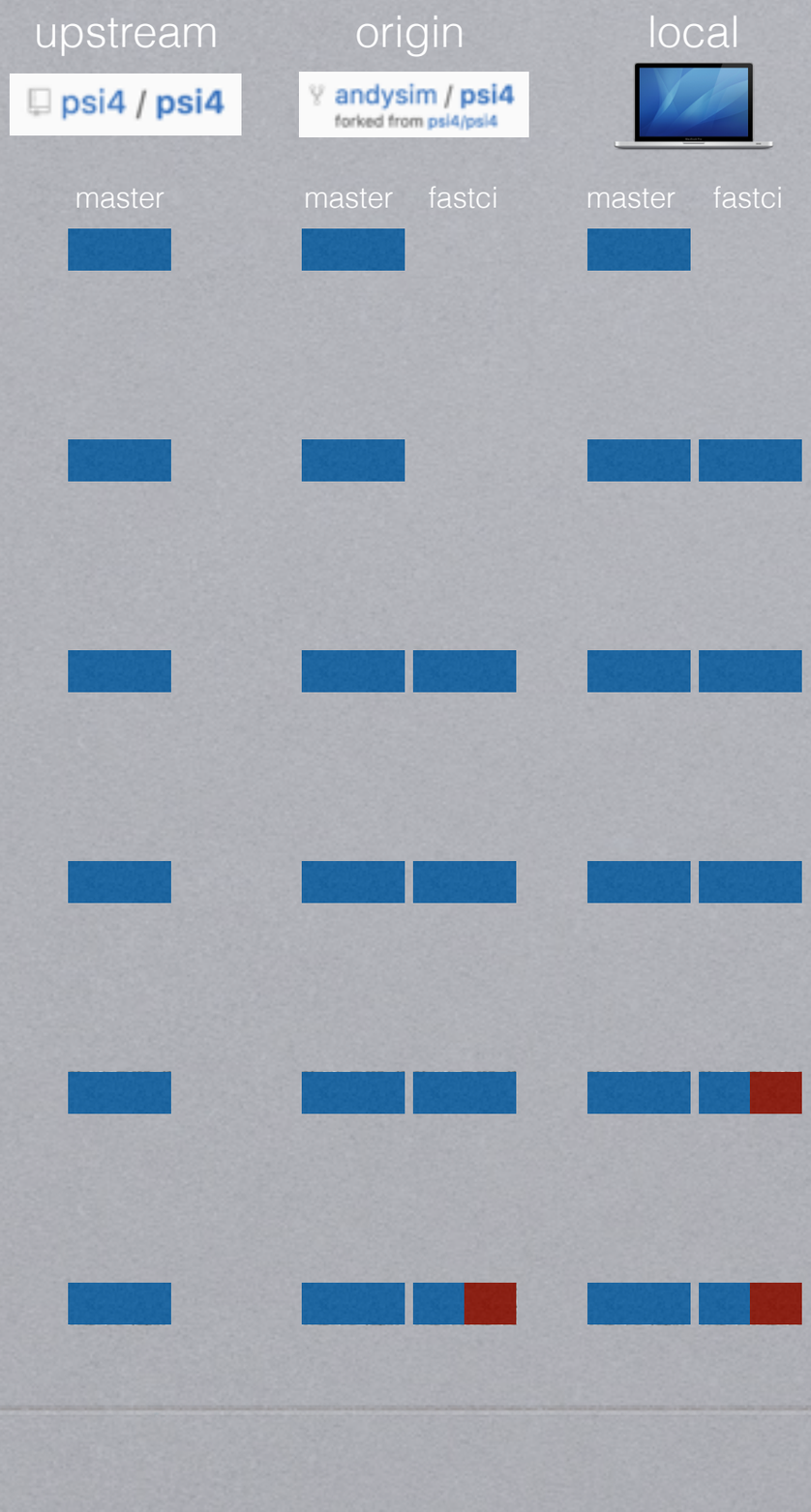
3) `git push origin fastci`

4) 

5) Add new code on fastci branch

WORKFLOW FOR CONTRIBUTING

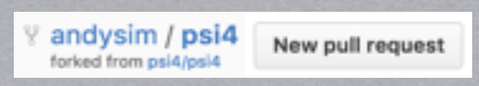
MAKING THE CHANGES/SETTING UP THE PR



1) `git clone git@github.com:andysim/psi4`
`git remote add upstream git@github.com:psi4/psi4`

2) `git checkout -b fastci`

3) `git push origin fastci`

4) 

5) Add new code on fastci branch

6) `git push origin fastci`

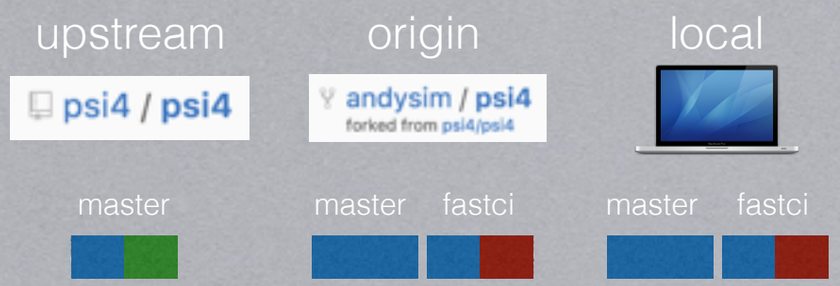
WORKFLOW FOR CONTRIBUTING

SYNCHRONIZING / CLEANING REPOSITORIES

7) New feature added on master by somebody else (via a PR)

WORKFLOW FOR CONTRIBUTING

SYNCHRONIZING / CLEANING REPOSITORIES



7) New feature added on master by somebody else (via a PR)

8) `git pull --rebase upstream master`

WORKFLOW FOR CONTRIBUTING

SYNCHRONIZING / CLEANING REPOSITORIES

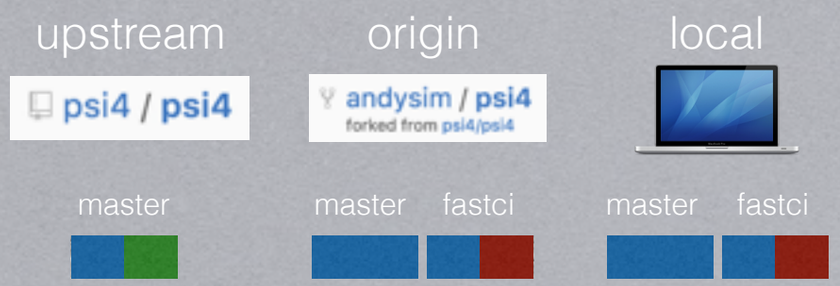
7) New feature added on master by somebody else (via a PR)

8) `git pull --rebase upstream master`

9) `git push origin fastci` (may need to add `--force`)

WORKFLOW FOR CONTRIBUTING

SYNCHRONIZING / CLEANING REPOSITORIES



7) New feature added on master by somebody else (via a PR)

8) `git pull --rebase upstream master`

9) `git push origin fastci (may need to add --force)`

10) PR accepted, after “ready to go” checked, tests, LGTM approval

WORKFLOW FOR CONTRIBUTING

SYNCHRONIZING / CLEANING REPOSITORIES

7) New feature added on master by somebody else (via a PR)

8) `git pull --rebase upstream master`

9) `git push origin fastci (may need to add --force)`

10) PR accepted, after “ready to go” checked, tests, LGTM approval

11)
```
git checkout master
git pull --rebase upstream master
git push origin master
```

WORKFLOW FOR CONTRIBUTING

SYNCHRONIZING / CLEANING REPOSITORIES

7) New feature added on master by somebody else (via a PR)

8) `git pull --rebase upstream master`

9) `git push origin fastci (may need to add --force)`

10) PR accepted, after “ready to go” checked, tests, LGTM approval

11)
```
git checkout master
git pull --rebase upstream master
git push origin master
```

12)
```
git branch -d fastci
git push origin :fastci
```

ADVANTAGES OF THE NEW WORKFLOW

- **For feature developers:-**
  - Feedback from the Psi4 team during development.
  - No fear of breaking the code for others.
  - Easy to see whether each commit breaks anything.
  - Intuitive for those familiar with other GitHub projects.

- **For the Psi4 team:-**
  - Easy way to track what people are working on.
  - Easy vetting / testing / merging of new contributions.
  - Code review means more consistent style.

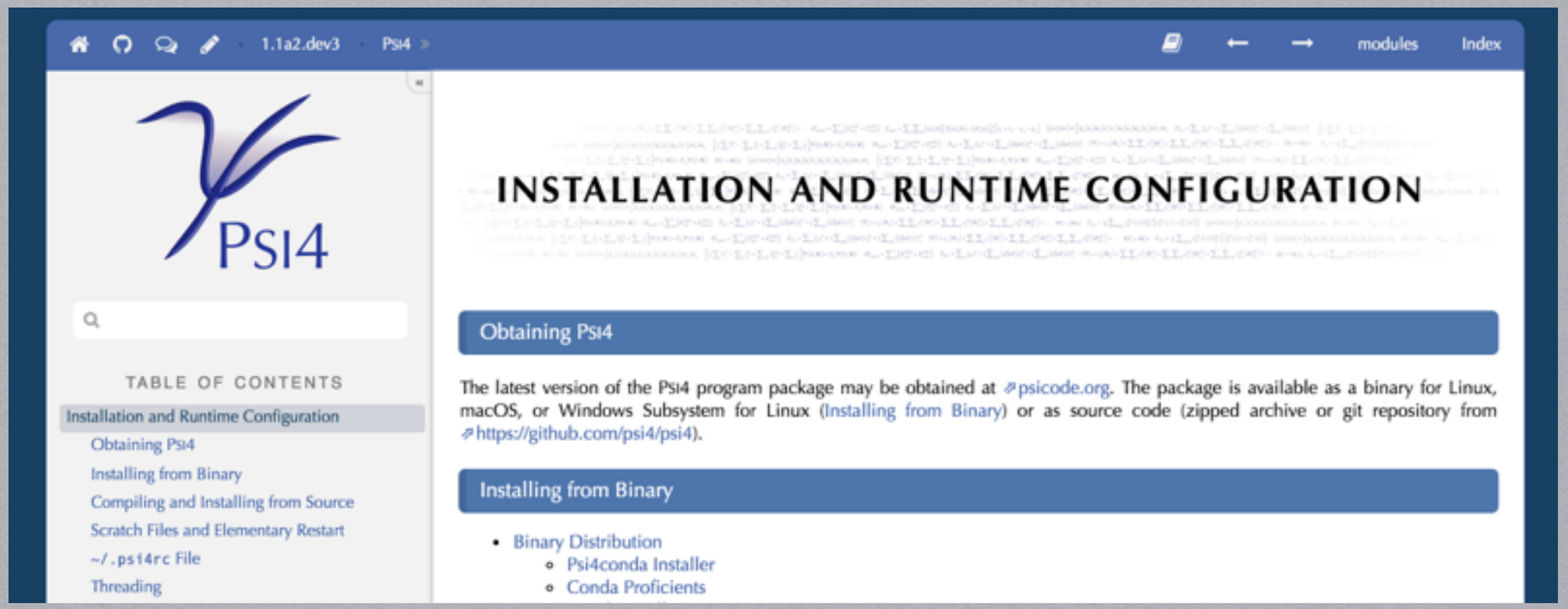
- **For end users:-**
  - Code from GitHub should always work.

