easybuild

building software with ease

EasyBuild hackathon @ Cyprus
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About HPC UGent:

- central contact for HPC at Ghent University
- part of central IT department (DICT)
- member of Flemish supercomputer centre (VSC)
  - collaboration between Flemish university associations

- six Tier2 systems, one Tier1 system
  - #163 in Top500 (Nov. 2012)
- team consists of 7 FTEs
- tasks include system administration of HPC infrastructure, user training, user support, ...

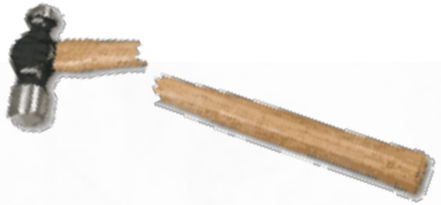
Building scientific software is... fun!

Scientists focus on the functionality of their software,
not on portability, build system, ...

Common **issues** with build procedures of scientific software:

- **incomplete**, e.g. no install step
- requiring human **interaction**
- heavily **customised** and **non-standard**
- uses **hard-coded** settings
- poor and/or outdated **documentation**

Very time-consuming for user support teams!



Current tools are lacking

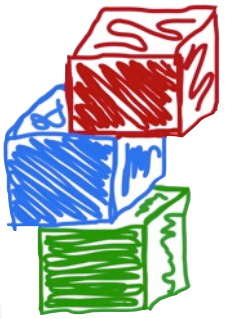
- building from **source** is preferred in an HPC environment
  - **performance** is critical, instruction selection is key (e.g. AVX)
- not a lot of packaged scientific software available (RPMs, ...)
  - requires **huge effort,** which is duplicated across distros
- existing build tools are
  - hard to **maintain** (e.g., bash scripts)
  - stand-alone, **no reuse** of previous efforts
  - **OS-dependent** (HomeBrew, *Ports, ...)
  - **custom** to (groups of) software packages

    e.g., Dorsal (DOLFIN), gmkpack (ALADIN)

Our build tool wish list

- **flexible** framework
- allows for **reproducible** builds
- supports **co-existence** of versions/builds
- **automated** builds and **dependency** resolution
- enables **sharing** of build procedure implementations

Building software with ease



a software build and installation framework

- written in **Python**
- developed in-house (HPC-UGent) for 2.5 years
- **open-source (GPLv2)** since April 2012
- **stable API** since Nov. 2012 (v1.0.0)
- continuously enhanced and extended
- *http://hpcugent.github.com/easybuild*

What does EasyBuild need?

- **Linux** / OS X
  - used daily on Scientific Linux 5.x/6.x (Red Hat-based)
  - also tested on Fedora, Debian, Ubuntu, CentOS, SLES, ...
  - a couple of known issues on OS X
  - no Windows support (and none planned for now)
- **Python 2.4** or more recent 2.x
- **environment modules** (lmod support planned)
- system C/C++ compiler to bootstrap a GCC toolchain

Installing EasyBuild

```
$ easy_install --user easybuild
```

error: option --user not recognized (only for recent setuptools)

You should be using pip!

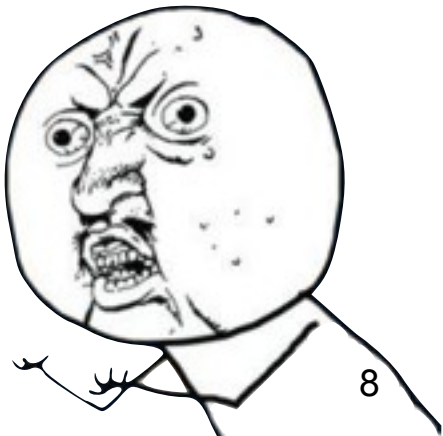
```
$ pip install --user easybuild
```

pip: No such file or directory (pip not installed)

Just use --prefix with easy_install!

```
$ easy_install --prefix=$HOME easybuild
$ export PATH=$HOME/bin:$PATH
$ eb --version
```

ERROR: Failed to locate EasyBuild's main script
(PYTHONPATH not set correctly)



Bootstrapping EasyBuild

Easily install EasyBuild by bootstrapping it.

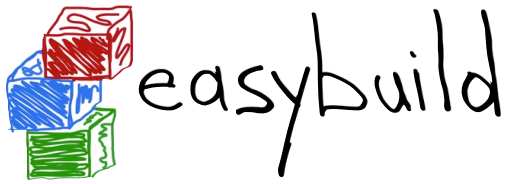
https://github.com/hpcugent/easybuild/wiki/Bootstrapping-EasyBuild

```
$ wget http://hpcugent.github.com/easybuild/bootstrap_eb.py
$ python bootstrap_eb.py $HOME
```

This will install EasyBuild with EasyBuild, and produce a module:

```
$ export MODULEPATH=$HOME/modules/all:$MODULEPATH
$ module load EasyBuild/1.2.0
$ eb --version
This is EasyBuild 1.2.0 (framework: 1.2.0, easyblocks: 1.2.0)
```

We're also looking into a packaged release (RPM, .deb, ...).



Configuring EasyBuild

By default, EasyBuild will install software to

`$HOME/.local/easybuild/software`

and produce modules files in

`$HOME/.local/easybuild/modules/all`

You can instruct EasyBuild otherwise by configuring it, using:

- a configuration file, e.g., `$HOME/.easybuild/config.py`
- environment variables, e.g., `$EASYBUILDINSTALLPATH`

https://github.com/hpcugent/easybuild/wiki/Configuration

‘Quick’ demo for the impatient

```
eb HPL-2.0-goalf-1.1.0-no-OFED.eb --robot
```

- downloads all required sources (best effort)
- constructs *goalf* toolchain, and builds HPL with it

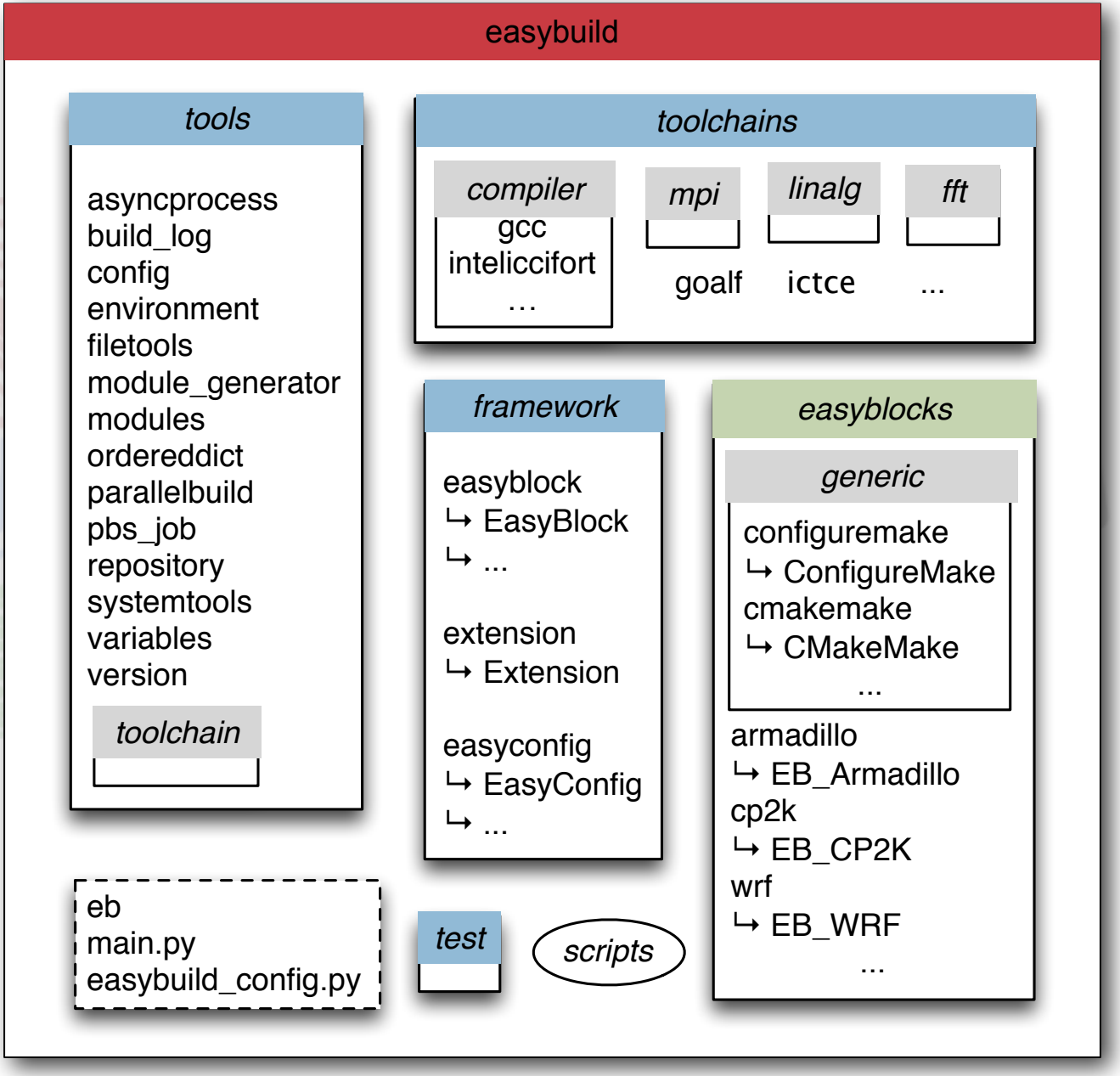
  goalf: GCC, OpenMPI, ATLAS, LAPACK, FFTW, ScaLAPACK, BLACS
- default: source/build/install dir in `$HOME/.local/easybuild`

note: we need a better *quick* demo (without ATLAS)

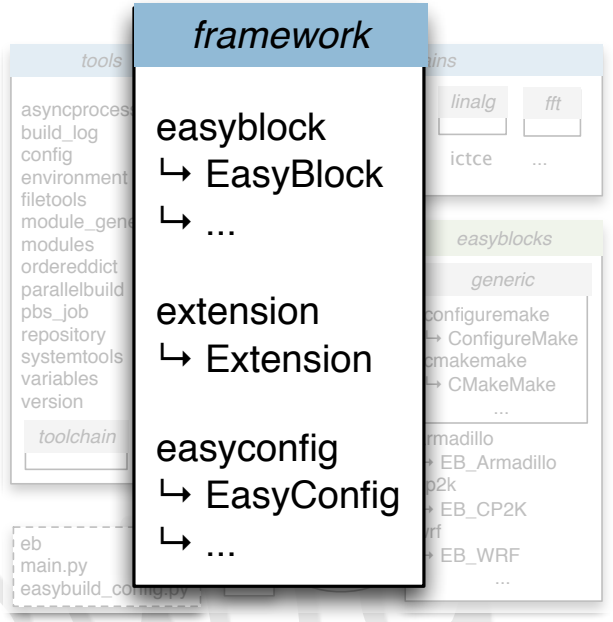
Terminology

- **framework**
  - Python packages and modules forming the heart of EasyBuild
  - provides (loads of) supporting functionality
  - very modular design w.r.t. toolchains and easyblocks
- **easyblock**
  - Python module providing implementation of a build procedure
  - can be generic or software-specific
- **easyconfig file (.eb)**
  - build specification: name, version, toolchain, build options, ...
  - simple text files, Python syntax

High-level design



High-level design



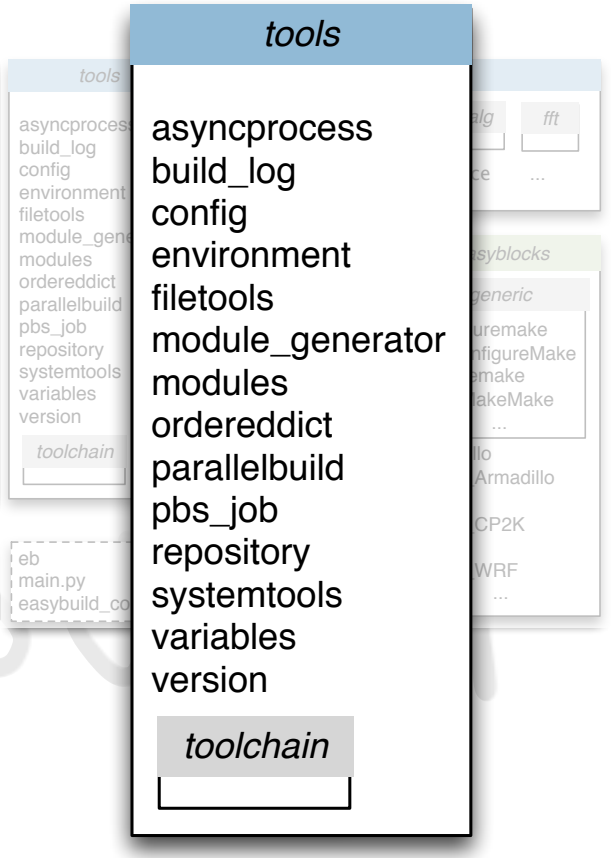
framework package

- core of EasyBuild
- 'abstract' class Easyblock
  - should be subclassed
- EasyConfig class
- Extension class
  - e.g., to build and install Python packages, R libraries, ...

High-level design

tools package

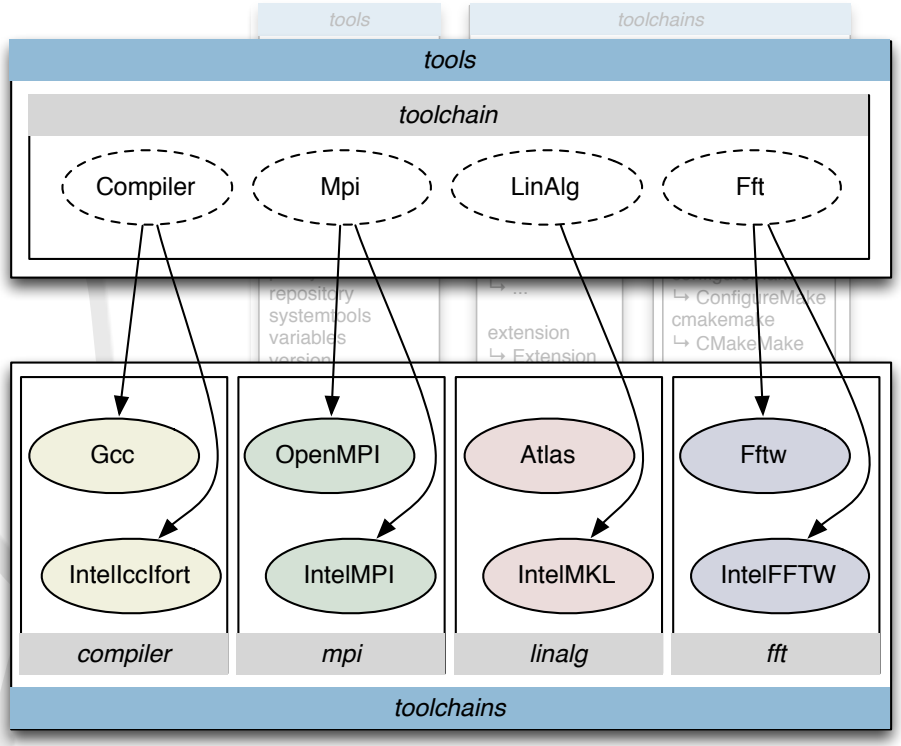
- supporting functionality, e.g.:
  - `run_cmd` for shell commands
  - `run_cmd_qa` for interaction
  - `extract_file` for unpacking
  - `apply_patch` for patching
- *tools.toolchain* for compiler toolchains



High-level design

toolchains package

- support for compiler toolchains
- relies on *tools.toolchain*
- toolchains are defined in here
- organized in subpackages:
  - *toolchains.compiler*
  - *toolchains.mpi*
  - *toolchains.linalg* (BLAS, LAPACK, ...)
  - *toolchains.fft*
- very modular design for allowing extensibility
- plug in a Python module for compiler/library to extend it



High-level design

test package

- unit testing of EasyBuild

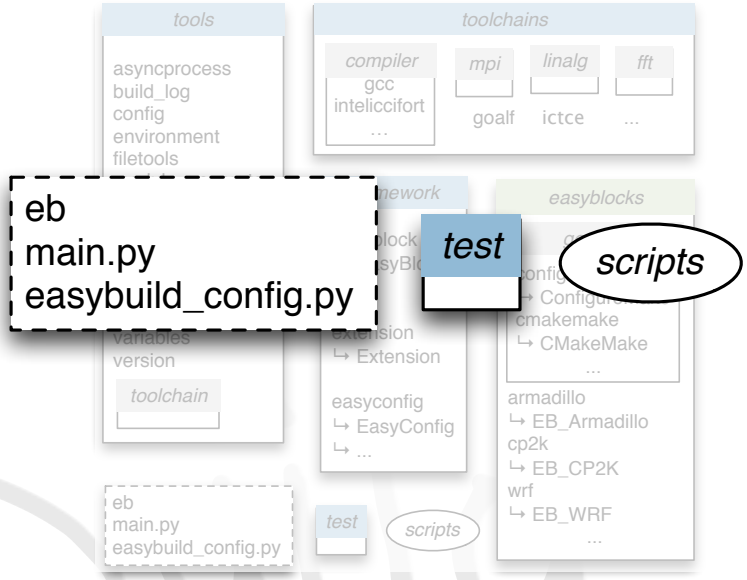
collection of scripts

- mainly for EasyBuild developers

main.py script + *eb* wrapper

default EasyBuild configuration file

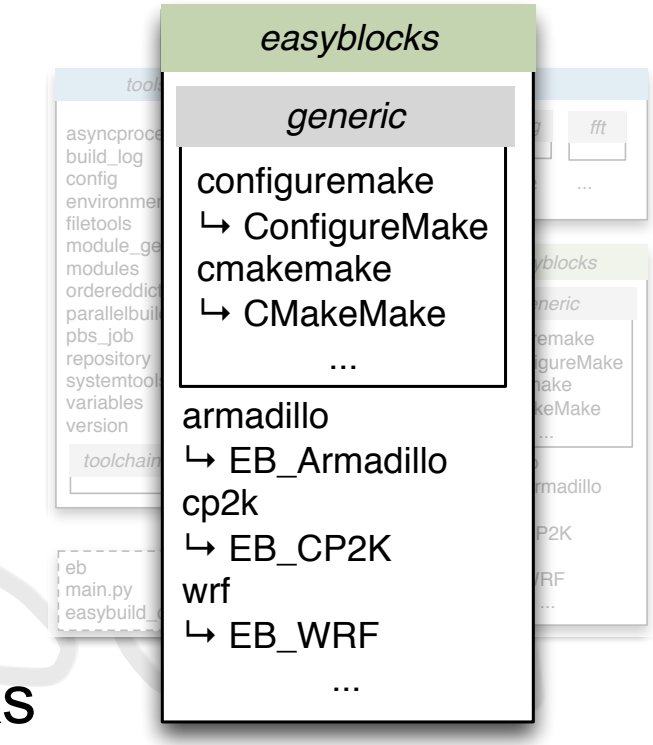
- can be used as a template for your own config file