PART II: CONDA & BRANCHES

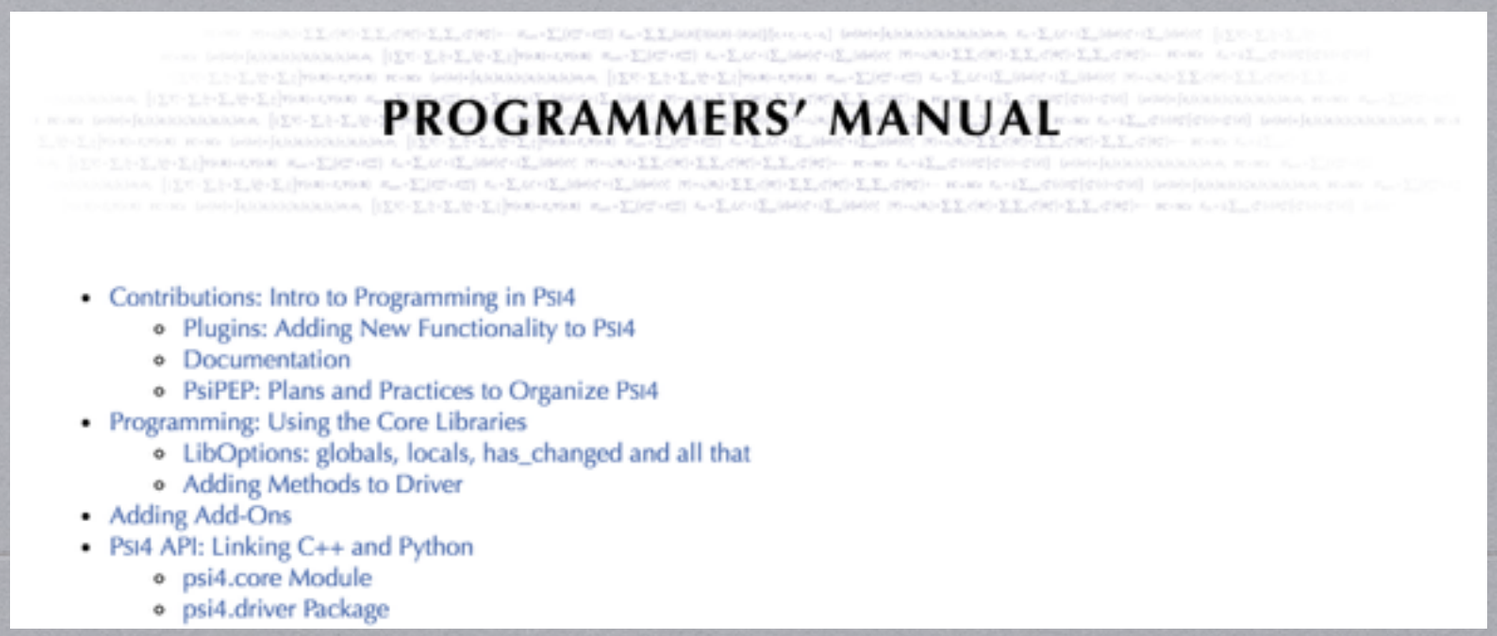
LORI A. BURNS

DOCUMENTATION REFRESH

HTTP://PSICODE.ORG/PSI4MANUAL/MASTER/INDEX.HTML



- API docs like **`help(psi4)`**
- NumPy docstrings in driver
- Sphinx (and Perl) only build dep