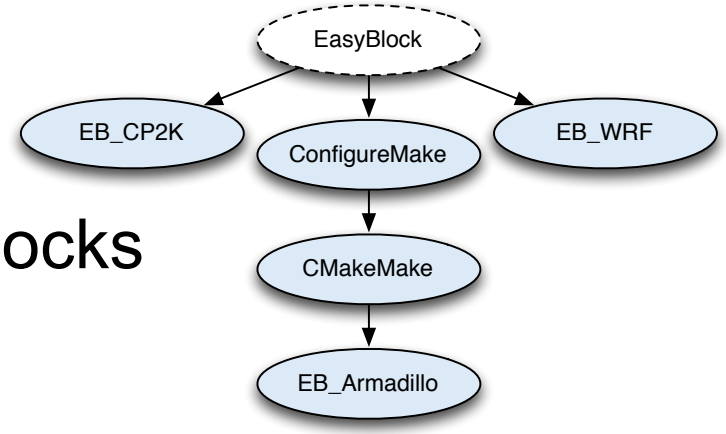


High-level design

easyblocks package

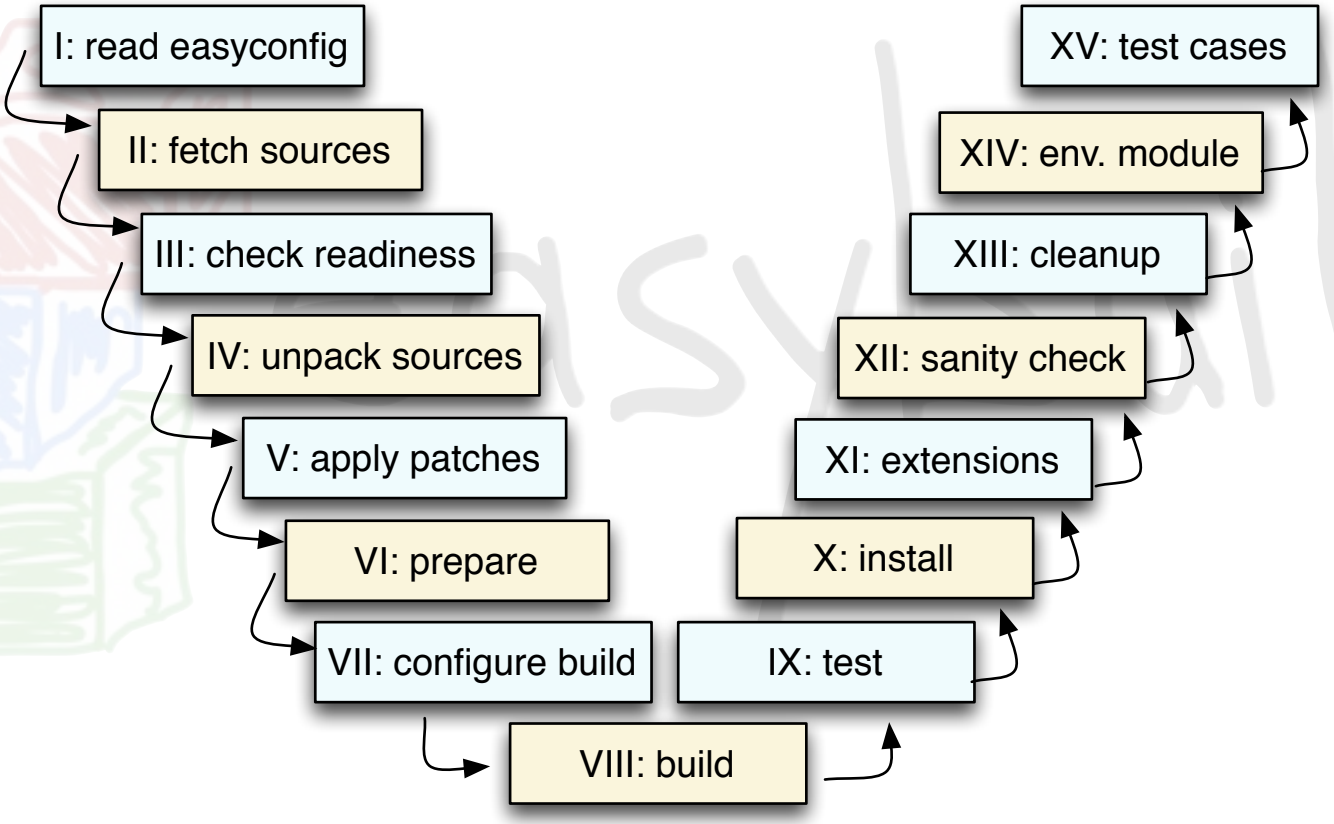
- build procedure implementations
- very modular design
  - add yours in the Python search path
  - EasyBuild will pick it up
- *easyblocks.generic*: generic easyblocks
  - custom support for groups of applications
  - e.g., ConfigureMake, CMakeMake, ...
- *easyblocks*: application-specific easyblocks
- object-oriented scheme
  - subclass from existing easyblocks or EasyBlock



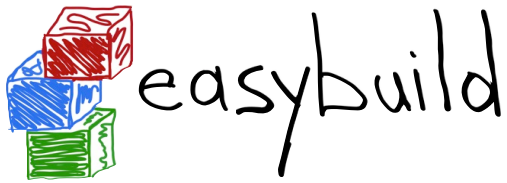


Step-wise install procedure

build and install procedure as implemented by EasyBuild



most of these steps can be customized if required

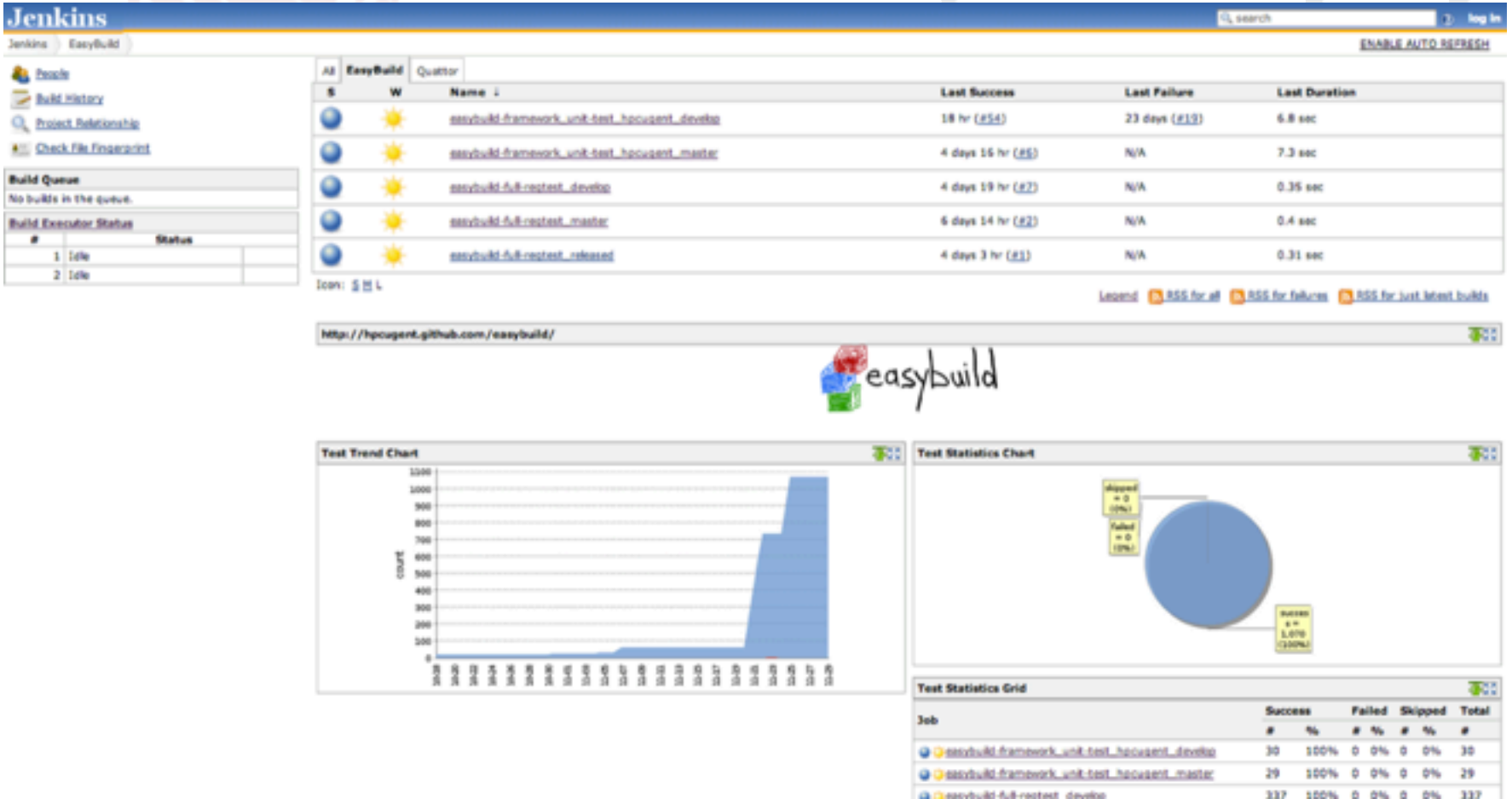


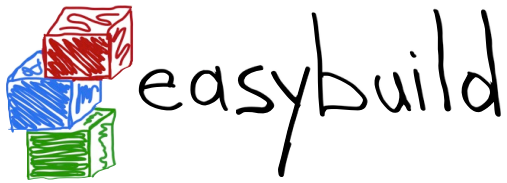
Features

- **logging** and archiving
  - entire build process is logged thoroughly, logs stored in install dir
  - easyconfig file used for build is archived (file/svn/git repo)
- **automatic dependency resolution**
  - software stack be built with a single command, using `--robot`
- running **interactive** installers **autonomously**
  - by passing a Q&A Python dictionary to the `run_cmd_qa` function
- building software in **parallel**
  - e.g., on a (PBS) cluster, by using `--job`
- comprehensive **testing**: unit tests, regression testing

Comprehensive testing

- unit tests are run automagically by Jenkins
- regression test results are pulled in
- publicly accessible: *https://jenkins1.ugent.be/view/EasyBuild*





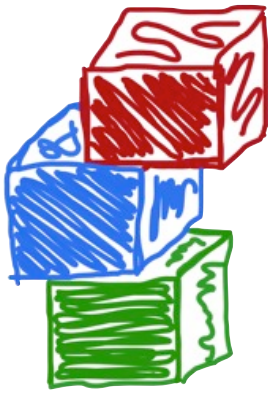
List of supported software (v1.2.0)

241 different software packages (619 example easyconfigs)

a2ps ABINIT ABySS ACML **ALADIN** AMOS AnalyzeFMRI ant aria2 Armadillo ASE ATLAS Autoconf Bash bbcp bbFTP bbftpPRO BEAGLE BFAST binutils BiSearch Bison BLACS BLAST Bonnie++ Boost Bowtie2 BWA byacc bzip2 ccache cflow CGAL cgdb Chapel CLHEP ClustalW2 CMake Corkscrew **CP2K** CPLEX Cufflinks cURL CVXOPT Cython Docutils **DOLFIN** Doxygen **EasyBuild** ECore Eigen ELinks EPD ESPResSo expat FASTX-Toolkit FFC FFTW FIAT flex FLUENT fmri freetype FSL g2clib g2lib GATE GCC GDAL GDB Geant4 GEOS GHC git glproto *gmacml* GMP *gmvapich2* gnuplot gnutls *goalf gompi* google-sparsehash GPAW gperf Greenlet grib_api GSL guile h5py h5utils Harminv HDF HDF5 HMMER HPL hwloc Hypre icc *iccifort ictce* ifort *iiqmpi* imkl impi Infernal Instant *iomkl* Iperf ipp *iqacml* itac JasPer Java Jinja2 JUnit LAPACK lftp libctl libdrm libffi libgtextutils libibmad libibumad libibverbs Libint libmatheval libpciaccess libpng libpthread-stubs libreadline libsmm libtool libunistring libxcb libxml2 libyaml lzo M4 makedepend Maple MATLAB matplotlib mc MCL MDP Meep MEME Mercurial Mesa MetaVelvet METIS MPFR mpiBLAST MrBayes MTL4 MUMmer MVAPICH2 nano NASM NCBI-Toolkit NCL ncurses netCDF netCDF-Fortran nettle **NEURON** numexpr numpy **NWChem** Oger **OpenFOAM** OpenMPI OpenPGM OpenSSL ORCA PAPI parallel ParMETIS Pasha paycheck PCRE **PETSc** petsc4py pkg-config Primer3 pyTables Python python-meep PyZMQ QLogicMPI **QuantumESPRESSO** R RNAz ROOT SAMtools ScaLAPACK ScientificPython scipy SCOOP SCOTCH setuptools Shapely SHRiMP SLEPc SOAPdenovo Sphinx Stow SuiteSparse SWIG Szip tbb Tcl tcsh Theano Tk Tophat Tornado TotalView Trilinos Trinity UFC UFL util-linux Valgrind Velvet ViennaRNA Viper VSC-tools VTK **WIEN2k** wiki2beamer **WPS WRF** xcb-proto XCrySDen XML xorg-macros xproto Yasm ZeroMQ zlib zsync

Current status

- **EasyBuild v1.2.0** released February 28th 2013
  - planned monthly releases (v1.x.0), bugfix releases as needed
  - v1.3.0 planned for March 29th, code freeze on March 20th
- various features pending:
  - **more flexibility**, e.g., module naming scheme, lmod support
  - bring **documentation** wiki up-to-date
  - support for **more software** and additional **compiler toolchains**
  - generate **packages** for supported software (RPMs, .deb, ...)
- small **community**, growing steadily
  - UGent + other Flemish university associations (VSC partners)
  - University of Luxembourg
  - Gregor Mendel Institute (Austria)
  - Cyprus Institute
  - ...



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HPC UGENT

UNIVERSITEIT GENT

VSC Vlaams Supercomputer Centrum

Do you want to know more?

website: *http://hpcugent.github.com/easybuild*

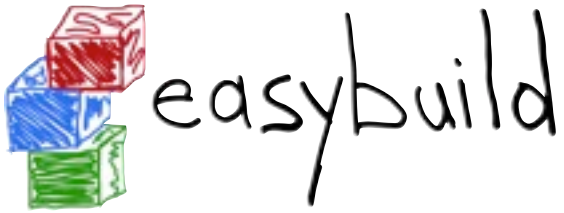
GitHub: *https://github.com/hpcugent/easybuild[-framework|-easyblocks|-easyconfigs]*

PyPi: *http://pypi.python.org/pypi/easybuild[-framework|-easyblocks|-easyconfigs]*

mailing list: *easybuild@lists.ugent.be*

Twitter: *@easy_build*

IRC: *#easybuild on freenode.net*



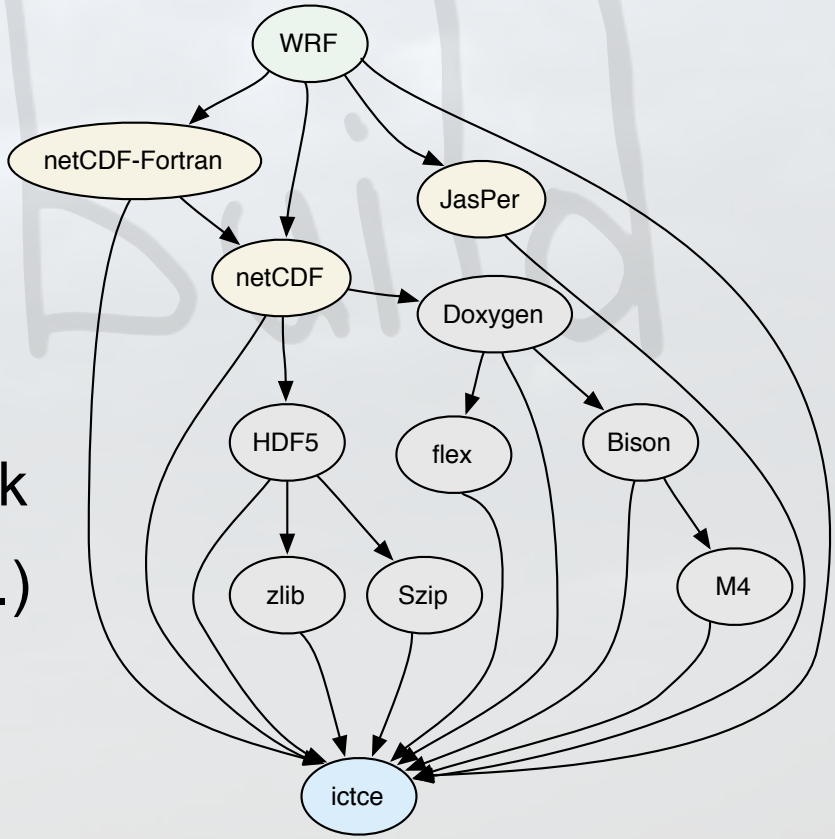
EasyBuild in practice: outline

- **Example use case**: an easyblock and easyconfig for WRF
- **Development workflow with git**: commit, pull request, ...
- Adding **support for accelerators** to EasyBuild
- Towards a more flexible **module naming scheme**
- **Hackathon** organization: task forces
- **Agenda** for the coming days

Example use case (1/2)

*building and installing **WRF** (Weather Research and Forecasting Model)*

- *http://www.wrf-model.org*
- complex(ish) **dependency graph**
- very **non-standard build procedure**
  - interactive `configure` script (!)
  - resulting `configure.wrf` needs work
    (hardcoding, tweaking of options, ...)
  - `compile` script (wraps around `make`)
  - no actual installation step



Example use case (2/2)

*building and installing **WRF** (Weather Research and Forecasting Model)*

- easyblock that comes with EasyBuild implements build procedure
  - running `configure` script **autonomously**
  - **building** with `compile` and **patching** configure.wrf
  - **testing** build with standard included tests/benchmarks
- various example easyconfig files available
  different versions, toolchains, build options, ...
- building and installing WRF becomes child's play, for example:

```
eb --software=WRF,3.4 --toolchain-name=ictce --robot
```