DOCUMENTATION CHALLENGE

A PLOY TO GET RID OF STALE FORKS

http://psicode.org/psi4manual/master/index.html

HOW TO EDIT

WHAT TO EDIT

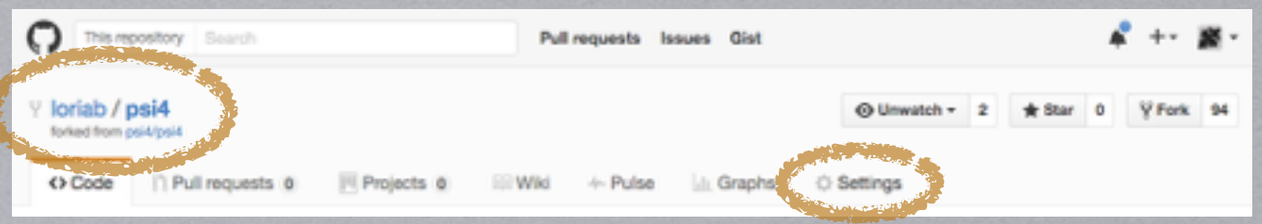
DOCUMENTATION CHALLENGE

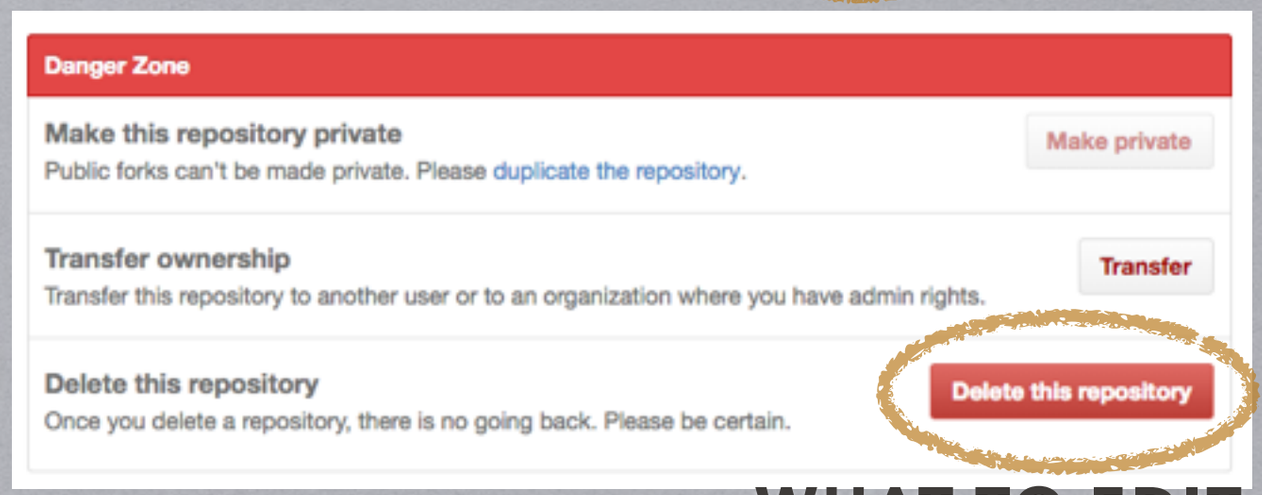
A PLOY TO GET RID OF STALE FORKS

http://psicode.org/psi4manual/master/index.html

HOW TO EDIT

1. Delete any existing GH fork





WHAT TO EDIT

DOCUMENTATION CHALLENGE

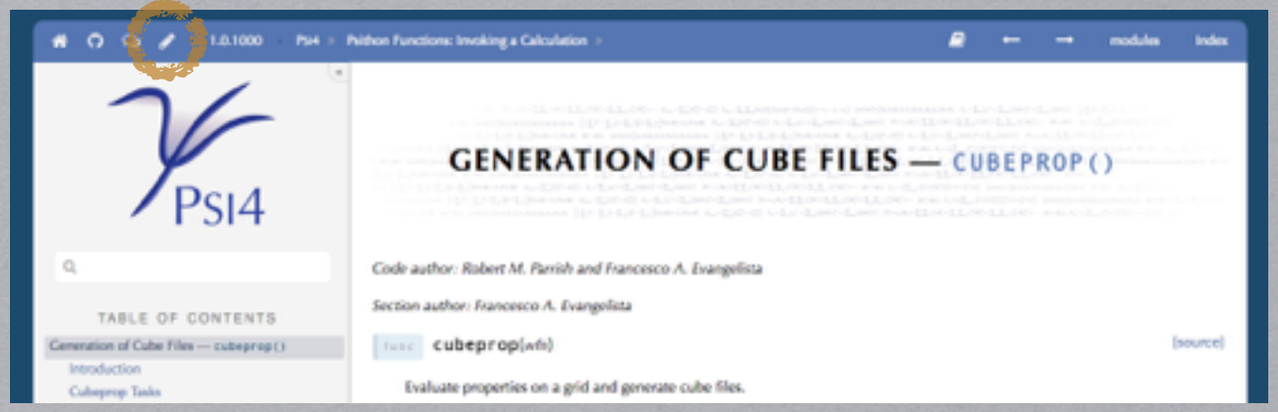
A PLOY TO GET RID OF STALE FORKS

http://psicode.org/psi4manual/master/index.html

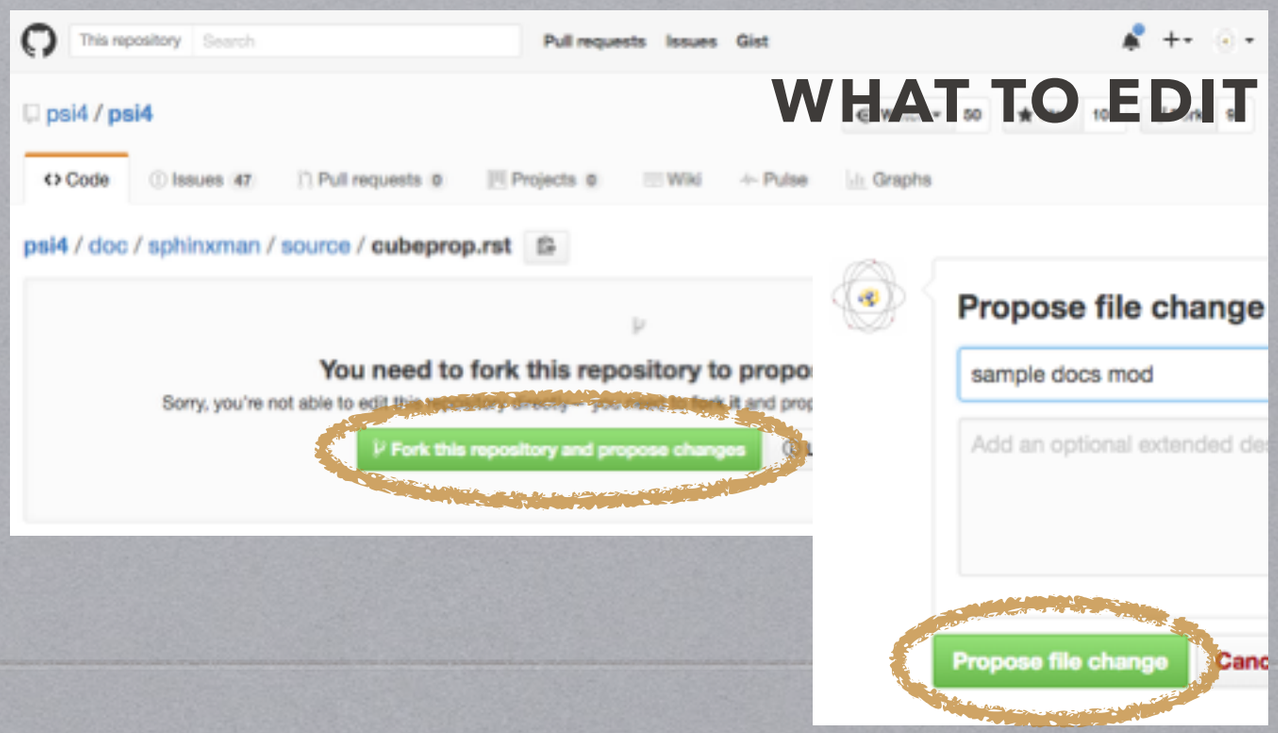
HOW TO EDIT

1. Delete any existing GH fork

2. Create a new fork, perhaps by editing a file online (no clone) from `docs/sphinxman/source/`



WHAT TO EDIT



DOCUMENTATION CHALLENGE

A PLOY TO GET RID OF STALE FORKS

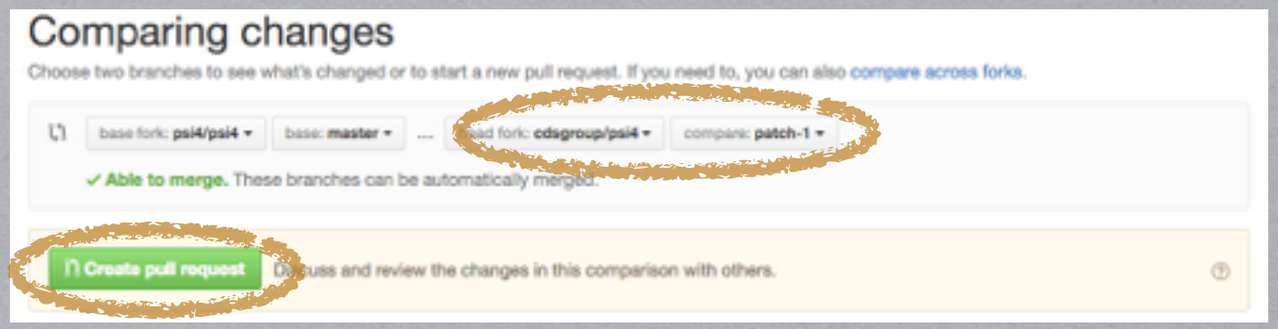
http://psicode.org/psi4manual/master/index.html

HOW TO EDIT

1. Delete any existing GH fork

2. Create a new fork, perhaps by editing a file online (no clone) from `docs/sphinxman/source/`

3. Submit a pull request from a *branch* of your fork



WHAT TO EDIT

DOCUMENTATION CHALLENGE

A PLOY TO GET RID OF STALE FORKS

http://psicode.org/psi4manual/master/index.html

HOW TO EDIT

1. Delete any existing GH fork

2. Create a new fork, perhaps by editing a file online (no clone) from `docs/sphinxman/source/`

3. Submit a pull request from a *branch* of your fork

4. If conflicts arise, clone and rebase to resolve them, independently or with advice

WHAT TO EDIT

DOCUMENTATION CHALLENGE

A PLOY TO GET RID OF STALE FORKS

http://psicode.org/psi4manual/master/index.html

HOW TO EDIT

1. Delete any existing GH fork

2. Create a new fork, perhaps by editing a file online (no clone) from `docs/sphinxman/source/`

3. Submit a pull request from a *branch* of your fork

4. If conflicts arise, clone and rebase to resolve them, independently or with advice

5. Once PR accepted, collect your sticker sheet

WHAT TO EDIT

DOCUMENTATION CHALLENGE

A PLOY TO GET RID OF STALE FORKS

http://psicode.org/psi4manual/master/index.html

HOW TO EDIT

1. Delete any existing GH fork

2. Create a new fork, perhaps by editing a file online (no clone) from `docs/sphinxman/source/`

3. Submit a pull request from a *branch* of your fork

4. If conflicts arise, clone and rebase to resolve them, independently or with advice

5. Once PR accepted, collect your sticker sheet

WHAT TO EDIT

- Anything that has confused you in narrative docs
- Any broken link
- Any docstring in driver
- Boost used 1-indexing for args, while Pybind11 uses 0-indexing, so many docstrings need adjusting in `psi4/src/`core.cc

2015		binary	docs
Tool	Linux	conda-build	Sphinx
Resource	Linux	psinet	psinet
Matrix	Linux	1 generic comp/gnu, py 2	
When		nightly crontab at 2AM	nightly crontab at 2AM
Runs		full tests AM 6; all must pass	full code scan all must build
Produces		Psi4 core conda package anaconda.org/psi4/psi4/files	Narrative & API Docs for Users & Py psicode.org/psi4manual/master/

PSINET (AKA. SPINET)

MACPSINET

2016		CI	binary	installer	stats	docs
Tool	L	Travis	conda-build	conda constructor	Codecov	Sphinx
	M	Distelli				
Resource	L	cloud	psinet	psinet	NYI, switch fr/mac	psinet
	M	mac-psinet	mac-psinet, NYI	mac-psinet	mac-psinet	*unneeded*
Matrix	L	5 comp/gnu, py 2	1 generic comp/gnu, py 2			
	M	1 comp/gnu, py 2			1 comp/gnu, py 2	
When		commit every latest commit	nightly crontab at 2AM	occasionally manually at new tag	occasionally manually	nightly crontab at 2AM
Runs		quicktests AM 4	full tests AM 6; all must pass	full tests AM 6; all must pass	full+processing AM 5	
Produces		Pass/Fail notice on GitHub commit github.com/psi4/psi4/pulls	Psi4 core conda package anaconda.org/psi4/psi4/files	Installer: Miniconda + P4core + Addons psicode.org/downloads2.html	Coverage Dash-board, Sunburst codecov.io/gh/psi4/psi4	Sphinx & Doxygen Autodocumenting psicode.org/psi4manual

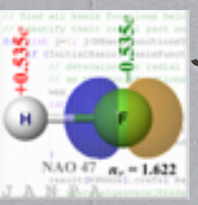
name: psi4conda

POST-PROCESSING

DFTD3 Grimme
dispersion correction
Fortran executable

GCP Grimme
small-basis correction
Fortran executable

GDMA Stone
multipole analysis
Fortran library



JANPA Nikolaienko
NBO bond analysis
Java executable

resp2 McGibbon
RESP charges
C++ Psi4 plugin

UPSTREAM

CHARMMing Woodcock
QM/MM web server
Python/HTML executable; calls Psi4

Pulsar Pritchard & Richards
datastructure interoperability
C++ framework; calls Psi4

WebMO Polik & Schmidt
GUI/web server
Perl/Java executable; calls Psi4

QC METHODS

Ambit Turney
tensor manipulations
Python/C++ library

Cfour Stanton & Gauss
$\langle CC|CC\rangle$
CC/MBPT/properties/etc.
Fortran executable

CheMPS2 Wouters
DMRG theory
Python/C++ library

DKH Wolf & Reiher
relativistic correction
Fortran library

Gaussian
many-body expansion
Fortran executable

MRCC Kállay
arbitrary order CC/CI
Fortran executable

v2rdm_casscf DePrince
active-space SCF
Fortran/C++ Psi4 plugin

libxc Marques
exchange-correlation fnctls.
C library

INTEGRALS

ERD Flocke
2e⁻ integrals
Fortran library

libint Valeev
2e⁻ integrals
C library

simint Pritchard
2e⁻ integrals
C++ library

SOLVATION

ADF Visscher
FDE solvation
Fortran/C executable

libefp Kaliman & Slipchenko
fragment potentials
C library

PCMSolver DiRemigio
solvation
Fortran library

STRUCTURE & VIS

MOLDEN Schaftenaar
MOLDEN orbital/density visualization
Fortran executable

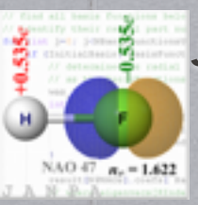
PubChem NIH
PubChem structure look-up
HTML

POST-PROCESSING

DFTD3 Grimme ★
dispersion correction
Fortran executable

GCP Grimme
small-basis correction
Fortran executable

GDMA Stone ★
multipole analysis
Fortran library



JANPA Nikolaienko
NBO bond analysis
Java executable

resp2 McGibbon
RESP charges
C++ Psi4 plugin

UPSTREAM

CHARMMing Woodcock
QM/MM web server
Python/HTML executable; calls Psi4

Pulsar Pritchard & Richards
datastructure interoperability
C++ framework; calls Psi4

WebMO Polik & Schmidt ★
GUI/web server
Perl/Java executable; calls Psi4

QC METHODS

Ambit Turney
tensor manipulations
Python/C++ library

Cfour Stanton & Gauss
$\langle CC|CC\rangle$ CC/MBPT/properties/etc.
Fortran executable