Use case: WRF - easyblock (1/3)

imports, class constructor,
custom easyconfig parameter

```
1  import fileinput, os, re, sys
2
3  import easybuild.tools.environment as env
4  from easybuild.easyblocks.netcdf import set_netcdf_env_vars
5  from easybuild.framework.easyblock import EasyBlock
6  from easybuild.framework.easyconfig import MANDATORY
7  from easybuild.tools.filetools import patch_perl_script_autoflush, run_cmd, run_cmd_qa
8  from easybuild.tools.modules import get_software_root
9
10 class EB_WRF(EasyBlock):
11
12   def __init__(self, *args, **kwargs):
13     super(EB_WRF, self).__init__(*args, **kwargs)
14     self.build_in_installdir = True
15
16   @staticmethod
17   def extra_options():
18     extra_vars = [('buildtype', [None, "Type of build (e.g., dmpar, dm+sm).", MANDATORY])]
19     return EasyBlock.extra_options(extra_vars)
20
```

import required functionality

class definition

class constructor, specify building in installation dir

define custom easyconfig parameters

Use case: WRF - easyblock (2/3)

configuration (part 1/2)

```
21  def configure_step(self):
22    # prepare to configure
23    set_netcdf_env_vars(self.log)
24
25    jasper = get_software_root('JasPer')
26    if jasper:
27      jasperlibdir = os.path.join(jasper, "lib")
28      env.setvar('JASPERINC', os.path.join(jasper, "include"))
29      env.setvar('JASPERLIB', jasperlibdir)
30
31    env.setvar('WRFIO_NCD_LARGE_FILE_SUPPORT', '1')
32
33    patch_perl_script_autoflush(os.path.join("arch", "Config_new.pl"))
34
35    known_build_types = ['serial', 'smpar', 'dmpar', 'dm+sm']
36    self.parallel_build_types = ["dmpar", "smpar", "dm+sm"]
37    bt = self.cfg['buildtype']
38
39    if not bt in known_build_types:
40      self.log.error("Unknown build type: '%s' (supported: %s)" % (bt, known_build_types))
41
```

configuration step function

set environment variables for dependencies

set WRF-specific env var for build options

patch configure script to run it autonomously

check whether specified build type makes sense

Use case: WRF - easyblock (2/3)

configuration (part 2/2)

```
42      # run configure script
43      bt_option = "Linux x86_64 i486 i586 i686, ifort compiler with icc"
44      bt_question = "\s*(?P<nr>[0-9]+).\s*%s\s*\(%s\)" % (bt_option, bt)
45
46      cmd = "./configure"
47      qa = {"(1=basic, 2=preset moves, 3=vortex following) [default 1]:": "1",
48            "(0=no nesting, 1=basic, 2=preset moves, 3=vortex following) [default 0]:": "0"}
49      std_qa = {r"%s.*\n(.*\n)*Enter selection\s*\[[0-9]+-[0-9]+\]\s*:" % bt_question: "%(nr)s"}
50
51      run_cmd_qa(cmd, qa, no_qa=[], std_qa=std_qa, log_all=True, simple=True)
52
53      # patch configure.wrf
54      cfgfile = 'configure.wrf'
55
56      comps = {
57               'SCC': os.getenv('CC'), 'SFC': os.getenv('F90'),
58               'CCOMP': os.getenv('CC'), 'DM_FC': os.getenv('MPIF90'),
59               'DM_CC': "%s -DMPI2_SUPPORT" % os.getenv('MPICC'),
60              }
61
62      for line in fileinput.input(cfgfile, inplace=1, backup='.orig.comps'):
63          for (k, v) in comps.items():
64              line = re.sub(r"^(%s\s*=\s*).*$" % k, r"\1 %s" % v, line)
65          sys.stdout.write(line)
66
```

prepare Q&A for configuring

run configure script autonomously

patch generated configuration file

Use case: WRF - easyblock (3/3)

build step & skip install step (since there is none)

build step function

```
67  def build_step(self):
68    # build WRF using the compile script
69    par = self.cfg['parallel']
70    cmd = "./compile -j %d wrf" % par
71    run_cmd(cmd, log_all=True, simple=True, log_output=True)
72
73    # build two test cases to produce ideal.exe and real.exe
74    for test in ["em_real", "em_b_wave"]:
75        cmd = "./compile -j %d %s" % (par, test)
76        run_cmd(cmd, log_all=True, simple=True, log_output=True)
77
78  def install_step(self):
79    pass
80
```

build WRF (in parallel)

build WRF utilities as well

no actual installation step (build in installation dir)

Use case: installing WRF

specify build details in easyconfig file (.eb)

software name and version

compiler toolchain specification and options

custom parameter for WRF

```
1  name = 'WRF'
2  version = '3.4'
3
4  homepage = 'http://www.wrf-model.org'
5  description = 'Weather Research and Forecasting'
6
7  toolchain = {'name': 'ictce','version': '3.2.2.u3'}
8  toolchainopts = {'opt': False, 'optarch': False}
9
10 sources = ['%sV%s.TAR.gz' % (name, version)]
11 patches = ['WRF_parallel_build_fix.patch',
12            'WRF-3.4_known_problems.patch',
13            'WRF_tests_limit-runtimes.patch',
14            'WRF_netCDF-Fortran_separate_path.patch']
15
16 dependencies = [('JasPer', '1.900.1'),
17                 ('netCDF', '4.2'),
18                 ('netCDF-Fortran', '4.2')]
19
20 buildtype = 'dmpar'
```

software website and description (informative)

list of source files

list of patches for sources

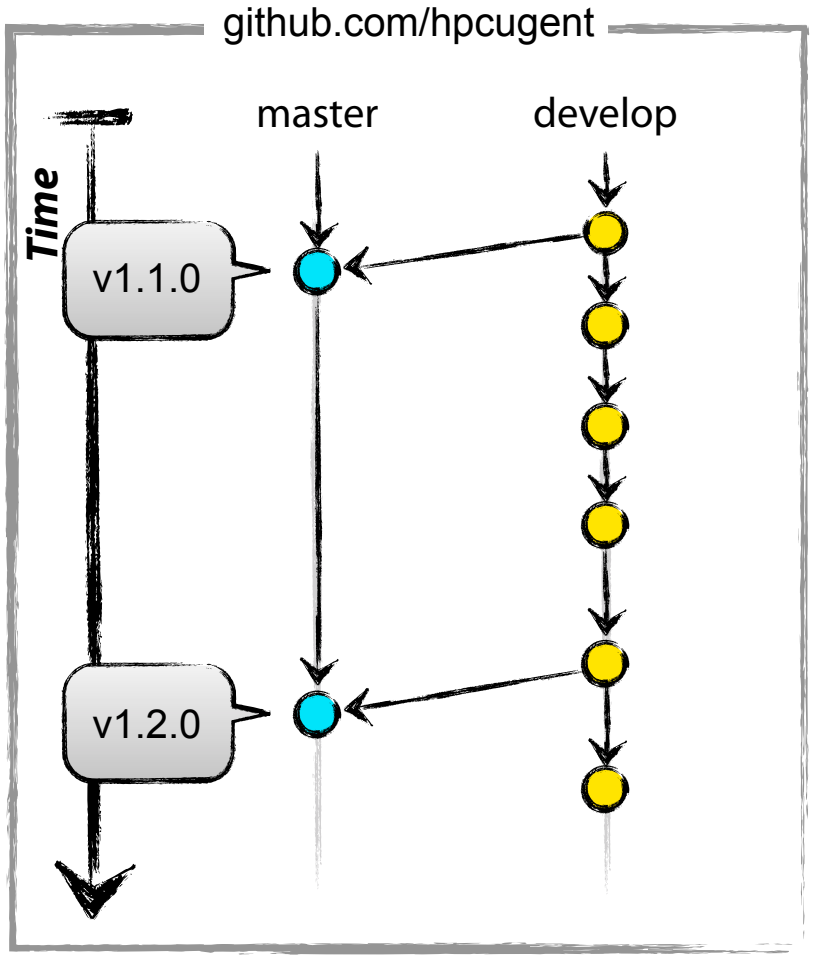
list of dependencies

```
eb WRF-3.4-ictce-3.2.2.u3-dmpar.eb --robot
```

Development workflow with git

Setting up

fork repository on GitHub,
and clone a working copy

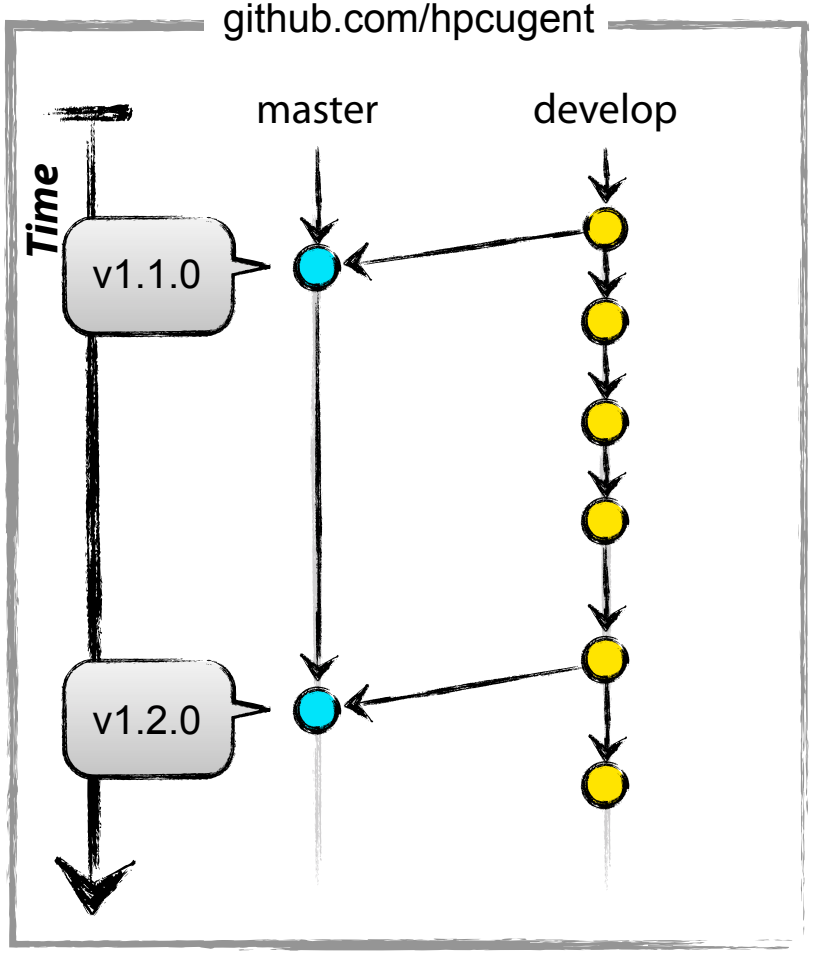


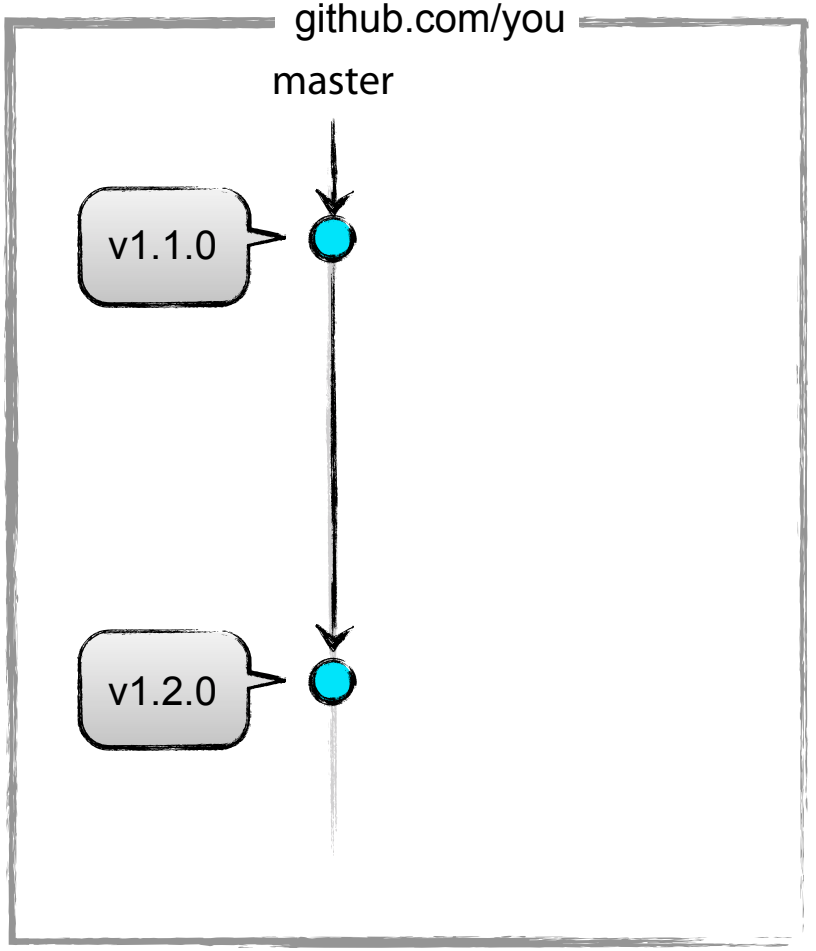
Development workflow with git

Setting up

fork repository on GitHub,
and clone a working copy


```
git clone git://github.com/you/reponame
```



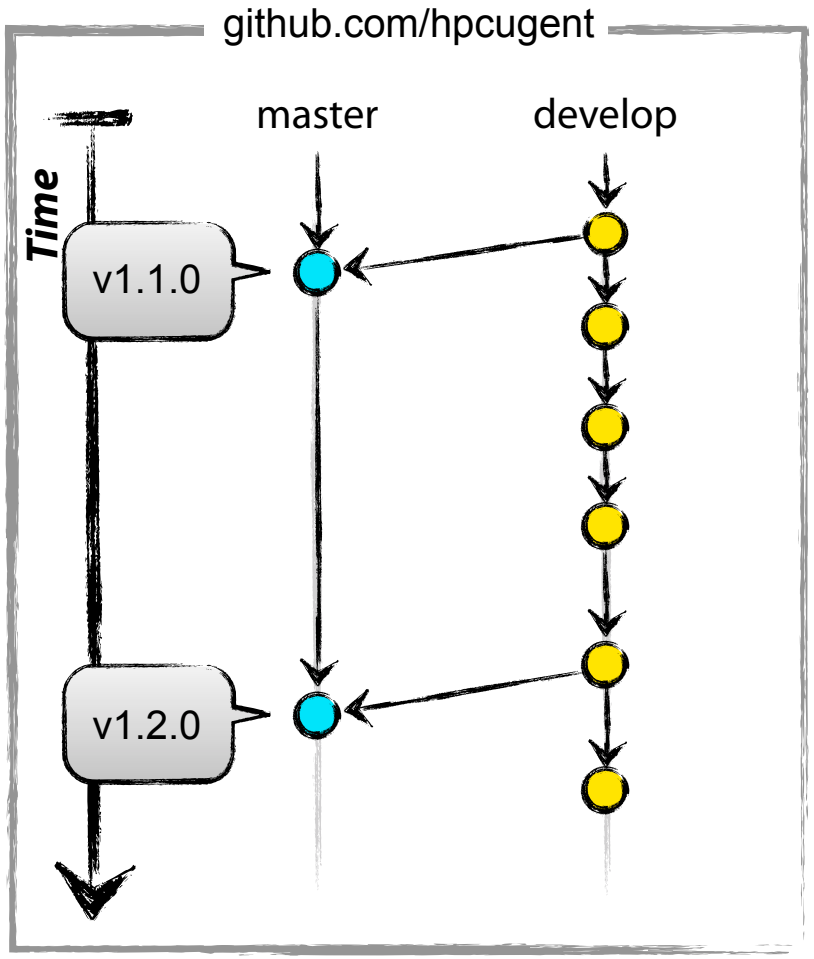


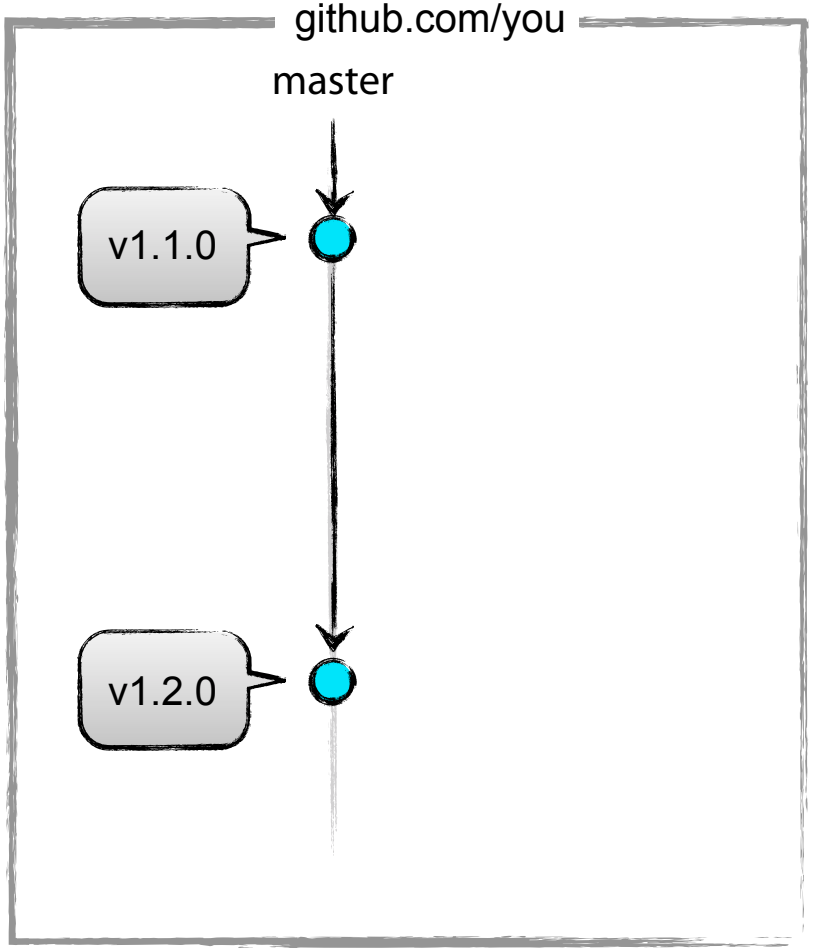
Development workflow with git

Setting up

define upstream remote repository

```
git remote add upstream
   git://github.com/hpcugent/reponame
```





Development workflow with git

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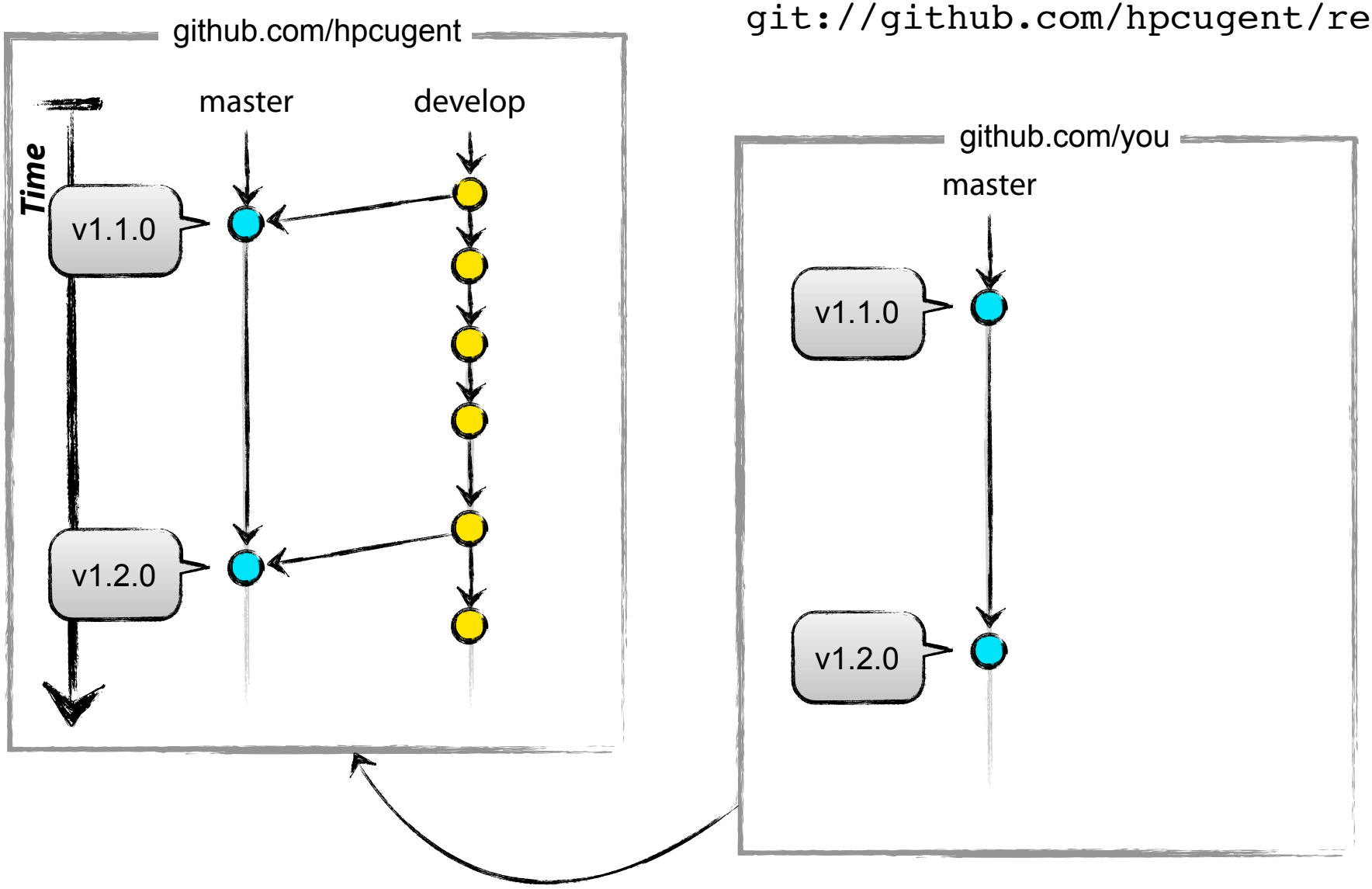
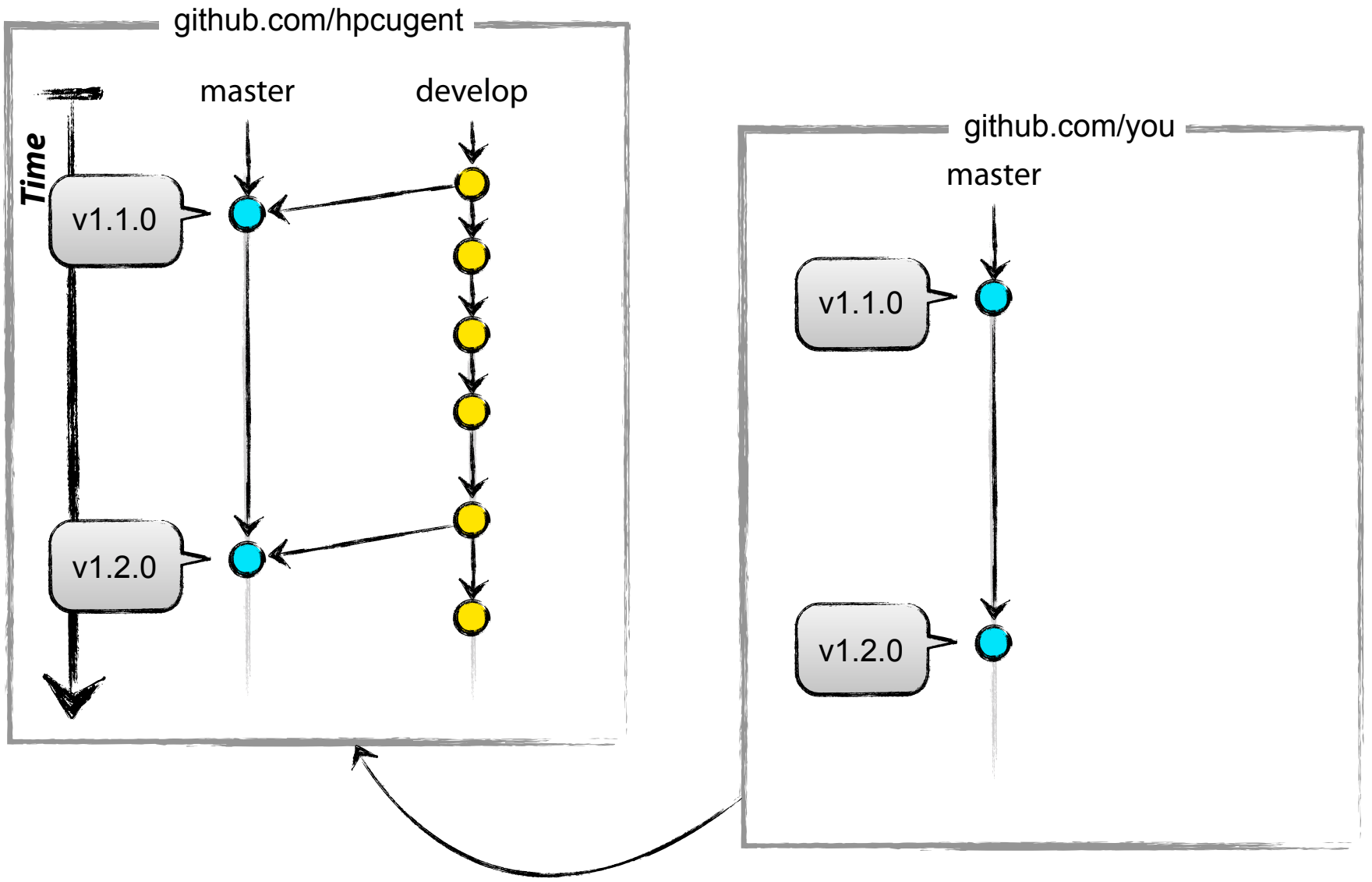


Development workflow with git

Setting up

pull in *develop* branch

```
git checkout -b develop
git pull upstream develop
```

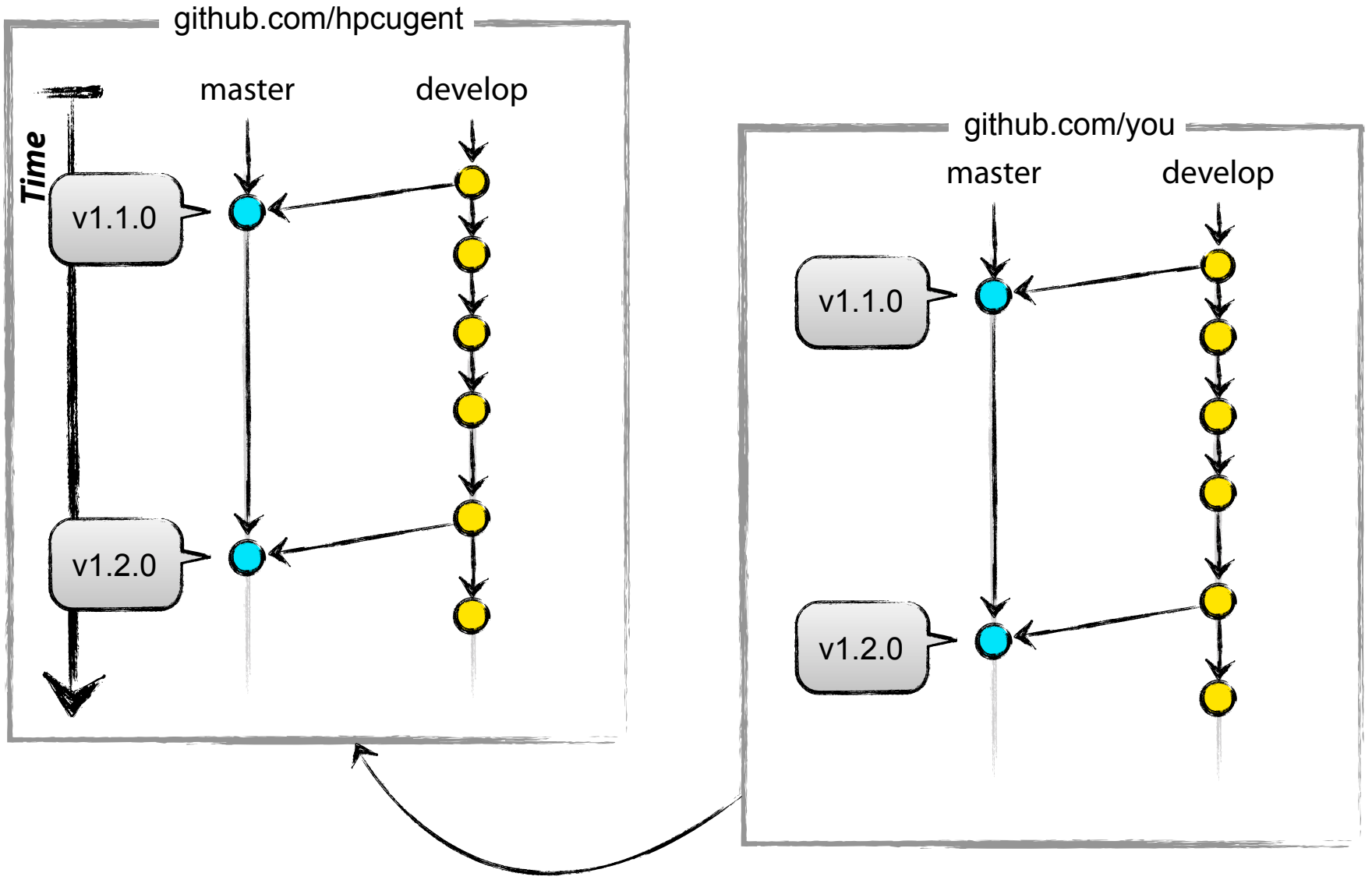


Development workflow with git

Setting up

pull in *develop* branch

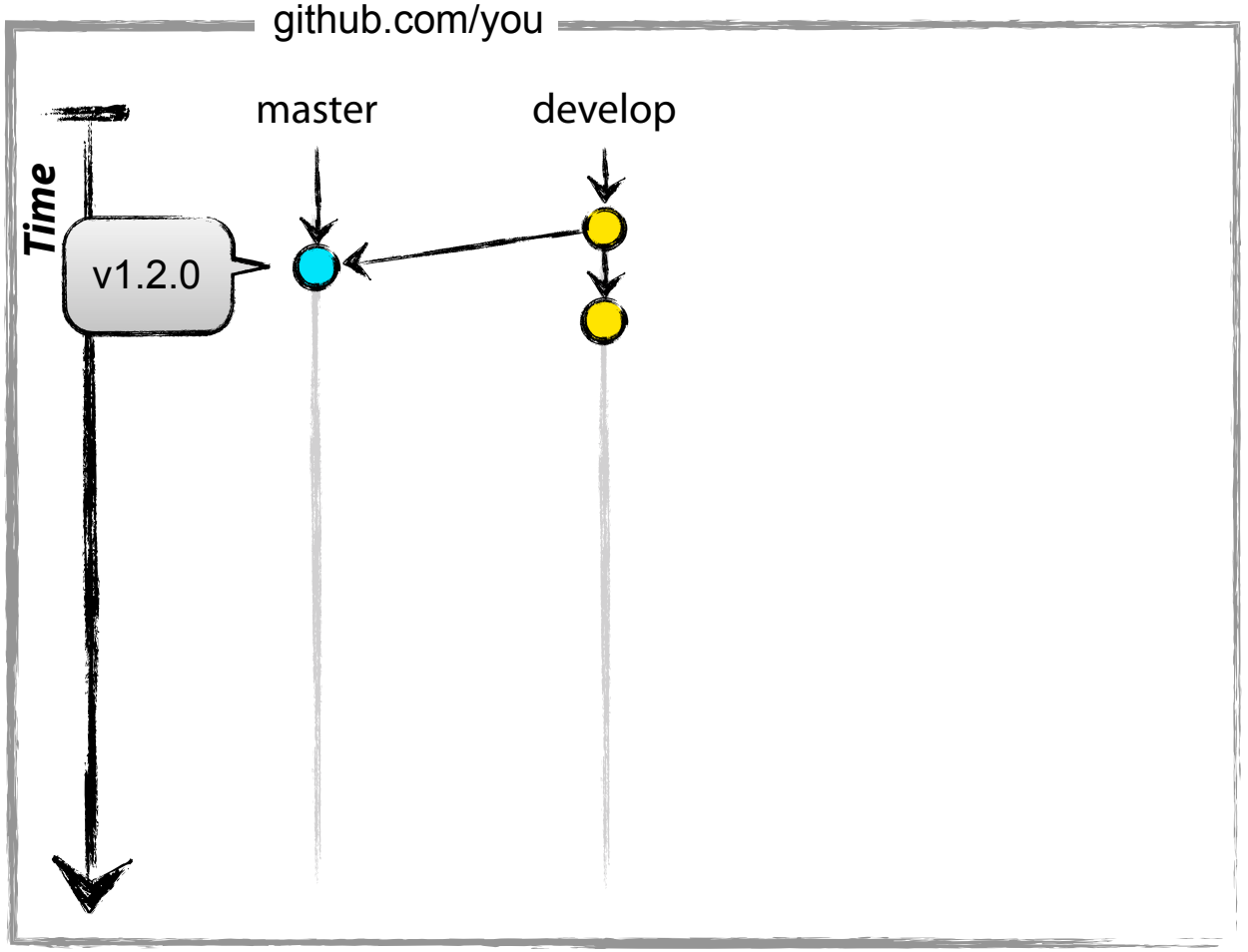
```
git checkout -b develop
git pull upstream develop
```



Development workflow with git

Implementing a feature

create a feature branch

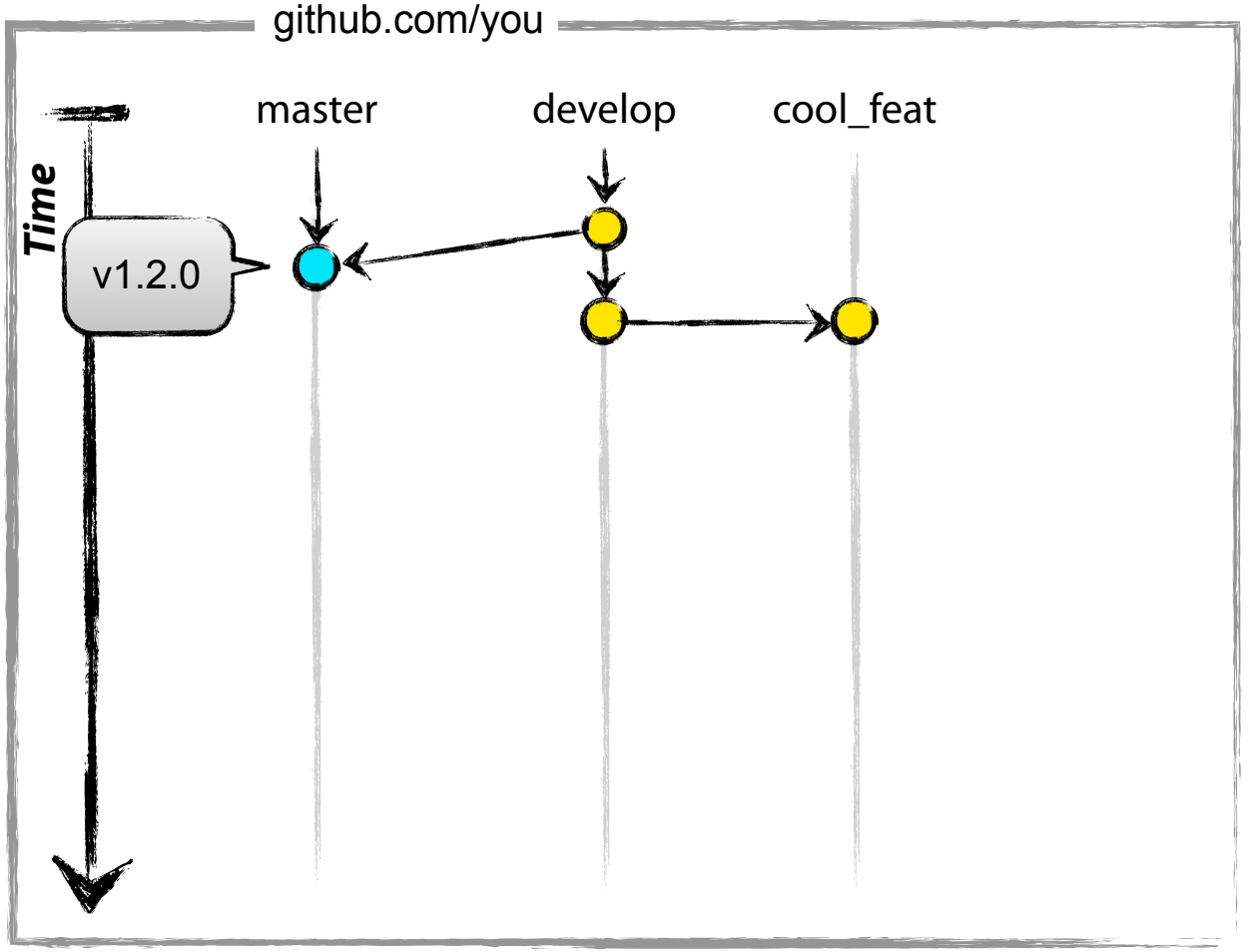


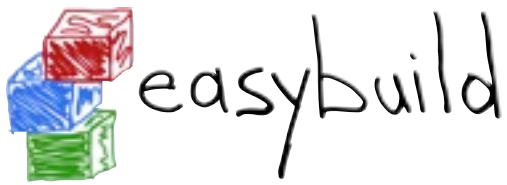
Development workflow with git

Implementing a feature

create a feature branch

```
git checkout develop
git branch cool_feat
git checkout cool_feat
```