CheMPS2 Wouters ★
DMRG theory
Python/C++ library

DKH Wolf & Reiher ★
relativistic correction
Fortran library

Gaussian
many-body expansion
Fortran executable

MRCC Kállay ★
arbitrary order CC/CI
Fortran executable

v2rdm_casscf DePrince ★
active-space SCF
Fortran/C++ Psi4 plugin

libxc Marques
exchange-correlation fnctls.
C library

INTEGRALS

ERD Flocke
2e⁻ integrals
Fortran library

libint Valeev ★
2e⁻ integrals
C library

simint Pritchard
2e⁻ integrals
C++ library

SOLVATION

ADF Visscher
FDE solvation
Fortran/C executable

libefp Kaliman & Slipchenko ★
fragment potentials
C library

PCMSolver DiRemigio ★
solvation
Fortran library

STRUCTURE & VIS

MOLDEN Schaftenaar
MOLDEN orbital/density visualization
Fortran executable

PubChem NIH ★
PubChem structure look-up
HTML

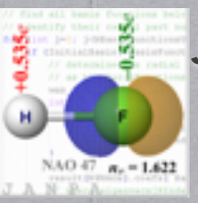
★ Psi4 actively performs build and integration testing

POST-PROCESSING

DFTD3 Grimme ★
dispersion correction
Fortran executable

GCP Grimme
small-basis correction
Fortran executable

GDMA Stone ★ ★
multipole analysis
Fortran library



JANPA Nikolaienko
NBO bond analysis
Java executable

resp2 McGibbon
RESP charges
C++ Psi4 plugin

UPSTREAM

CHARMMing Woodcock
QM/MM web server
Python/HTML executable; calls Psi4

Pulsar Pritchard & Richards
datastructure interoperability
C++ framework; calls Psi4

WebMO Polik & Schmidt ★
GUI/web server
Perl/Java executable; calls Psi4

QC METHODS

Ambit Turney
tensor manipulations
Python/C++ library

Cfour Stanton & Gauss
$\langle CC|CC\rangle$ CC/MBPT/properties/etc.
Fortran executable

CheMPS2 Wouters ★ ★
$\mathbb{C}he[\mathcal{M}][\mathcal{P}][\mathcal{S}]\,2$ DMRG theory
Python/C++ library

DKH Wolf & Reiher ★ ★
relativistic correction
Fortran library

Gaussian
many-body expansion
Fortran executable

MRCC Kállay ★
arbitrary order CC/CI
Fortran executable

v2rdm_casscf DePrince ★
active-space SCF
Fortran/C++ Psi4 plugin

libxc Marques
exchange-correlation fnctls.
C library

INTEGRALS

ERD Flocke
2e⁻ integrals
Fortran library

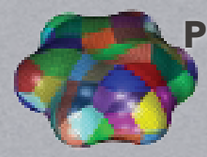
libint Valeev ★ ★
2e⁻ integrals
C library

simint Pritchard
2e⁻ integrals
C++ library

SOLVATION

ADF Visscher
FDE solvation
Fortran/C executable

libefp Kaliman & Slipchenko ★ ★
fragment potentials
C library



PCMSolver DiRemigio ★
solvation
Fortran library

STRUCTURE & VIS

MOLDEN Schaftenaar
MOLDEN orbital/density visualization
Fortran executable

PubChem NIH ★
PubChem structure look-up
HTML

★ Psi4 actively performs build and integration testing ★ library and integrated into Psi4 CMake

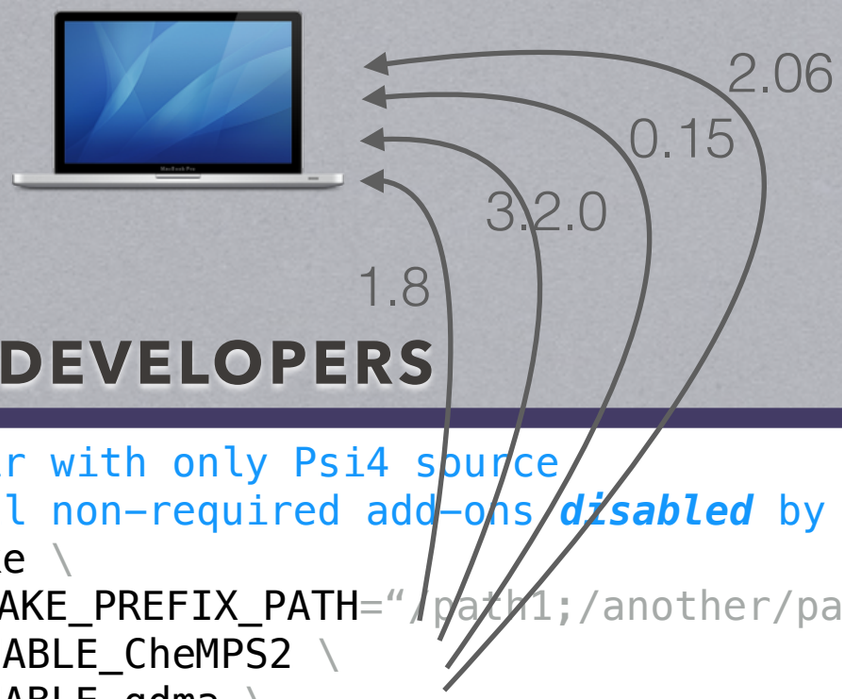
INTEGRATIONS FOR ALL

CORE DEVELOPERS

```
>>> # dir with only Psi4 source
>>> # all non-required add-ons disabled by default
>>> cmake \
    -DCMAKE_PREFIX_PATH="/path1;/another/path2" \
    -DENABLE_CheMPS2 \
    -DENABLE_gdma \
    ...
    # CMake downloads external projects' source from internet
>>> make
>>> ctest -L addons
    Psi4 core.....................................................PASSED
    Psi4 + DFTD3 executable.......................................PASSED
    Psi4 + CheMPS2 library........................................PASSED
    Psi4 + PCMSolver library......................................PASSED
    Psi4 + V2RDM_CASSCF plugin....................................PASSED
    Psi4 + Ambit library..........................................PASSED
    Psi4 library..................................................PASSED
>>> # working Psi4 executable complete with add-ons, customized for local
hardware & software
```

INTEGRATIONS FOR ALL

seeking *built* in **CMAKE_PREFIX_PATH**



CORE DEVELOPERS

```
>>> # dir with only Psi4 source
>>> # all non-required add-ons disabled by default
>>> cmake \
    -DCMAKE_PREFIX_PATH="/path1;/another/path2" \
    -DENABLE_CheMPS2 \
    -DENABLE_gdma \
    ...
    # CMake downloads external projects' source from internet
>>> make
>>> ctest -L addons
    Psi4 core.....................................................PASSED
    Psi4 + DFTD3 executable.......................................PASSED
    Psi4 + CheMPS2 library........................................PASSED
    Psi4 + PCMSolver library......................................PASSED
    Psi4 + V2RDM_CASSCF plugin....................................PASSED
    Psi4 + Ambit library..........................................PASSED
    Psi4 library..................................................PASSED
>>> # working Psi4 executable complete with add-ons, customized for local
hardware & software
```

INTEGRATIONS FOR ALL

seeking *built* in **CMAKE_PREFIX_PATH**

seeking *source* from internet

research homepage

GitHub

BitBucket

GitHub/psi4

1.8

3.2.0

0.15

2.06

CORE DEVELOPERS

```
>>> # dir with only Psi4 source
>>> # all non-required add-ons disabled by default
>>> cmake \
    -DCMAKE_PREFIX_PATH="/path1;/another/path2" \
    -DENABLE_CheMPS2 \
    -DENABLE_gdma \
    ...
    # CMake downloads external projects' source from internet
>>> make
>>> ctest -L addons
    Psi4 core.....................................................PASSED
    Psi4 + DFTD3 executable.......................................PASSED
    Psi4 + CheMPS2 library........................................PASSED
    Psi4 + PCMSolver library......................................PASSED
    Psi4 + V2RDM_CASSCF plugin....................................PASSED
    Psi4 + Ambit library..........................................PASSED
    Psi4 library..................................................PASSED
>>> # working Psi4 executable complete with add-ons, customized for local
hardware & software
```

INTEGRATIONS FOR ALL

linking *built* in **CMAKE_PREFIX_PATH**

downloading *source* from internet

research homepage

GitHub

BitBucket

GitHub/psi4

Psi4 CONDA INSTALL

tarball

clone

library

clone

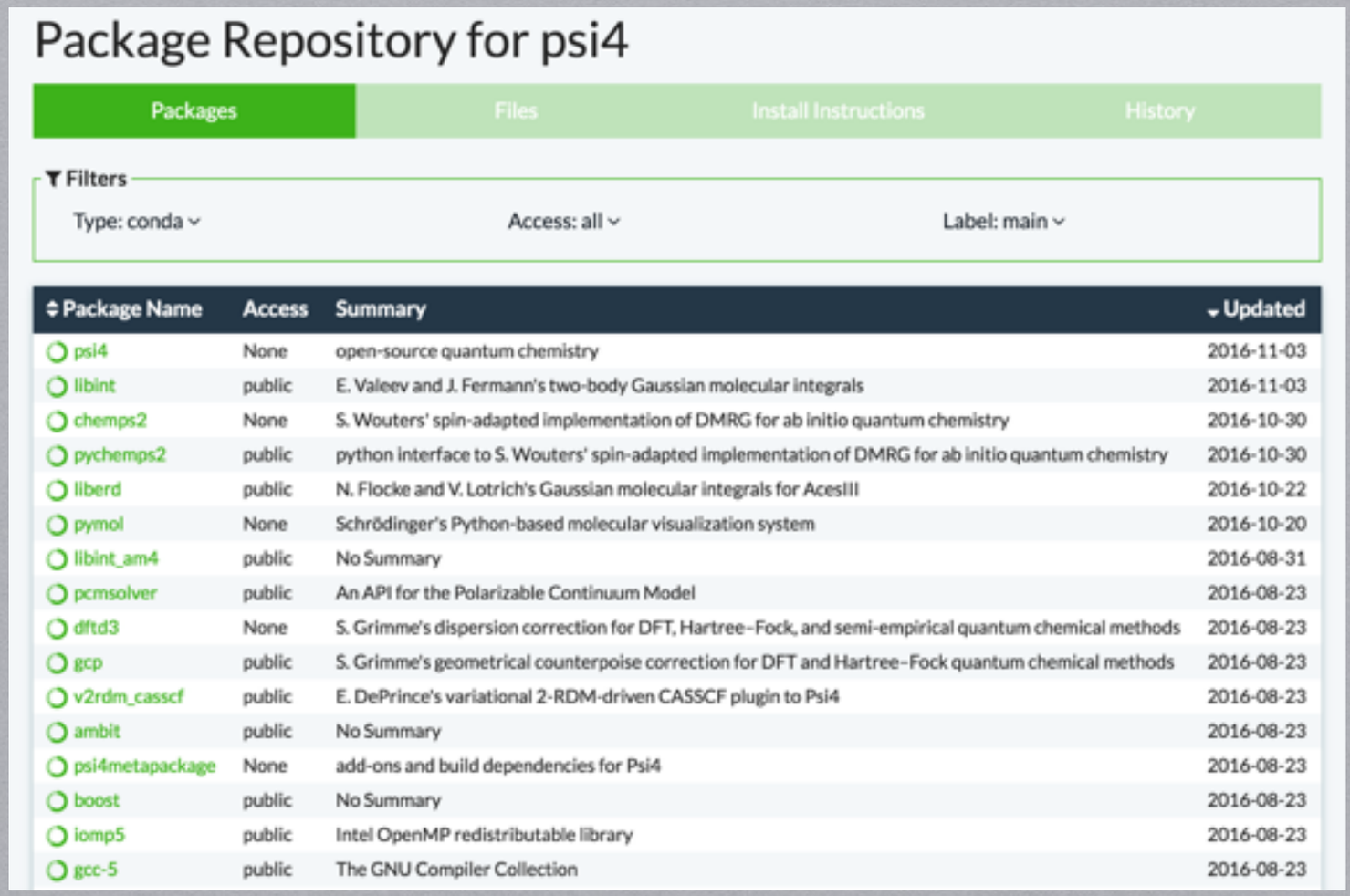
CORE DEVELOPERS

```
>>> # dir with only Psi4 source
>>> # all non-required add-ons disabled by default
>>> cmake \
    -DCMAKE_PREFIX_PATH="/path1;/another/path2" \
    -DENABLE_CheMPS2 \
    -DENABLE_gdma \
    ...
    # CMake downloads external projects' source from internet
>>> make
>>> ctest -L addons
    Psi4 core.....................................................PASSED
    Psi4 + DFTD3 executable.......................................PASSED
    Psi4 + CheMPS2 library........................................PASSED
    Psi4 + PCMSolver library......................................PASSED
    Psi4 + V2RDM_CASSCF plugin....................................PASSED
    Psi4 + Ambit library..........................................PASSED
    Psi4 library..................................................PASSED
>>> # working Psi4 executable complete with add-ons, customized for local
hardware & software
```

ctest -L addons NYI

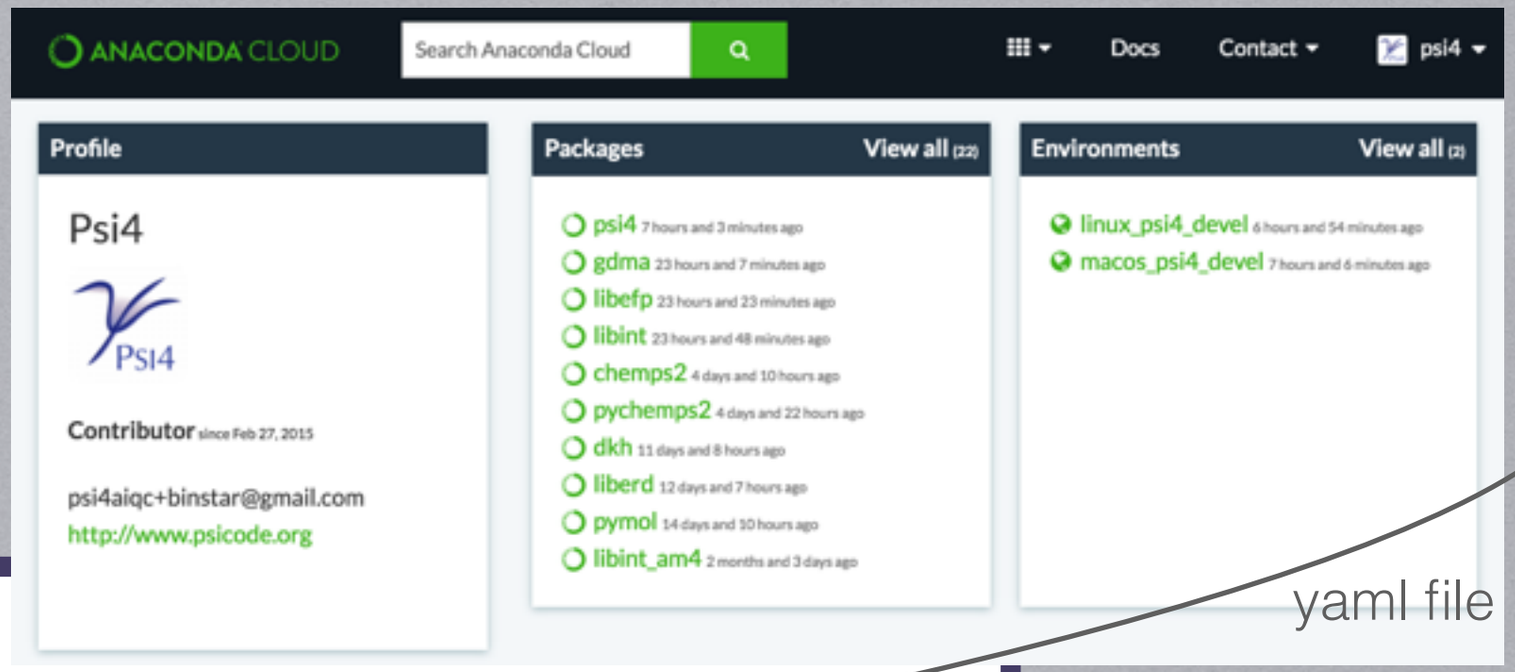
INTEGRATIONS FOR ALL
ENTER CONDA

- nothing so far has saved compile time, unless you built all those pkgs separately (and compatibly)
- you're probably not using many of the addons, so why bother maintaining their build
- conda's already got them built. why not reuse?



Package Name	Access	Summary	Updated
psi4	None	open-source quantum chemistry	2016-11-03
libint	public	E. Valeev and J. Fermann's two-body Gaussian molecular integrals	2016-11-03
chemps2	None	S. Wouters' spin-adapted implementation of DMRG for ab initio quantum chemistry	2016-10-30
pychemps2	public	python interface to S. Wouters' spin-adapted implementation of DMRG for ab initio quantum chemistry	2016-10-30
liberd	public	N. Flocke and V. Lotrich's Gaussian molecular integrals for AcesIII	2016-10-22
pymol	None	Schrödinger's Python-based molecular visualization system	2016-10-20
libint_am4	public	No Summary	2016-08-31
pcmsolver	public	An API for the Polarizable Continuum Model	2016-08-23
dftd3	None	S. Grimme's dispersion correction for DFT, Hartree–Fock, and semi-empirical quantum chemical methods	2016-08-23
gcp	public	S. Grimme's geometrical counterpoise correction for DFT and Hartree–Fock quantum chemical methods	2016-08-23
v2rdm_casscf	public	E. DePrince's variational 2-RDM-driven CASSCF plugin to Psi4	2016-08-23
ambit	public	No Summary	2016-08-23
psi4metapackage	None	add-ons and build dependencies for Psi4	2016-08-23
boost	public	No Summary	2016-08-23
iomp5	public	Intel OpenMP redistributable library	2016-08-23
gcc-5	public	The GNU Compiler Collection	2016-08-23

INTEGRATIONS FOR ALL



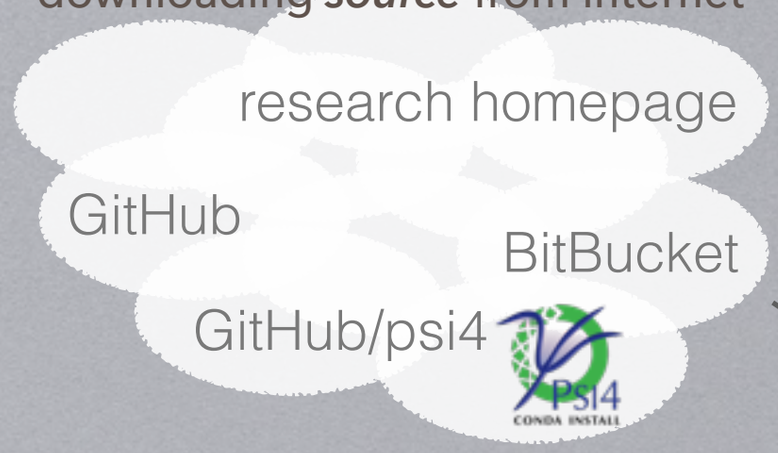

```
>>> # install a mini/anaconda
>>> # update it (conda update conda)
>>> # if “conda env create” below fails, conda install anaconda-client -or-
>>> # download file from site and save as environment.yml
>>> cat environment.yml
name: linux_psi4_devel
channels: !!python/tuple
- !!python/unicode 'defaults'
dependencies:
- mkl=11.3.3=0
- numpy=1.11.2=py27_0
- psi4/label/test::gdma=2.2.06=0
- psi4/label/test::psi4=1.1a2.dev3+20605d7=py27_0
- psi4::dftd3=3.2.0=7
- psi4::gcc-5=5.2.0=1
- psi4::libint=1.1.6=0
- python=2.7.12=1
      ...
>>> conda env create psi4/linux_psi4_devel (or macos_psi4_devel)
>>> source activate linux_psi4_devel
>>> # working Psi4 executable complete with add-ons
```