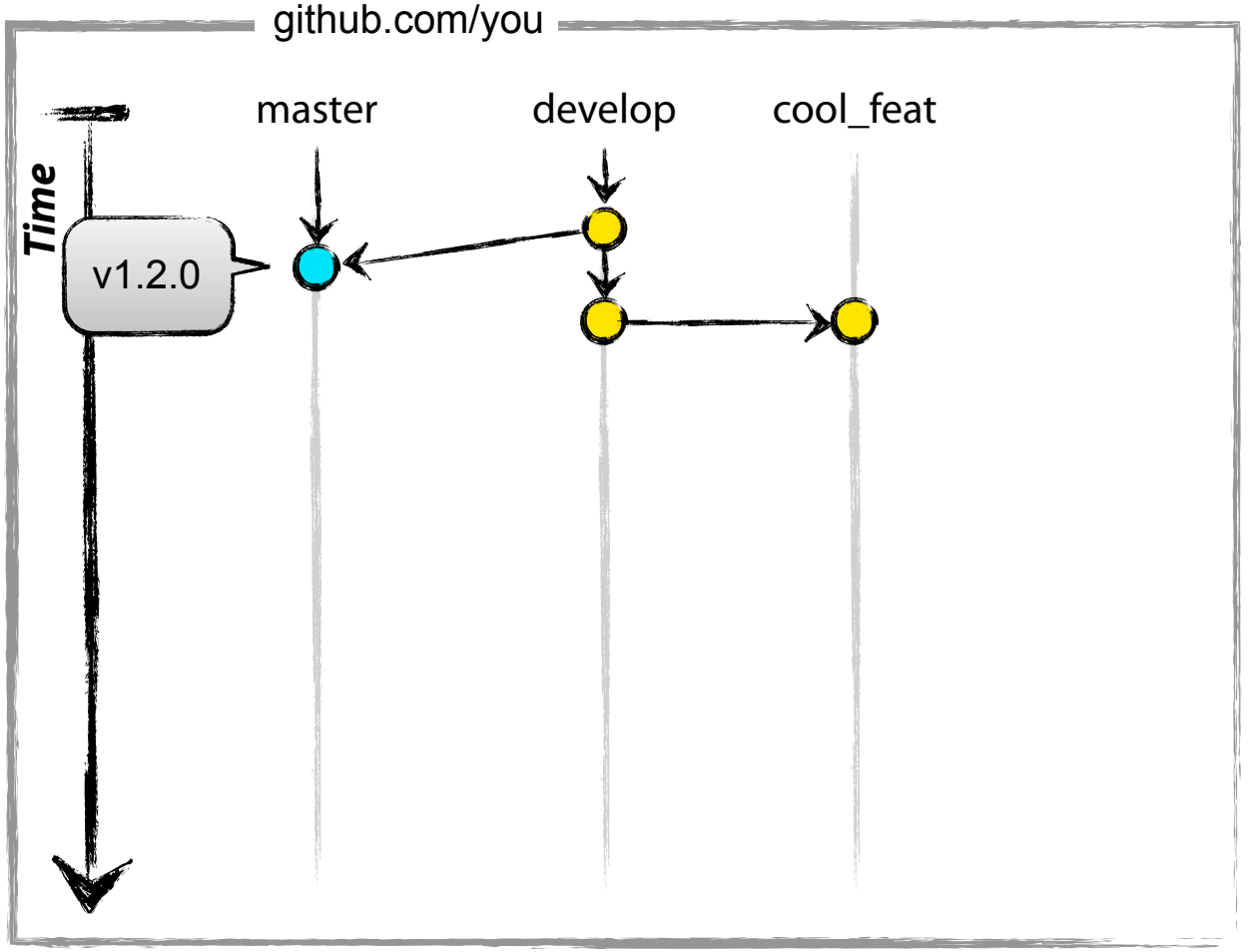




Development workflow with git

Implementing a feature

adjust code, stage and commit

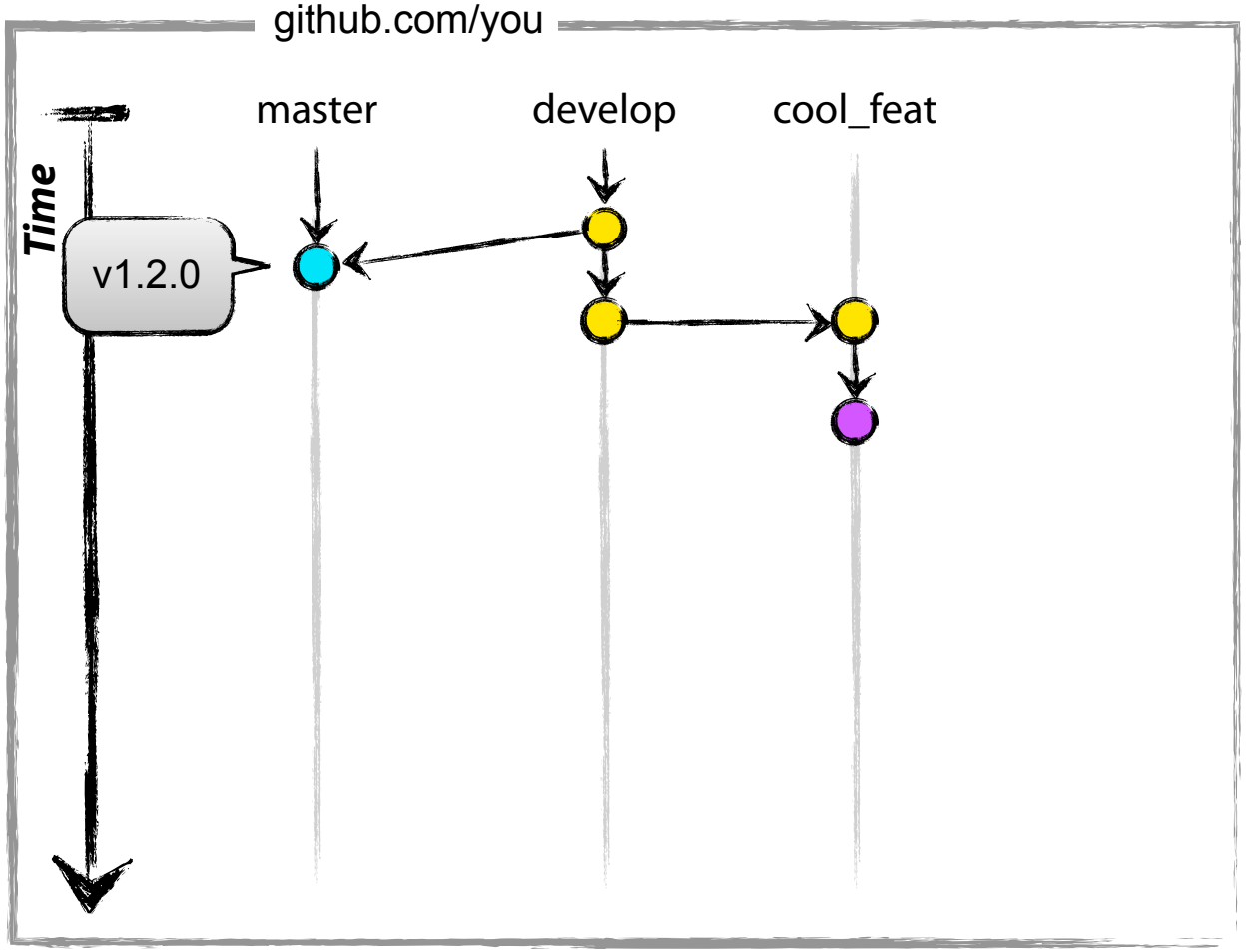


Development workflow with git

Implementing a feature

adjust code, stage and commit

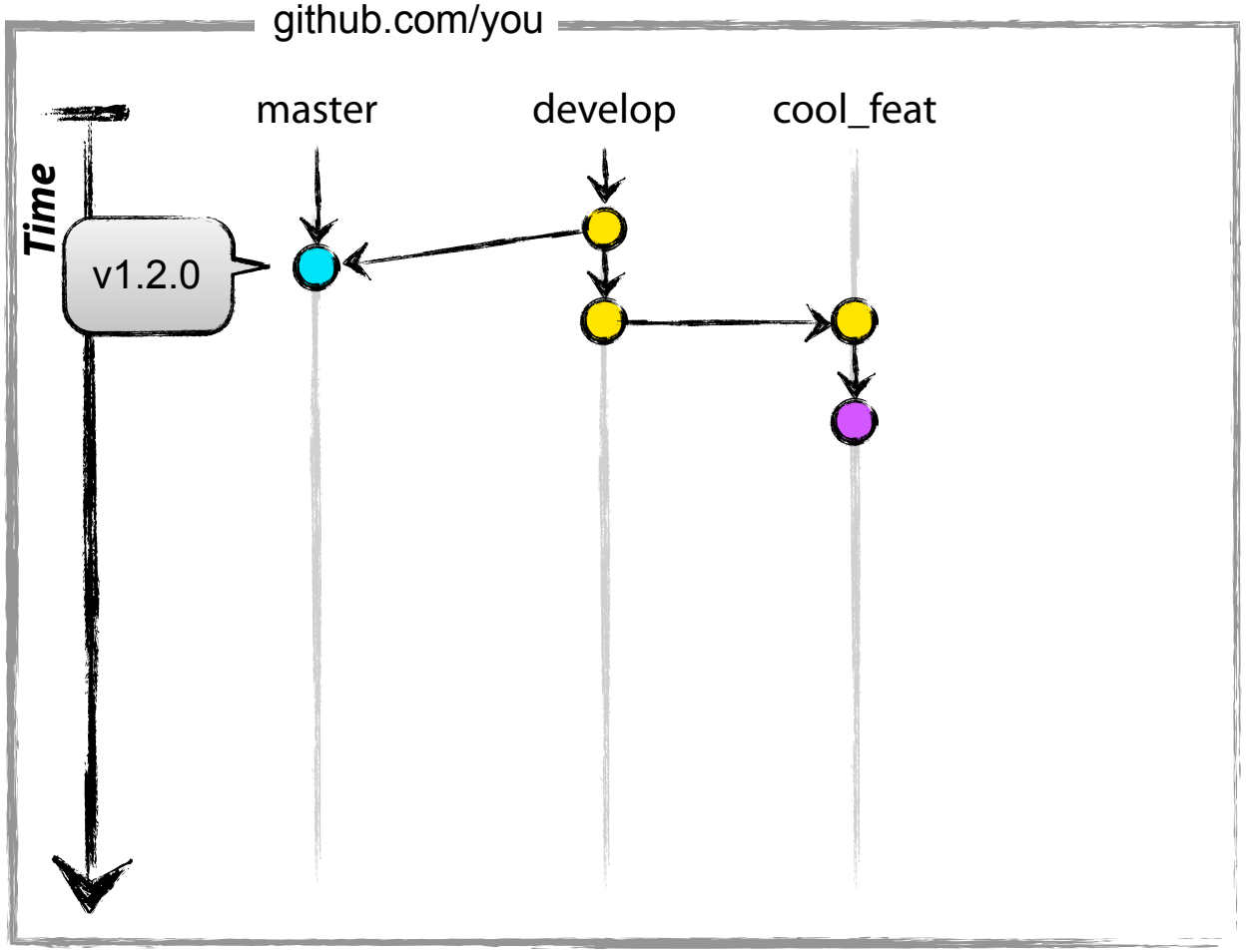
```
vim code.py
git add code.py
git commit -m “new stuff”
```



Development workflow with git

Implementing a feature

adjust code, stage and commit,
and fix that bug

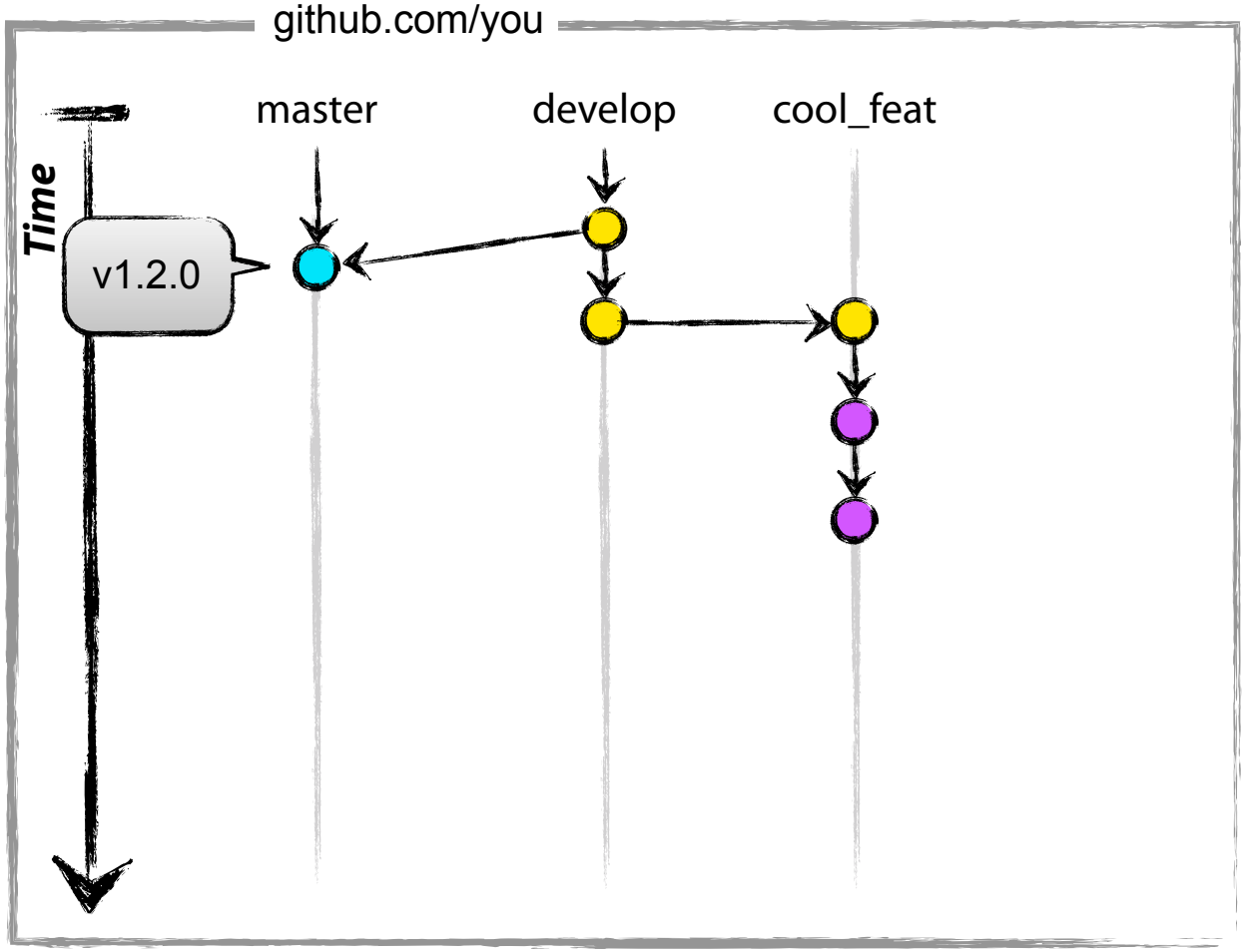


Development workflow with git

Implementing a feature

adjust code, stage and commit, and fix that bug

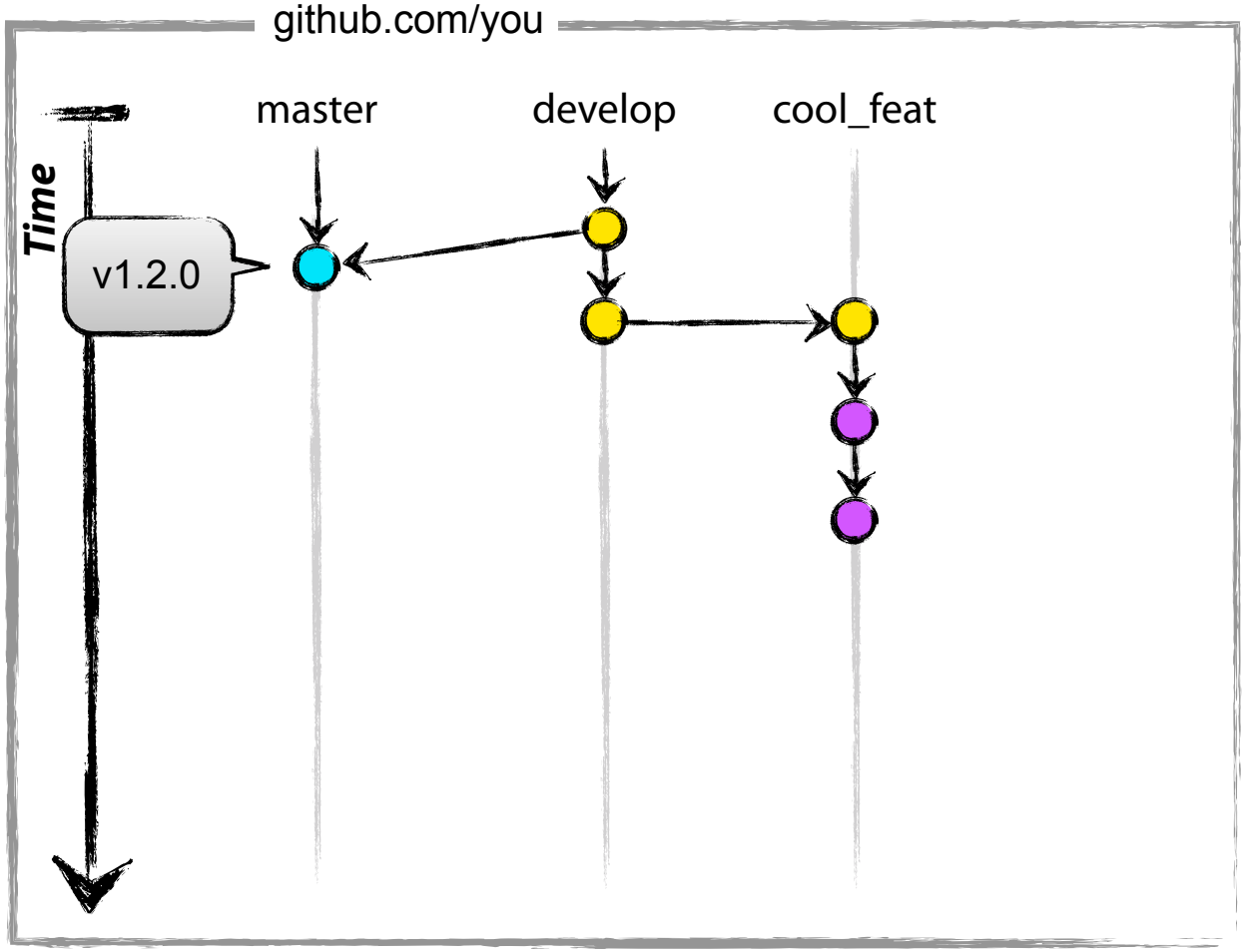
```
vim code.py
git add code.py
git commit -m “bugfix”
```