INTEGRATIONS FOR ALL

linking *built* in **CMAKE_PREFIX_PATH**

libraries

downloading *source* from internet



clone

CORE DEVELOPERS

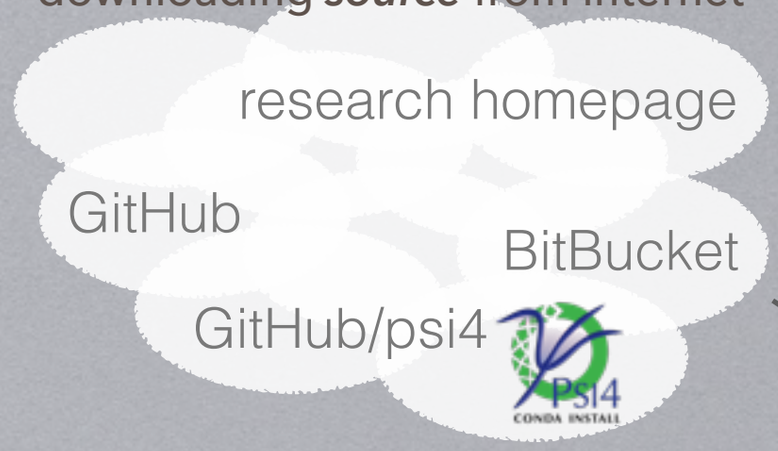
```
>>> # dir with only Psi4 source
>>> export PREFIX=/home/miniconda/envs/linux_psi4_devel
>>> cmake \
    -DCMAKE_PREFIX_PATH="${PREFIX}" \
    -DENABLE_CheMPS2=ON \
    -DENABLE_gdma=ON \
    -DMAX_AM_ERI=6 \
    -DPYTHON_EXECUTABLE=${PREFIX}/bin/python2.7 \
    ...
    # CMake collects mostly built conda libraries, internet src as fallback
>>> make
>>> ctest -L addons
    Psi4 core.....................................................PASSED
    Psi4 + DFTD3 executable.......................................PASSED
    Psi4 + CheMPS2 library........................................PASSED
    Psi4 + PCMSolver library......................................PASSED
    Psi4 + V2RDM_CASSCF plugin....................................PASSED
    Psi4 + Ambit library..........................................PASSED
    Psi4 library..................................................PASSED
>>> # working Psi4 executable complete with add-ons, Psi4 core customized
for local hardware & software
```

INTEGRATIONS FOR ALL

linking *built* in **CMAKE_PREFIX_PATH**

libraries

downloading *source* from internet



CORE DEVELOPERS

```
>>> # dir with only Psi4 source
>>> export PREFIX=/home/miniconda/envs/linux_psi4_devel
>>> cmake \
    -DCMAKE_PREFI
    -DENABLE_Che
    -DENABLE_gdm
    -DMAX_AM_ERI
    -DPYTHON_EXE
    ...
    # CMake coll
>>> make
>>> ctest -L add
    Psi4 core...
    Psi4 + DFTD3
    Psi4 + CheMP
    Psi4 + PCMSo
    Psi4 + V2RDM
    Psi4 + Ambit
    Psi4 library
>>> # working Ps
for local hardware & software
```

```
>>> export PREFIX=/home/user/miniconda/envs/linux_psi4_devel
    # cmake itself
>>> ${PREFIX}/bin/cmake \
    -DCMAKE_PREFIX_PATH="${PREFIX}" \
    -DENABLE_gdma=ON \
    -DMAX_AM_ERI=6 \
    -DPYTHON_EXECUTABLE=${PREFIX}/bin/python2.7 \
    # c/c++ compilers (linux only)
    -DCMAKE_C_COMPILER=${PREFIX}/bin/gcc \
    -DCMAKE_CXX_COMPILER=${PREFIX}/bin/g++ \
    # fortran compilers (linux & mac)
    -DCMAKE_Fortran_COMPILER=${PREFIX}/bin/gfortran \
    # sphinx for docs build
    -DSPHINX_ROOT=${PREFIX} \
    # gcc c++11 libraries, if compiler needs them
    -DCMAKE_C_FLAGS="-gcc-name=${PREFIX}/bin/gcc" \
    -DCMAKE_CXX_FLAGS="-gcc-name=${PREFIX}/bin/gcc -gxx-name=${PREFIX}/bin/g++"
```

INTEGRATIONS FOR ALL

USERS

```
>>> # download Psi4 installer
>>> bash Psi4conda-latest.sh
    ...
    Psi4 core.....................................................PASSED
    Psi4 + DFTD3 executable.......................................PASSED
    Psi4 + CheMPS2 library........................................PASSED
    Psi4 + PCMSolver library......................................PASSED
    Psi4 + V2RDM_CASSCF plugin....................................PASSED
    Psi4 + Ambit library..........................................PASSED
    Psi4 library..................................................PASSED
>>> # working Psi4 executable complete with add-ons
```

PERIPHERAL DEVELOPERS

```
>>> # working Psi4 executable complete with add-ons (from above)
>>> conda install gcc
>>> psi4 -new-plugin mygreatcode
>>> cd mygreatcode
>>> make
Attention! This SCF may be density-fitted.
>>> # working compiling development environment ready for extension
```

VERSIONING

PRAY I DON'T ALTER IT ANY FURTHER

- **DEVELOPMENT SNAPSHOT** on master; passes quicktests, may break features;
  - **FORMAT** `M.m+1.devN`
  - **UPDATE VIA** `conda update psi4 -c psi4/label/level`
- **PRE-RELEASE** on master; passes quicktests; conda devel channel
  - **ALPHA** much of the milestone is in
  - **RC** much a plausible release candidate
    - conda devel channel
- **RELEASE** on master or maintenance; all tests pass, never less capable than its predecessor
  - **FORMAT** master (`M.m`) or maintenance (`M.m.p`)
  - **UPDATE VIA** `conda update psi4`

- want to be able to break things on psi4/psi4 master occasionally (e.g., plugins, mints9) without those commits being a released version (implied by 1.0.101)
- want to be able to do bug fixes on releases (pulled off as 1.0.x) without naming conflicts)
- want to accommodate those who only want stable versions
- you can ignore tags if you like. but locally computed v will be wrong

equivalent

1.0.0

RELEASE

1.0

PRE-RELEASE

1.1a1

PRE-RELEASE

1.1rc1

RELEASE

1.1

A B C D E F G H I J K L M

1.1.dev2 1.1.dev3 1.1.dev5 1.1a1.dev1 1.1rc1.dev2 1.2.dev1

Development **master** not readily accessed

RELEASE

1.0.1

RELEASE

1.0.2

A D′ E′ F′ H′

Maintenance **1.0.x**

- always has a tag at its head
- only bug fixes

L

Maintenance **1.1.x**

PART III: PLUGINS & LAYOUT

JUSTIN M. TURNEY

PLUGINS

Plugins continue to be the best way to add new functionality to Psi4.

Your code is developed as a standalone entity, which is compiled independently of Psi4, but can still make sure of Psi4's vast library.

Plugins are loaded at runtime by Psi4 from any location.

PLUGINS

```
% psi4 --help
  --new-plugin NEW_PLUGIN
                    Creates a new directory with files for writing a new
                    plugin.
  --new-plugin-template
{aointegrals,basic,dfmp2,mointegrals,scf,sointegrals,wavefunction}
                          New plugin template to use.


% psi4 --new-plugin mydfmp2 --new-plugin-template dfmp2
-- Creating "mydfmp2" with "dfmp2" template. --------------------
==> Created plugin files:
  __init__.py, CMakeLists.txt, doc.rst, input.dat, plugin.cc, pymodule.py
```

The ability to create just a Makefile for an existing plugin as been removed.

PLUGINS

```
project(mydfmp2 CXX)

find_package(psi4 1.0 REQUIRED)

add_psi4_plugin(mydfmp2 plugin.cc)
```

- Plugins now make use of CMake for configuring and building.

```
export CMAKE_PREFIX_PATH=\
   /Users/jtturney/Install/psi4
```

- If you install Psi4 into a non-standard location you will likely need to define CMAKE_PREFIX_PATH

PLUGINS

```
% cd mydfmp2

% cmake .
-- The CXX compiler identification is AppleClang 8.0.0.8000042
-- Check for working CXX compiler: /usr/bin/c++
-- Check for working CXX compiler: /usr/bin/c++ -- works
-- Detecting CXX compiler ABI info
-- Detecting CXX compiler ABI info - done
-- Detecting CXX compile features
-- Detecting CXX compile features - done
-- Psi4 include directory: /Users/jtturney/Install/psi4/include
-- Psi4 executable: /Users/jtturney/Install/psi4/bin/psi4
-- Psi4 core library: /Users/jtturney/Install/psi4/lib/psi4/core.so
-- Python executable: /Users/jtturney/anaconda3/bin/python
-- Configuring done
-- Generating done
-- Build files have been written to: /Users/jtturney/mydfmp2

% make

% psi4
```

PART IV: DIRECTORY LAYOUT

JUSTIN M. TURNEY

BINARIES AND LIBRARIES
MERGED

C. 2015

```
src/lib/
libdiis/
libdpd/
libfock/
libmints/
libpsio/
...
src/bin/
ccenergy/
detci/
dfmp2/
dmrg/
occ/
sapt/
scf/
...
```

```
psi4/src/psi4/
ccenergy/
detci/
dfmp2/
dmrg/
libdiis/
libdpd/
libfock/
libmints/
libpsio/
occ/
sapt/
scf/
...
```

NOW

- **WHAT** modules/libraries of C++ code, written by us
- **WHY** bin/lib distinguished by names; mirror installed header paths
- **NEW** *binaries* get built; *libraries* get their headers installed

C++ CORE

RAISED ABOVE MODULES AND CLEANED

C. 2015

```
src/bin/psi4/
clean.cc
export_blas_lapack.cc
export_functional.cc
export_mints.cc
export_oeprop.cc
...
psi4.cc
psi4.h
psi_start.cc
psi_stop.cc
python.cc
read_options.cc
script.cc
script.h
set_memory.cc
```

NOW

```
psi4/src/
core.cc
export_blas_lapack.cc
export_functional.cc
export_mints.cc
export_oeprop.cc
...
psi4/
read_options.cc
```

- WHAT module-running code
- WHY sanity and CMake like dependencies as subdirectories
- NEW **`python.cc`** (`BOOST_PYTHON_MODULE(psi4)`) becomes **`core.cc`** (`PYBIND11_PLUGIN(core)`); most else gone

PSIDATADIR

SPLIT BY LANGUAGE, PURPOSE, & PROJECT

C. 2015

```
lib/
basis/
databases/
efpfrag/
fsapt/
grids/
plugin/
psi4/
python/
quadratures/
scripts/
```

```
psi4/share/psi4/
basis/
databases/
fsapt/
grids/
plugin/
quadratures/
scripts/

psi4/
driver/
```

NOW

- WHAT the pieces that didn't need compilation
- WHY separate python and data; mirror GNU install directory structure in source
- NEW **python/** becomes **driver/**; envvar PSI4DATADIR defunct; efp evicted

HEADERS
WINNOWED AND NAMESPACE

C. 2015

```
include/
Z_to_element.h
chkpt_params.h
compiler.h
cov_radii.h
element_to_Z.h
exception.h
fragment.h
masses.h
molecular_system.h
physconst.h
process.h
psi4-dec.h
psi4-def.h
psifiles.h
psitypes.h
...
```

NOW

```
psi4/include/psi4/
masses.h
physconst.h
pragma.h
psi4-dec.h
psifiles.h
pybind11.h

psi4/src/psi4/libmints/
element_to_Z.h
psi4/src/psi4/optking/
cov_radii.h
psi4/src/psi4/libpsi4util/
exception.h
psi4/src/psi4/libparallel/
process.h
```

- WHAT global (supra-module) headers
- WHY mirror GNU install directory structure in source
- NEW now actually installed! useable by plugins

EXTERNAL PROJECTS
TENTACLES SEVERED

C. 2015

```
boost/
boost_1_57_0.tar.bz2
cmake/
FindCHEMPS2.cmake
FindPCMSolver.cmake
ConfigPCMSolver.cmake
ConfigChemps2.cmake
ConfigBoost.cmake
interfaces/
libefp/
lib/
efpfrag/
src/lib/
libderiv/
liberd/
libint/
libmints/dkh2-dkh4_main.F90
```

NOW

```
external/
ambit/CMakeLists.txt
chemps2/CMakeLists.txt
dkh/CMakeLists.txt
gdma/CMakeLists.txt
gtfock/CMakeLists.txt
libefp/CMakeLists.txt
liberd/CMakeLists.txt
libint/CMakeLists.txt
pcmsolver/CMakeLists.txt
pybind11/CMakeLists.txt
```

- WHAT everything we didn't write that we depend on or use as enhancement
- WHY good practice, sanity for maintainers (LAB), and avoid possessing others' code
- NEW no external code stored locally, even tarballs & share; "config" CMake proj., not "module"

VERSION, HEADER, CL-ARGS

SPLIT BY LANGUAGE, PURPOSE, & PROJECT

C. 2015

```
src/bin/psi4/
gitversion.py
version.cc
psi_start.cc
```

```
Psi4: An Open-Source Ab Initio Electronic Structure Package
Psi4 1.0 Driver

Git: Rev dirty

J. M. Turney, A. C. Simmonett, R. M. Parrish, E. G. Hohenstein,
F. A. Evangelista, J. T. Fermann, B. J. Mintz, L. A. Burns, J. J. Wilke,
M. L. Abrams, N. J. Russ, M. L. Leininger, C. L. Janssen, E. T. Seidl,
W. D. Allen, H. F. Schaefer, R. A. King, E. F. Valeev, C. D. Sherrill,
and T. D. Crawford, WIREs Comput. Mol. Sci. 2, 556-565 (2012)
(doi: 10.1002/wcms.93)

                    Additional Contributions by
A. E. DePrince, U. Bozkaya, A. Yu. Sokolov, D. G. A. Smith, R. Di Remigio,
R. M. Richard, J. F. Gonthier, H. R. McAlexander, M. Saitow, and
B. P. Pritchard
-------------------------------------------------------------------------


Psi4 started on: Monday, 17 October 2016 10:40AM

Process ID:  68092
PSIDATADIR: /Users/loriab/linux/psihub/psi4inversion/psi4/objdir1/stage/Use
(inversion/install-psi4/share/psi4
Memory:     500.0 MiB
Threads:    1
```

```
psi4/
run_psi4.py.in
versioner.py
metadata.py
```

```
usage: psi4 [-h] [-i INPUT] [-o OUTPUT] [-v] [-V] [-k] [-m] [-r] [-s SCRATCH]
            [-a] [-l PSIDATADIR] [-n NTHREAD] [-p PREFIX] [--inplace]
            [--new-plugin NEW_PLUGIN]
            [--new-plugin-makefile NEW_PLUGIN_MAKEFILE]

 hybrid C++/Python quantum chemistry module.

ptional arguments:
  -h, --help            show this help message and exit
  -i INPUT, --input INPUT
                        Input file name. Default input.dat.
  -o OUTPUT, --output OUTPUT
                        Redirect output elsewhere. Default filename.out if
                        input is filenamefilename.out if input is filename.in
                        or filename.dat output.dat if input is input.dat
  -v, --verbose         Print a lot of information.
  -V, --version         Print version information.
  -k, --skip-preprocessor
                        Skips input preprocessing. Expert mode.
  -m, --messy           Leave temporary files after the run is completed.
  -r, --restart         Number to be used instead of process id.
  -s SCRATCH, --scratch SCRATCH
                        Psi4 scratch directory to use.
  -a, --append          Append results to output file. Default Truncate first
  -l PSIDATADIR, --psidatadir PSIDATADIR
                        Specify where to look for the Psi data directory.
                        Overrides PSIDATADIR.
  -n NTHREAD, --nthread NTHREAD
                        Number of threads to use (overrides OMP_NUM_THREADS)
  -p PREFIX, --prefix PREFIX
                        Prefix name for psi files. Default psi
  --inplace             Runs psi4 from the source directory.!Warning! expert
                        option.
  --new-plugin NEW_PLUGIN
                        Creates a new directory with files for writing a new
                        plugin. You can specify an additional argument that
                        specifies a template to use, for example --new-plugin
                        name +mointegrals
  --new-plugin-makefile NEW_PLUGIN_MAKEFILE
                        Creates Makefile that can be used to compileplugins.
                        The Makefile is placed in the currentdirectory.
```

NOW

- **WHAT** initial run-time probes
- **WHY** everyone from Py, CM, GNU has versioning prefs; easier to control env through Py
- **NEW** wait for versioning lightning talk

DIRECTORY STRUCTURE

CONCERNING C-SIDE CORE

```
psi4/src/
core.cc (make py-mod, top exports)
export_mints.cc   (module exports)
export_blas_lapack.cc              (“)
                  al.cc            (“)
                  c                (“)
                                   (“)
                                    (module source)
                                    (module options)
```

CONCERNING PSI4 WHOLE

```
psi4/
__init__.py (import Py- & C-sides)
driver/                  (Py-side Psi4)
import_core.py (import C- details)
include/                   (C-side headers)
                  (build config help)
                  e.in (CM detection)
                  (simulate psi4 exe)
                  (text data library)
                        (C-side Psi4)
                  eader & versioning)
```

CONCERNING PSI4+EXT SUPERBUILD

```
/
LICENSE                          (GPLv2+)
cmake/  (superbuild build support)
doc/                  (documentation)
external/       (external projects)
media/                         (logos)
plugins/              (model plugins)
psi4/   (Psi4 proj. in superbuild)
samples/          (tests less CMake)
tests/  (Psi4 core & add-on tests)
```

DIRECTORY STRUCTURE
NOT MEANT TO BE CRUEL

psi4/psi4/src/psi4

- constrained by GitHub repository name
- contains the CMake project

psi4/psi4/src/psi4

- constrained by Python module name
- contains the Python project

psi4/psi4/src/psi4

psi4/psi4/share/psi4

psi4/psi4/include/psi4

- constrained by GNU project name
- contains the C++ project
- new namespace pad dirs, but tab-able

PART V: A BRIEF HISTORY OF VERSIONING Psi4

OR, WHY THINGS KEEP GETTING MORE COMPLICATED

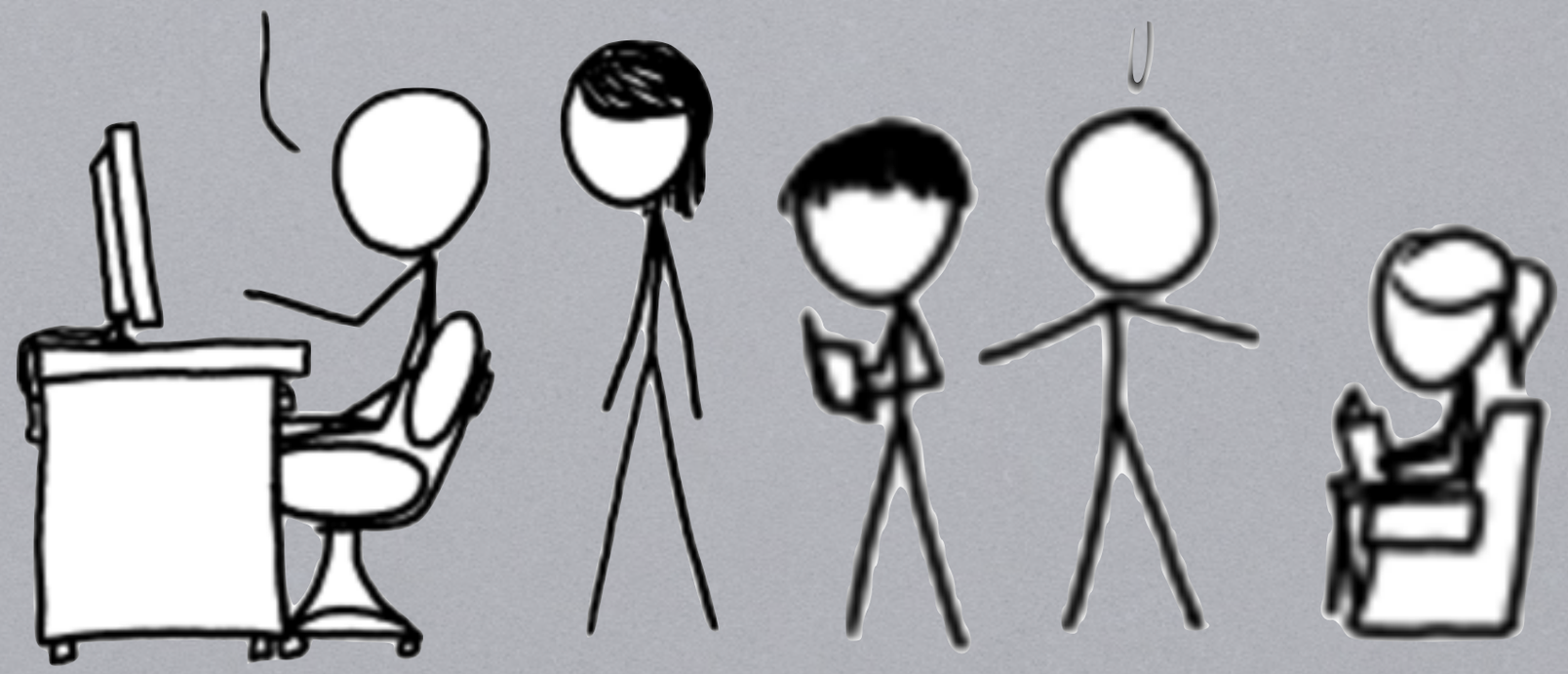
LORI A. BURNS

IN THE BEGINNING
JET NEEDED NO VERSIONING

- CONSTRAINTS None: only one person. Plus, SVN numbers sequentially.