Development workflow with git

Implementing a feature

adjust code, stage and commit,
and fix that bug, and the typo too

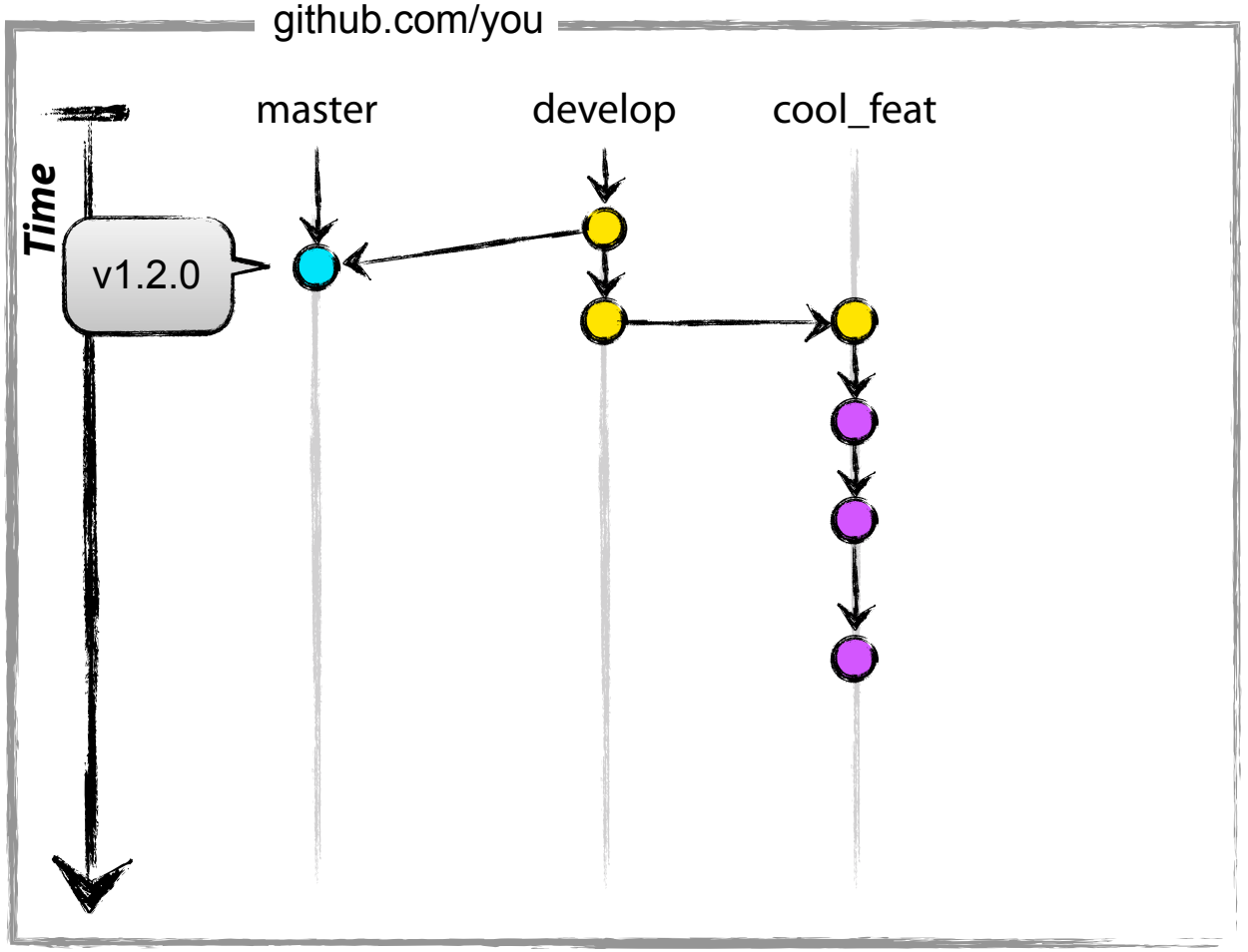


Development workflow with git

Implementing a feature

adjust code, stage and commit,
and fix that bug, and the typo too

```
vim code.py
git add code.py
git commit -m “typo (grr)”
```

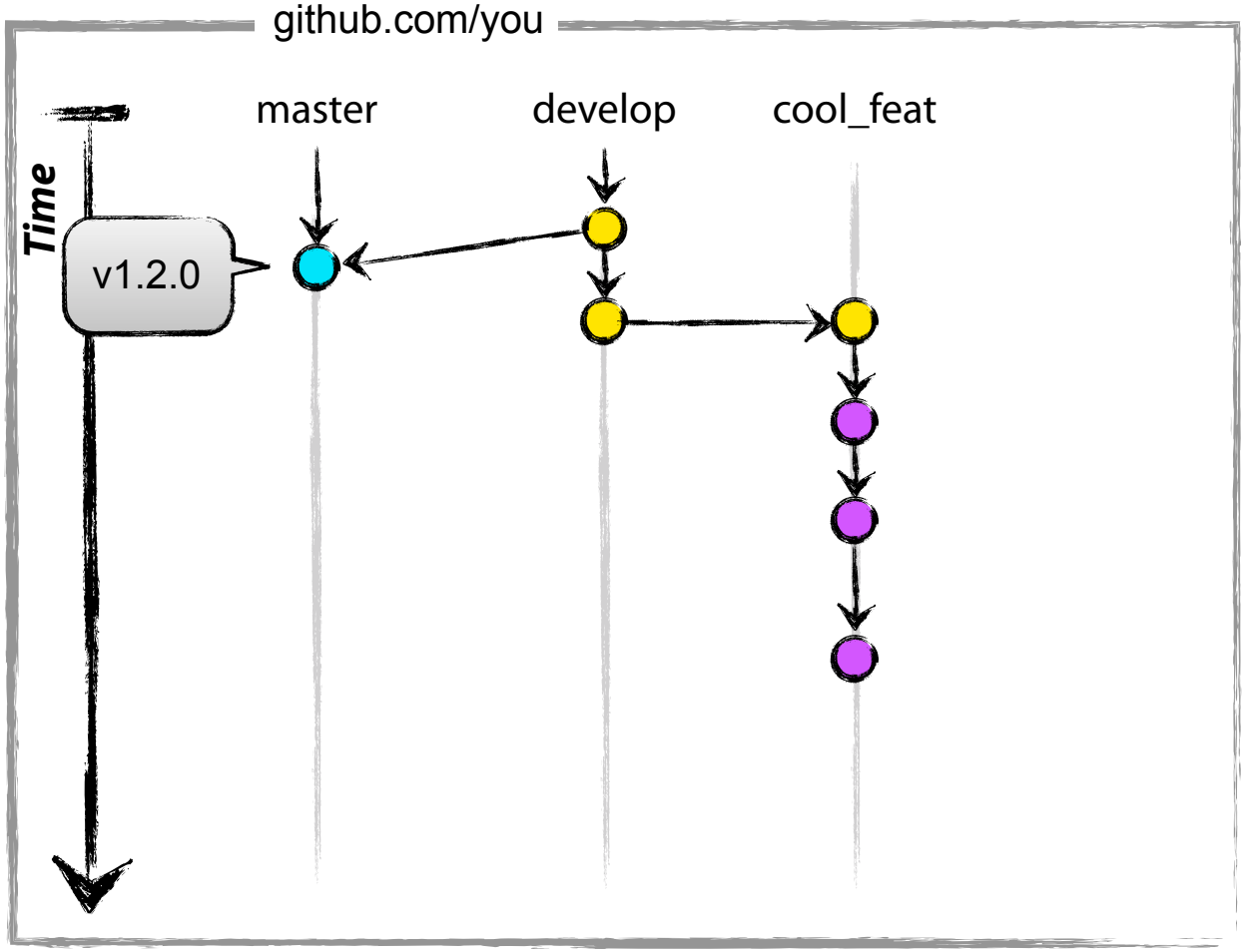


Development workflow with git

Contribute back!

push your feature branch
to your repository

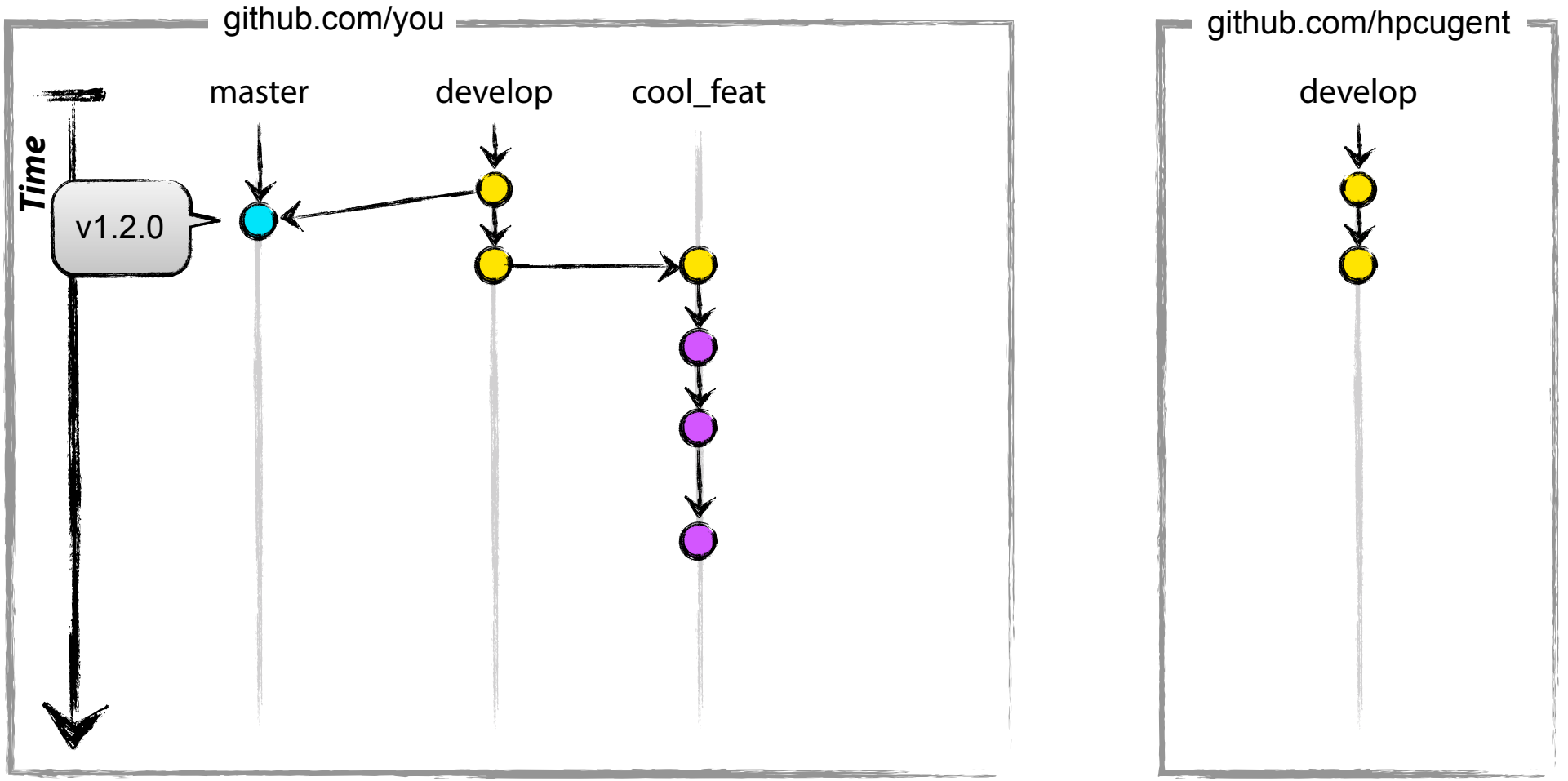
```
git push origin cool_feat
```



Development workflow with git

Contribute back!

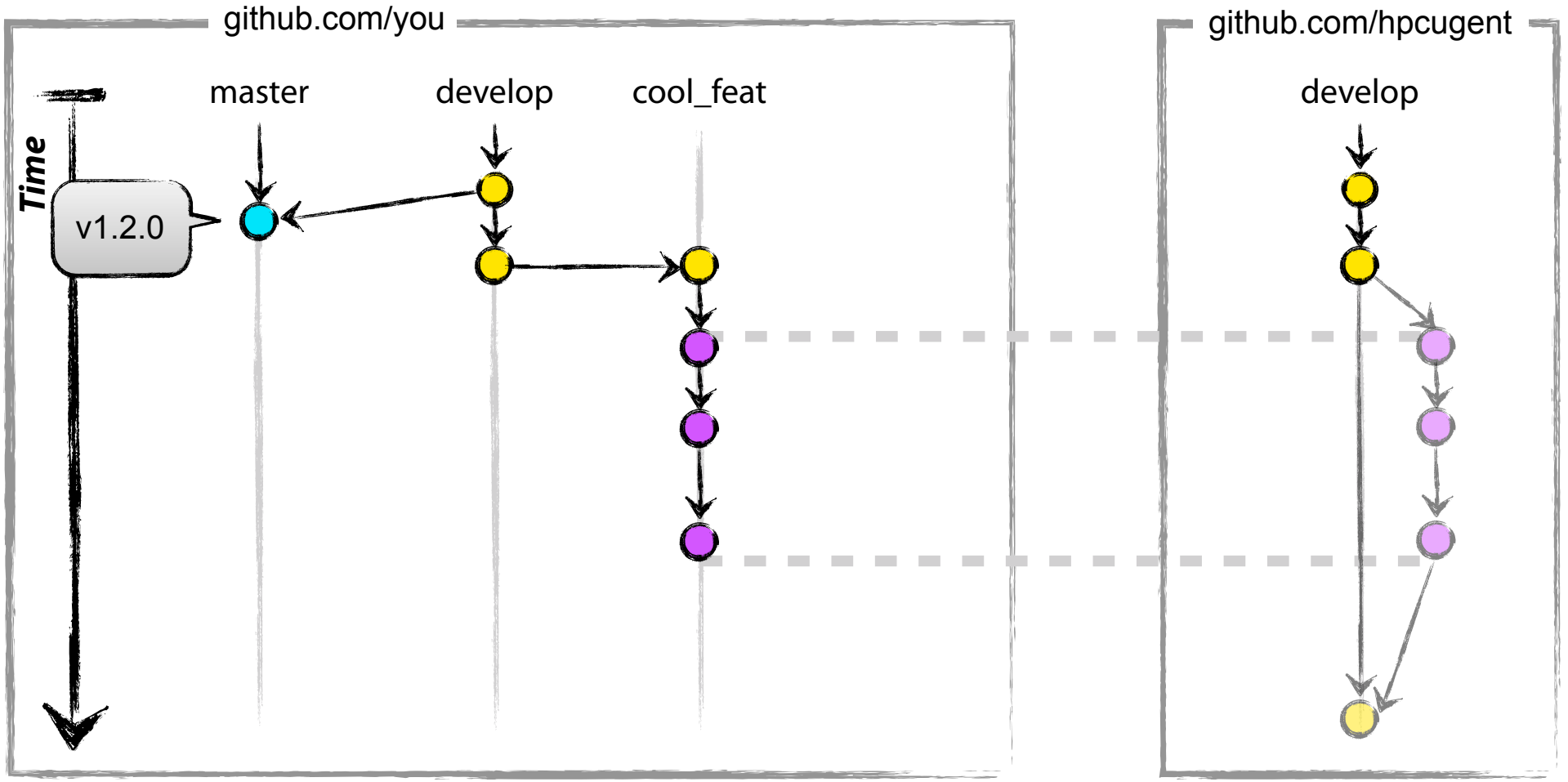
create a pull request via GitHub



Development workflow with git

Contribute back!

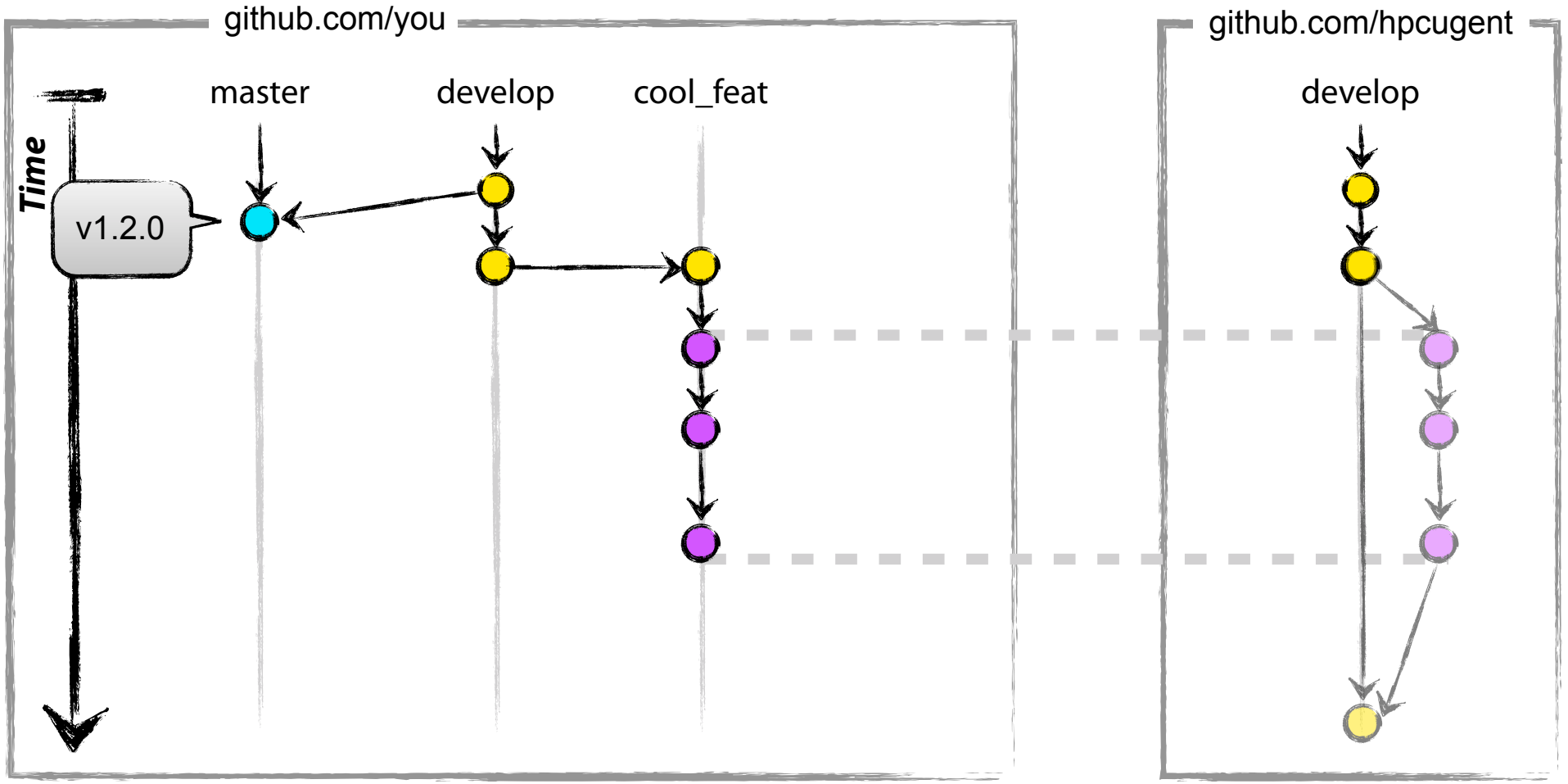
create a pull request via GitHub



Development workflow with git

Contribute back!

await code review, fix remarks



Development workflow with git

Contribute back!