THE INTERREGNUM

TRUE DEVELOPERS ONLY NEED GIT HASHES



- CONSTRAINTS Minimal: only need to ID the code so git hash suffices.

VERSIONING CIRCA 2015
ENTER CONDA & SORTABILITY

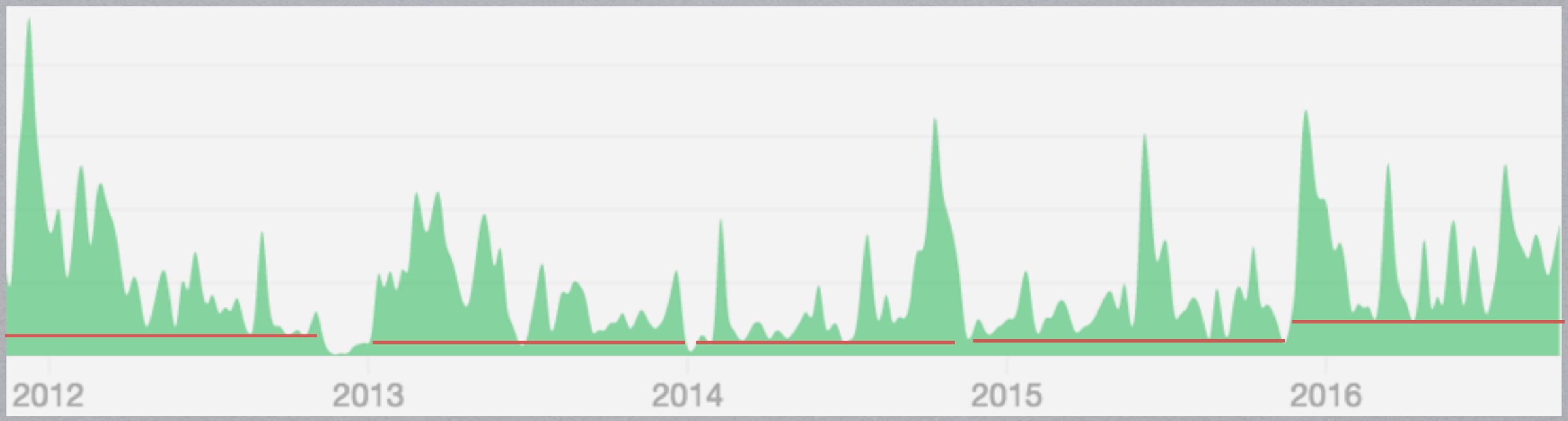
- CONSTRAINTS `conda update psi4` needs a sortable version to act upon

VERSIONING CIRCA 2015
ENTER CONDA & SORTABILITY

- CONSTRAINTS `conda update psi4` needs a sortable version to act upon

VERSIONING IN THE AGE OF CHANGE

I HAVE ALTERED THE VERSIONING



- CONSTRAINTS
  - want to break things on master occasionally (e.g., plugins, cc14) without implying a released version
  - want to do bug fixes on tagged releases without naming conflicts
  - want to accommodate users who only want stable versions

THE FINE PRINT: you can ignore tags if you like. but locally computed version will be undefined

VERSIONING

PRAY I DON'T ALTER IT ANY FURTHER

DEVELOPMENT SNAPSHOT on master; passes quicktests, may break features;

FORMAT `M.m+1.devN`

UPDATE VIA `conda update psi4 -c psi4/label/level`

PRE-RELEASE on master; passes quicktests; conda devel channel

ALPHA much of the milestone is in

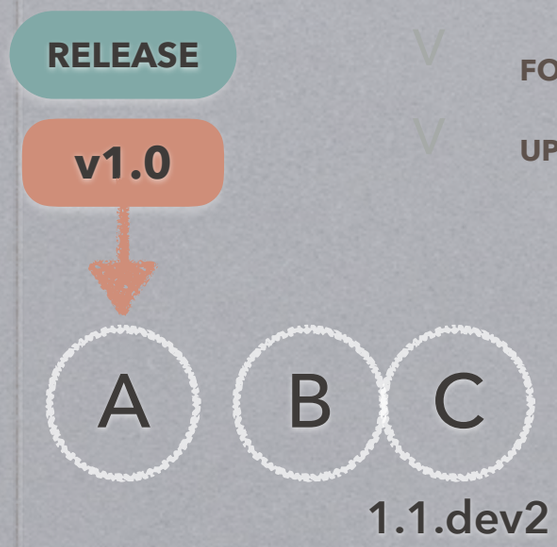
RC much a plausible release candidate

conda devel channel

RELEASE on master or maintenance; all tests pass, never less capable than its predecessor

FORMAT master (`M.m`) or maintenance (`M.m.p`)

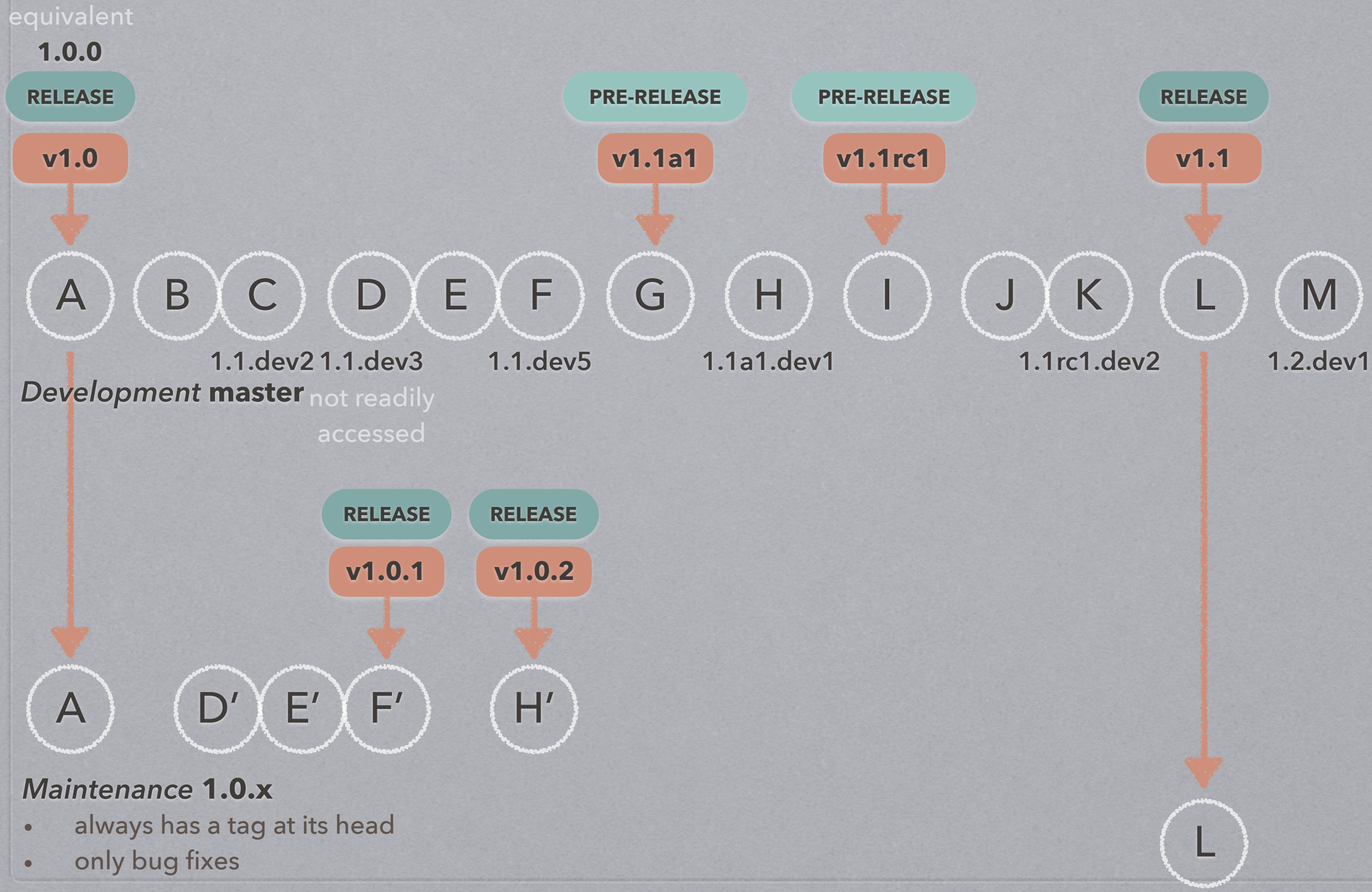
UPDATE VIA `conda update psi4`



DEVELOPMENT SNAPSHOT — on master; passes quicktests, may break features; `M.m+1.devN` format; `conda update psi4 -c psi4/label/devel`

PRE-RELEASE — on master; passes quicktests; conda devel channel

RELEASE — on master (`M.m`) or maintenance (`M.m.p`) branch; all tests pass, always excepting deprecations, never less capable than its predecessor; `conda update psi4`



V DEVELOPMENT SNAPSHOT — on master; passes quicktests, may break features; `M.m+1.devN` format; `conda update psi4 -c psi4/label/devel`

V PRE-RELEASE — on master; passes quicktests; conda devel channel

V RELEASE — on master (`M.m`) or maintenance (`M.m.p`) branch; all tests pass, always excepting deprecations, never less capable than its predecessor; `conda update psi4`

equivalent

1.0.0

RELEASE **v1.0** — A

PRE-RELEASE **v1.1a1** — G

PRE-RELEASE **v1.1rc1** — I

RELEASE **v1.1** — L

B C D E F G H I J K L M

1.1.dev2 1.1.dev3 1.1.dev5 1.1a1.dev1 1.1rc1.dev2 1.2.dev1

Development **master** not readily accessed

RELEASE **v1.0.1** — F′

RELEASE **v1.0.2** — H′

A D′ E′ F′ H′

Maintenance **1.0.x**

- always has a tag at its head
- only bug fixes

L

Maintenance **1.1.x**