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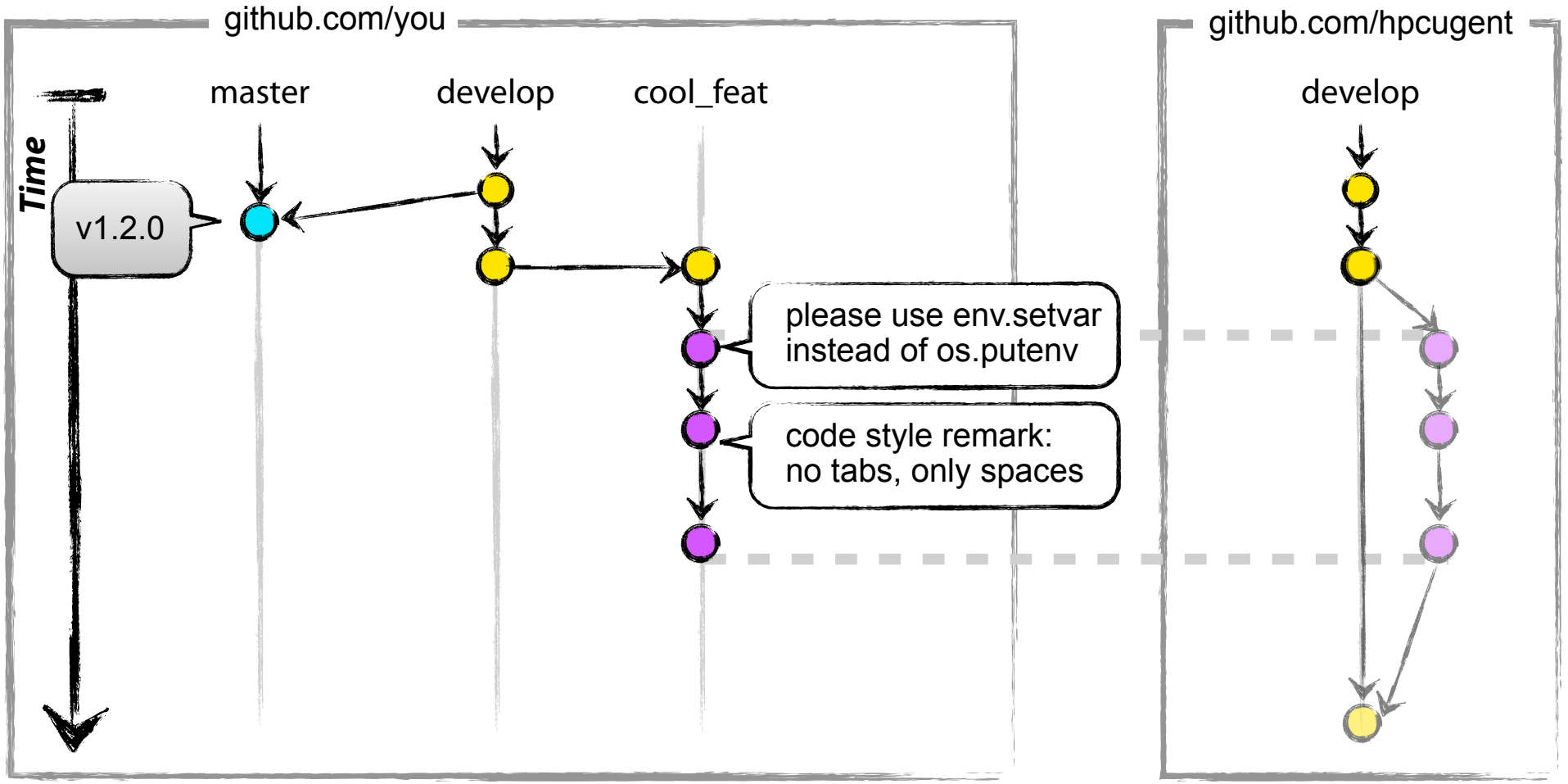
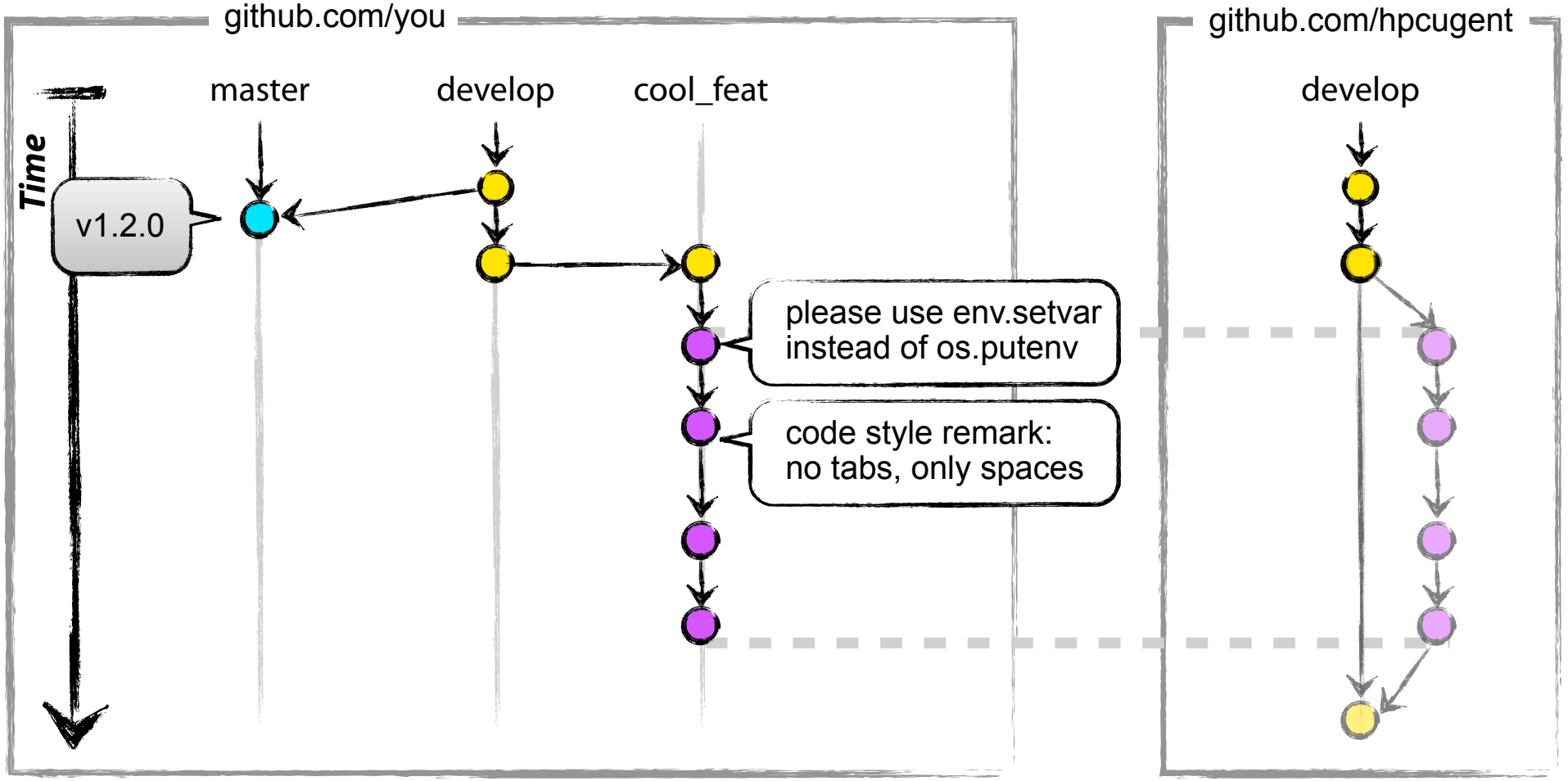


Development workflow with git

Contribute back!

await code review, fix remarks

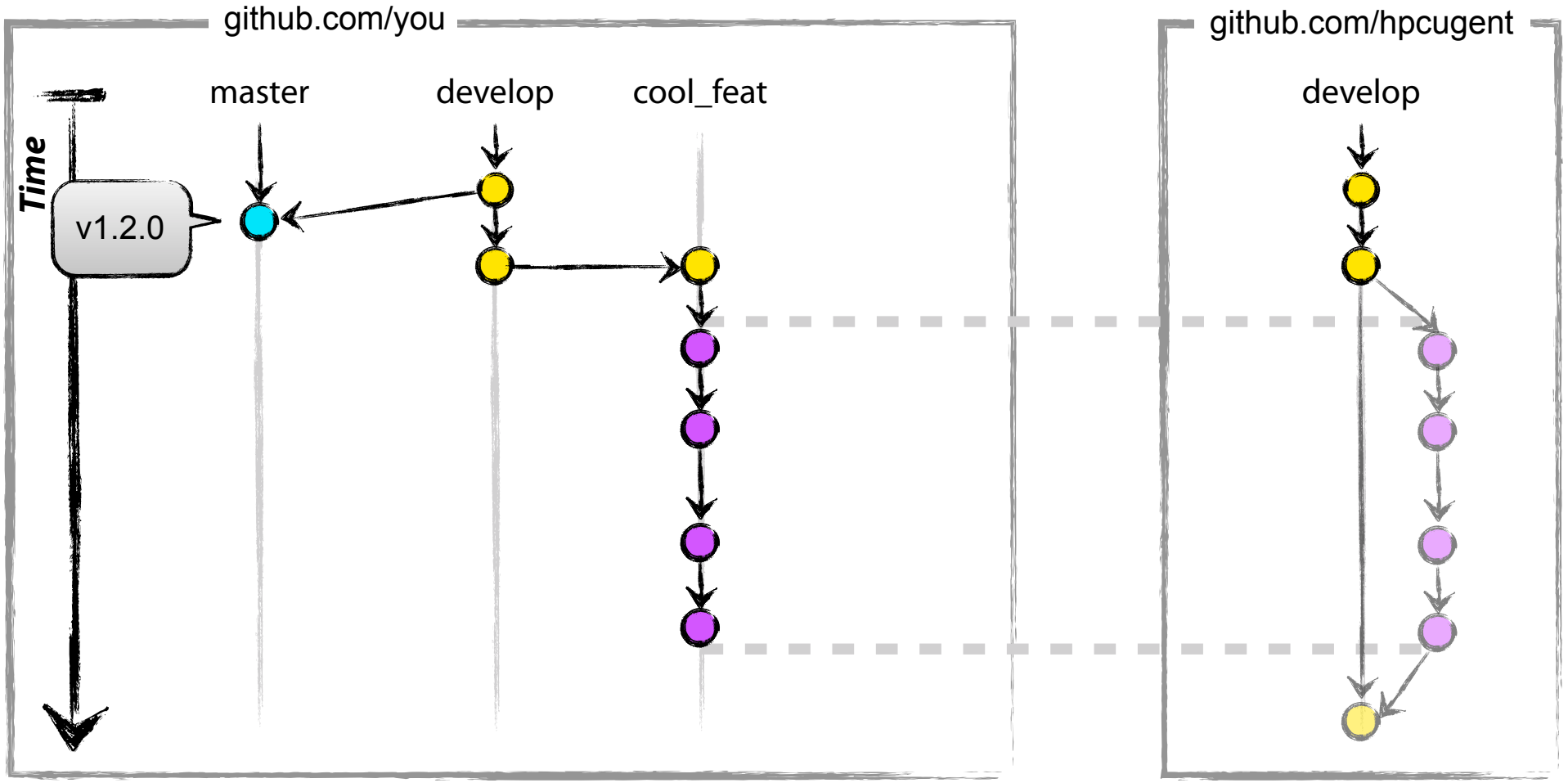
```
vim code.py
git add code.py
git commit -m “fixed remarks”
git push origin cool_feat
```



Developing workflow with git

Contribute back!

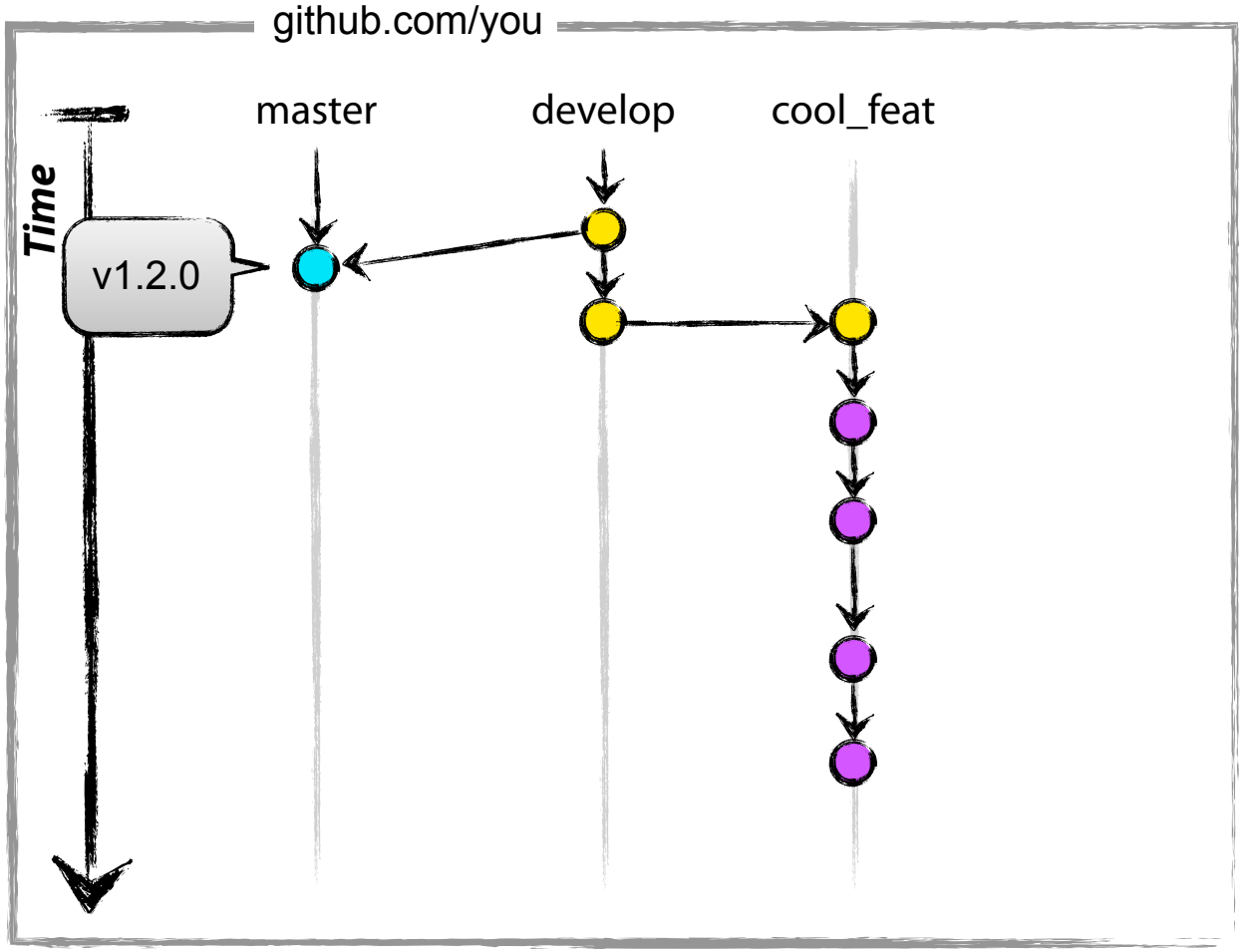
await the merge, update,
and clean up

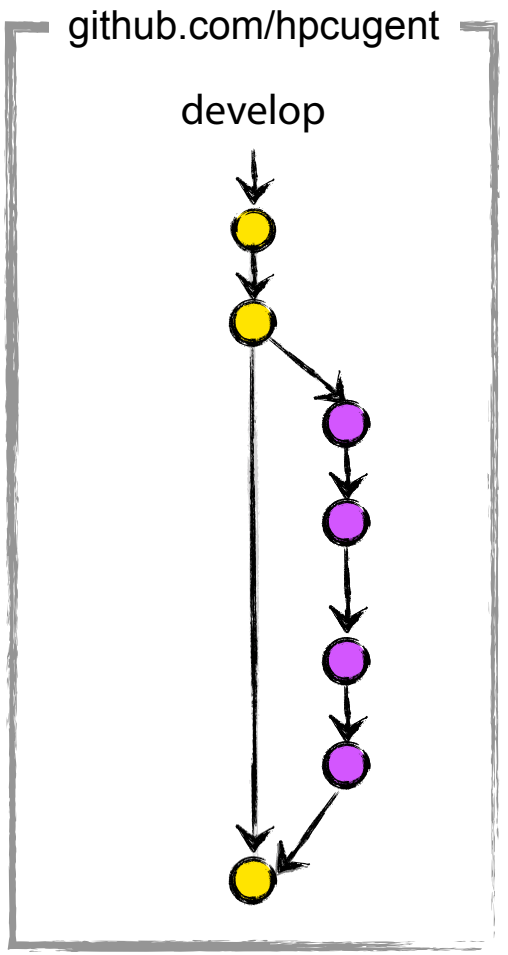


Developing workflow with git

Contribute back!

await the merge, update,
and clean up



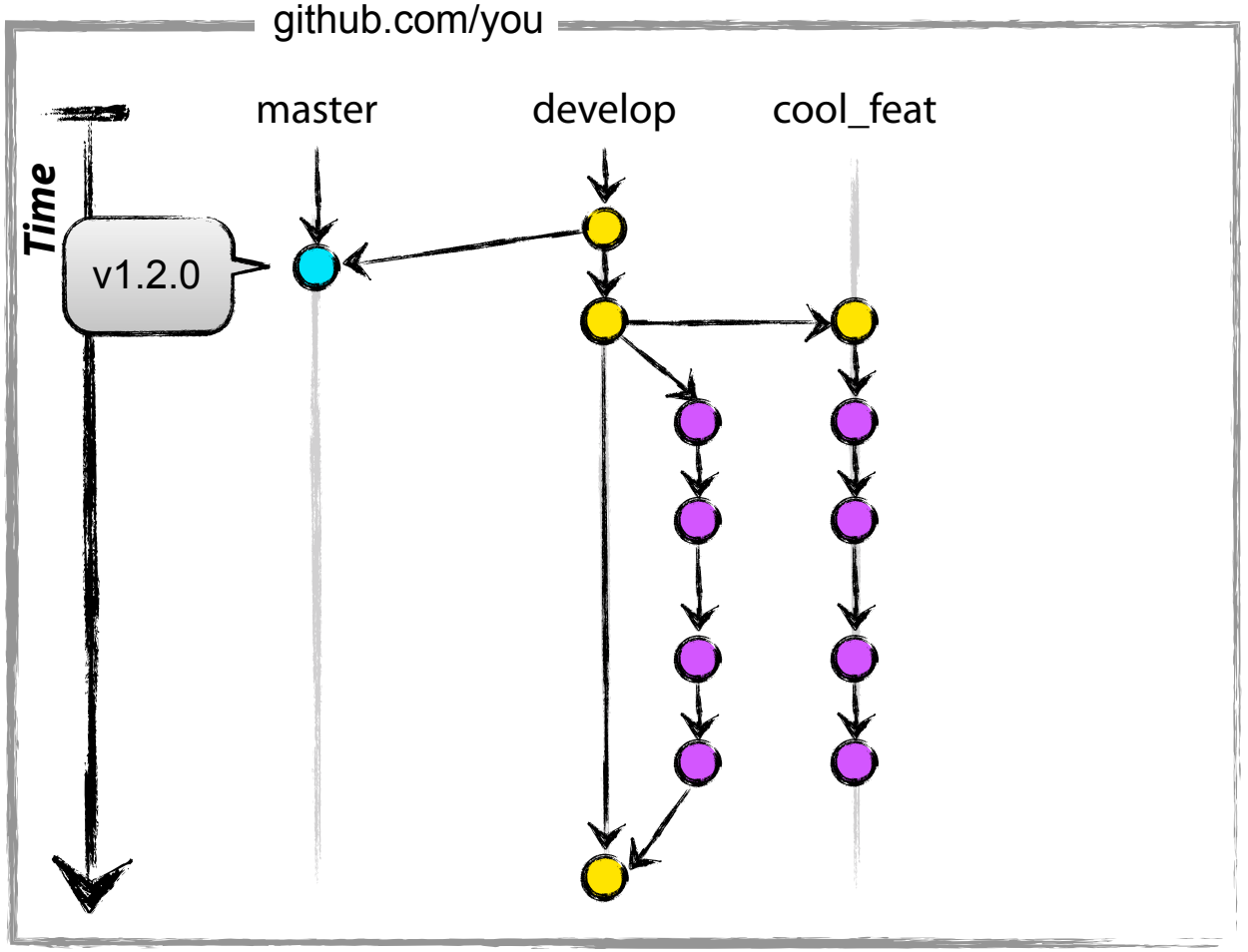


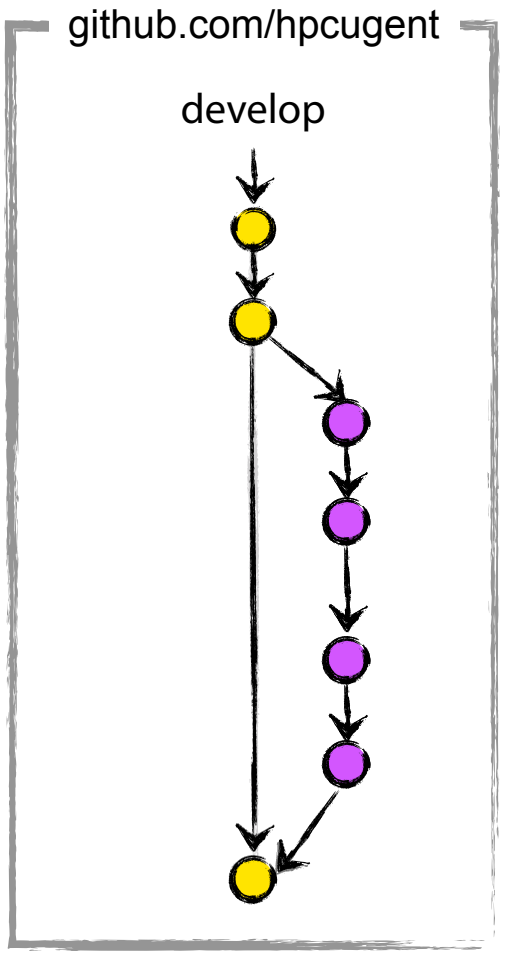
Developing workflow with git

Contribute back!

await the merge, update,
and clean up

```
git checkout develop
git pull upstream develop
```



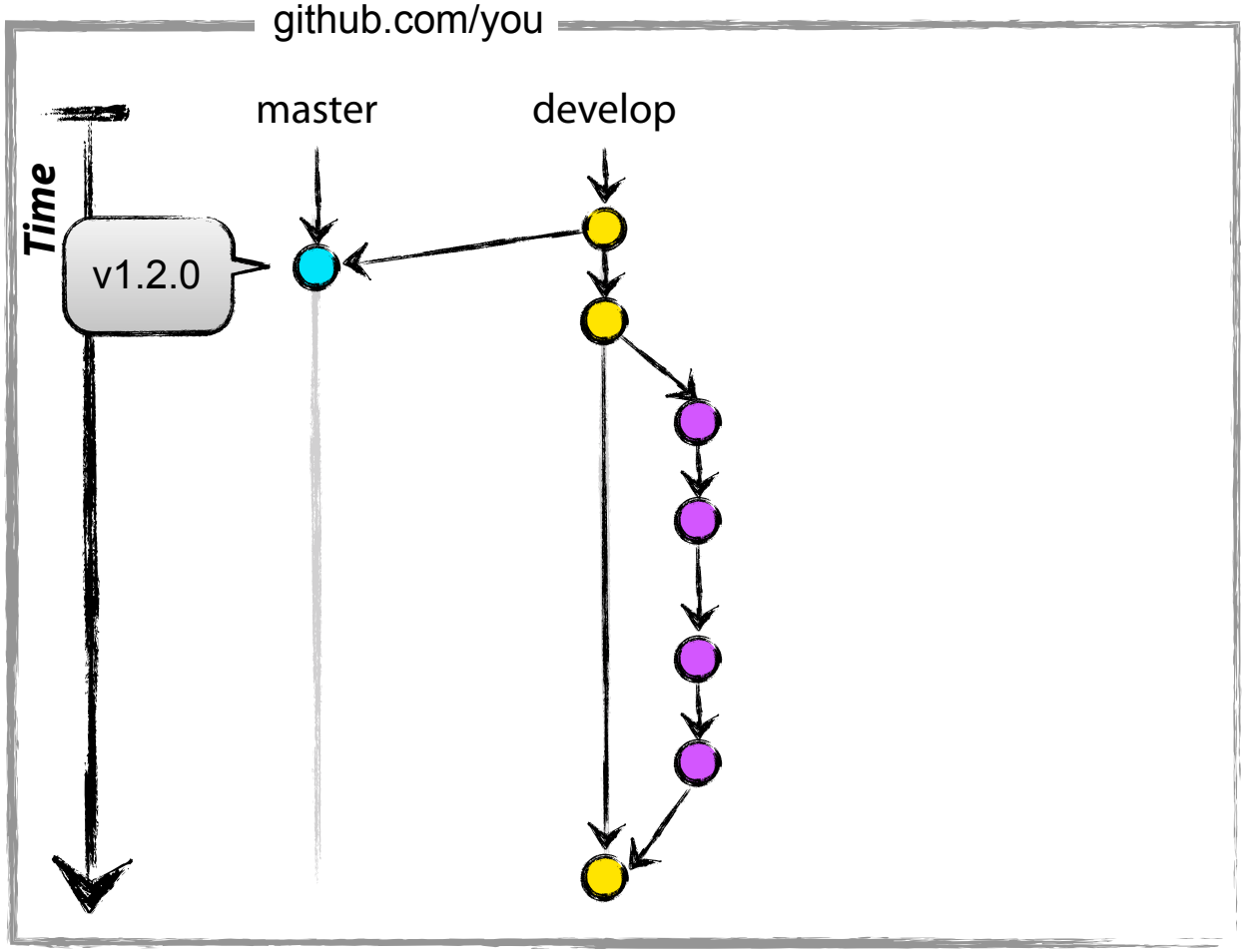


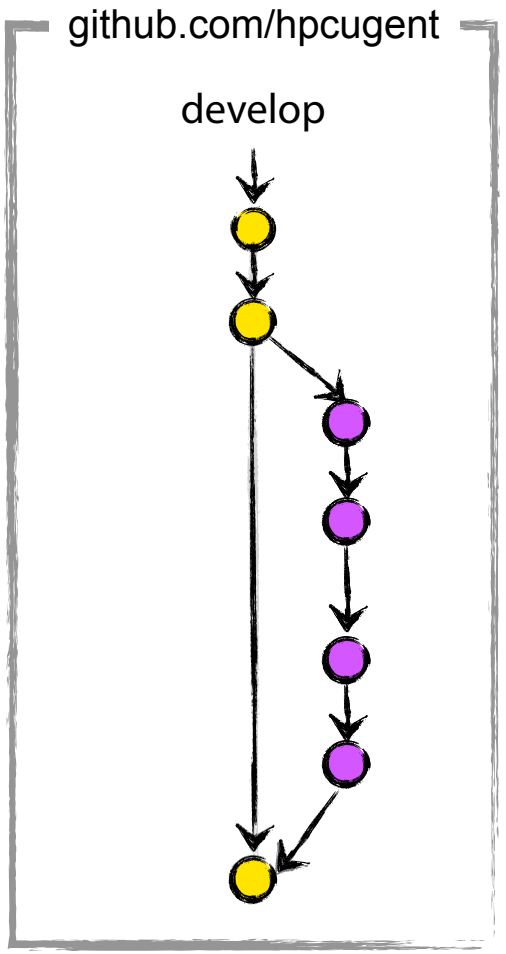
Developing workflow with git

Contribute back!

await the merge, update, and clean up

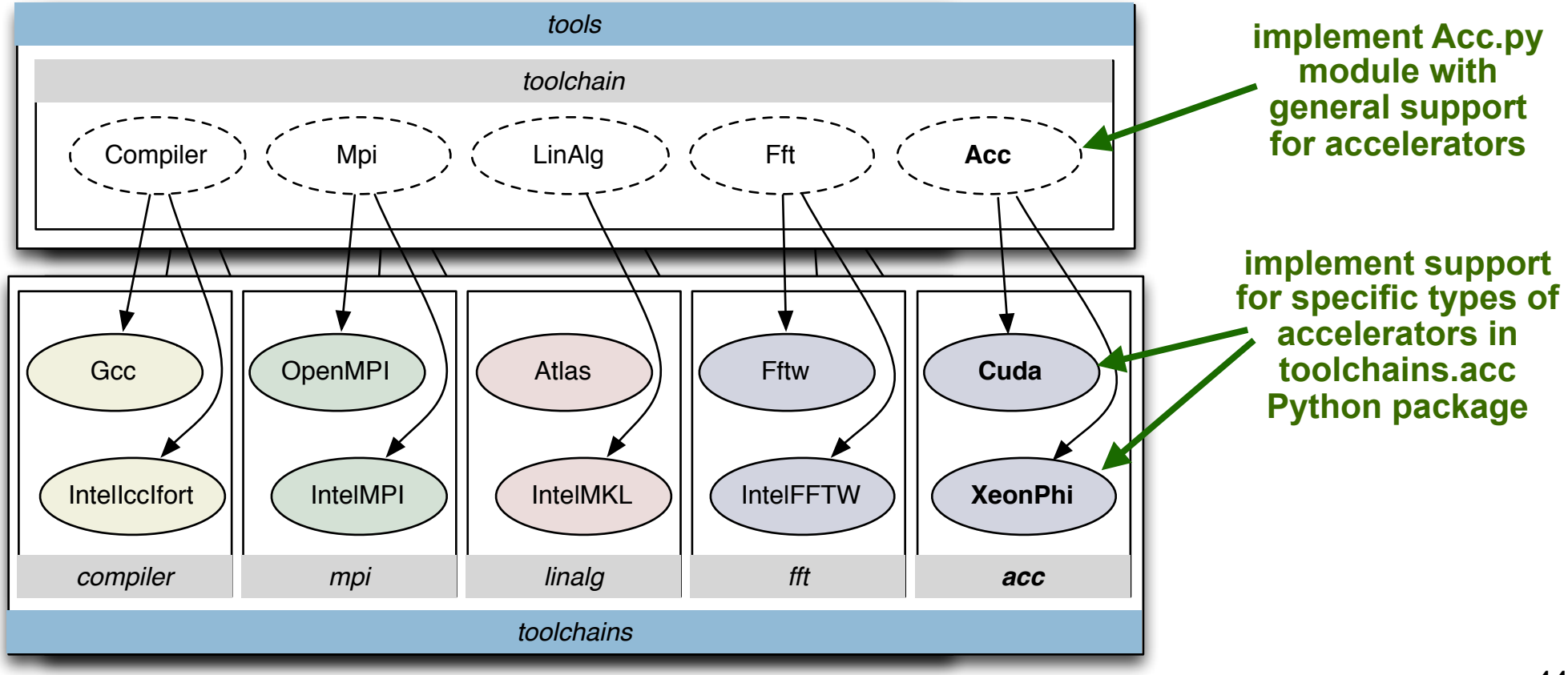
```
git checkout develop
git pull upstream develop
git branch -d cool_feat
```

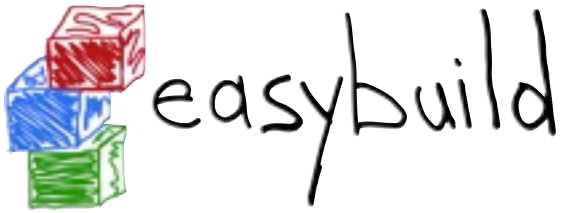




Adding support for accelerators

1. extend toolchain support in easybuild-framework
   - figure out what is needed (compiler commands, libraries, ...)
   - use implemented MPI support for inspiration





Adding support for accelerators

1. extend toolchain support in easybuild-framework
   - figure out what is needed (compiler commands, libraries, ...)
   - use implemented MPI support for inspiration
2. extend supported toolchain options

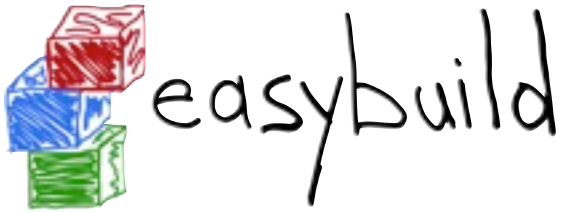
   for example:

```
toolchainopts = {'use_cuda': True}

toolchainopts = {'use_xeonphi': True}
```

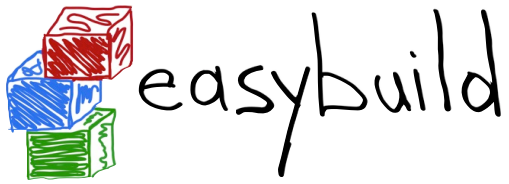
or

```
toolchainopts = {'with_acc': CUDA}
```



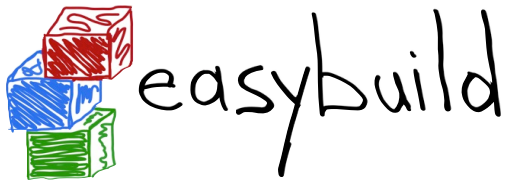
Adding support for accelerators

1. extend toolchain support in easybuild-framework
   - figure out what is needed (compiler commands, libraries, ...)
   - use implemented MPI support for inspiration
2. extend supported toolchain options
3. construct a CUDA-enabled toolchain
   - add support for installing CUDA with EasyBuild
   - add a toolchain definition and write an easyconfig file
     - e.g., ictce**c** (Intel tools + CUDA), goalf**c**, iomkl**c**, goolf**c**, ...
4. test, fix, commit, repeat



Module naming scheme
call for feedback

- currently still hard-wired in EasyBuild
  - more flexibility planned, to allow tailoring to site setup
- support for customisation hopefully by v1.3 (end of March)
- current status:
  - trying to understand what is needed
  - thinking about best way to incorporate this into current design
- most likely solution:
  - modular/object-oriented, just plug in a custom naming scheme
  - customization via self-defined ModuleNamingScheme (sub)class



Module naming scheme
call for feedback

flat (non-hierarhical) naming scheme

<name>/[verpre]**<version>**[-<tcname-tcver>][<versuf>]

Examples:

GCC/4.6.3

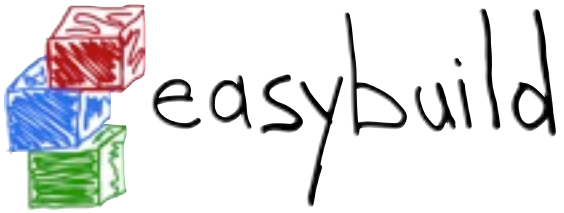
ictce/4.0.6

bzip2/1.0.6-ictce-4.0.6

WRF/3.4.1-iqacml-3.7.3-dmpar

How does your module naming scheme look like?

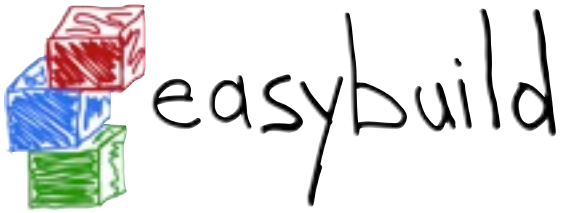
What does EasyBuild need to support?



Hackathon task forces

- accelerator support in the EasyBuild framework
- easyconfigs/easyblocks for software of interest
  - GPGPU software (see NVIDIA notes on wiki)
  - open issues: PRACE software, OpenBLAS, ...
- enhance framework: tackle open issues
- test and get familiar with EasyBuild on your own system(s)

Work on something ***you*** care about!



Agenda

https://github.com/hpcugent/easybuild/wiki/3rd-easybuild-hackathon

- today:
  - before lunch: **EasyBuild in Cyprus/Julich** (George / Alan)
  - after lunch: **technical discussions** on open issues
  - **NVIDIA presentation** via conference call: 5pm - 6pm
- Tuesday/Wednesday (10am - 6pm): **actual hackathon**
  - focus on support for accelerators and local interests
  - Jens T. and myself are here for questions and helping out

easybuild

building software with ease

EasyBuild hackathon @ Cyprus
March 11th 2013

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