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EasyBuild at the Fred Hutch

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Using EasyBuild at the Fred Hutch

- Using EasyBuild since 2015
- Many issues with library consistency early in usage
 - pkg-config and multiple library versions
 - Line between OS packages and EasyBuild as blurry
- Local R and Python module lists are very large
- Developed EasyUpdate to manage R and Python
- Update R within a week of each new release
- Significant support for Bioinformatics Packages

<https://github.com/FredHutch/easybuild-life-sciences>

EasyUpdate for R and Python

Initial use of EasyBuild as a build tool – not focused on library support

During 2019 Hutch changed how we support local R and Python modules – Using foss-2018b

Switched from a single EasyConfig to using Bundles

Support building of the community release of R and Python

Contribute as much as possible

Utilize existing EasyConfigs

Local Support for latest R and Python – BioConductor

Custom R and Python EasyConfig

```
easyblock = 'PythonBundle'

name = 'Python'
version = '3.7.4'
versionsuffix = '-fh1'

dependencies = [
    ('Python', '3.7.4'),
    ('pytest', '5.0.1', '-Python-%(pyver)s'),
    ('pybind11', '2.3.0', '-Python-%(pyver)s'),
    ('matplotlib', '3.1.1', '-Python-%(pyver)s'),
    ('Biopython', '1.74', '-Python-%(pyver)s'),
    ('Pysam', '0.15.3', '-Python-%(pyver)s'),
    ('pybedtools', '0.8.0', '-Python-%(pyver)s'),
    ('jupyter', '1.0.0', '-Python-%(pyver)s'),
    ...
]
exts_defaultclass = 'PythonPackage'

exts_list = [
    ('only local differences', '1.0.0'),
]
```

Updated EasyUpdate

- Refactor easy_update to read dependencies
- Read exts_list from dependencies
- Python is becoming a significant dependency for BioInformatics
- exts_defaultclass = 'PythonPackage'

Easy Update Dependency Checking

Dependency Checking Single Library

```
./easy_update.py --rver 3.6 --search rstan
```

```
BioConductor version: biocver not set
```

```
('Rcpp', '1.0.3'),  
('lattice', '0.20-38'),  
('Matrix', '1.2-18'),  
('RcppEigen', '0.3.3.7.0'),  
('BH', '1.72.0-3'),  
('StanHeaders', '2.21.0-1'),  
('digest', '0.6.23'),  
('gtable', '0.3.0'),  
('lazyeval', '0.2.2'),  
('MASS', '7.3-51.5'),  
('nlme', '3.1-143'),  
('mgcv', '1.8-31'),  
('plyr', '1.8.5'),  
('glue', '1.3.1'),  
('magrittr', '1.5'),  
('stringi', '1.4.5'),  
('stringr', '1.4.0'),  
('reshape2', '1.4.3'),  
('rlang', '0.4.2'),  
('farver', '2.0.3'),  
('labeling', '0.3'),  
('colorspace', '1.4-1'),  
('munsell', '0.5.0'),  
('R6', '2.4.1'),  
('RColorBrewer', '1.1-2'),  
('viridisLite', '0.3.0'),  
('lifecycle', '0.1.0'),  
('scales', '1.1.0'),  
('assertthat', '0.2.1'),  
('crayon', '1.3.4'),  
('fansi', '0.4.1'),  
('cli', '2.0.1'),  
('utf8', '1.1.4'),  
('backports', '1.1.5'),
```

```
('ellipsis', '0.3.0'),  
('zeallot', '0.1.0'),  
('vctrs', '0.2.1'),  
('pillar', '1.4.3'),  
('pkgconfig', '2.0.3'),  
('tibble', '2.1.3'),  
('withr', '2.1.2'),  
('ggplot2', '3.2.1'),  
('inline', '0.3.15'),  
('gridExtra', '2.3'),  
('checkmate', '1.9.4'),  
('matrixStats', '0.55.0'),  
('loo', '2.2.0'),  
('ps', '1.3.0'),  
('processx', '3.4.1'),  
('callr', '3.4.0'),  
('rprojroot', '1.3-2'),  
('desc', '1.2.0'),  
('prettyunits', '1.1.0'),  
('pkgbuild', '1.0.6'),  
('rstan', '2.19.2'),
```

48 Dependencies for rstan

Easy Update Dependency Checking

Dependency Checking Single Library with an EasyConfig file
exts_list is populated from EasyConfig

```
./easy_update.py R-3.6.2-foss-2018b.eb --search rstan  
  ('StanHeaders', '2.21.0-1'),  
  ('inline', '0.3.15'),  
  ('loo', '2.2.0'),  
  ('rstan', '2.19.2'),
```

- Only 3 Dependencies for rstan
- First 46 dependencies are in the base EasyConfig

EasyUpdate PythonBundle

```
/easy_update.py --verbose wot-1.0.8-foss-2018b-Python-3.6.6.eb
```

```
- dependency: Python-3.6.6-foss-2018b.eb
- dependency: pybind11-2.2.4-foss-2018b-Python-3.6.6.eb
- dependency: python-igraph-0.7.1.post6-foss-2018b-Python-3.6.6.eb
- dependency: h5py-2.10.0-foss-2018b-Python-3.6.6.eb
- dependency: matplotlib-3.0.0-foss-2018b-Python-3.6.6.eb
- dependency: SWIG-3.0.12-foss-2018b-Python-3.6.6.eb
- dependency: GDAL-2.2.3-foss-2018b-Python-3.6.6.eb
- dependency: GEOS-3.6.2-foss-2018b-Python-3.6.6.eb
- dependency: Arrow-0.15.1-foss-2018b-Python-3.6.6.eb
- dependency: PyTables-3.4.4-foss-2018b-Python-3.6.6.eb
```

```
PyYAML : 5.3 (keep) [49, 1]
python-lzo : 1.12 (keep) [49, 2]
anndata : 0.6.22.post1 -> 0.7.1 (update) [49, 3]
fisher : 0.1.9 (keep) [49, 4]
forceatlas2-python : 1.0 (keep) [49, 5]
hnsplib : 0.3.4 (keep) [49, 6]
lightgbm : 2.3.1 (keep) [49, 7]
numpy-groupies : 0.9.10 (keep) [49, 8]
loompy : 3.0.6 (keep) [49, 9]
louvain-github : 0.6.1.post1 (keep) [49, 10]
MulticoreTSNE-modified : 0.1.post2 (keep) [49, 11]
natsort : 7.0.0 (keep) [49, 12]
llvmlite : 0.31.0 (keep) [49, 13]
numba : 0.47.0 (keep) [49, 14]
retrying : 1.3.3 (keep) [49, 15]
plotly : 4.5.0 (keep) [49, 16]
ply : 3.11 (keep) [49, 17]
thriftpy : 0.3.9 (keep) [49, 18]
backports.csv : 1.0.7 (keep) [49, 19]
parquet : 1.2 (keep) [49, 20]
statsmodels : 0.11.0 (keep) [49, 21]
scikit-learn : 0.22.1 (keep) [49, 22]
scikit-misc : 0.1.1 (keep) [49, 23]
```

```
configparser : 4.0.2 from entrypoints (add) [49, 24]
entrypoints : 0.3 (keep) [49, 25]
pyflakes : 2.1.1 (keep) [49, 26]
pycodestyle : 2.5.0 (keep) [49, 27]
mccabe : 0.6.1 (keep) [49, 28]
flake8 : 3.7.9 (keep) [49, 29]
param : 1.9.3 (keep) [49, 30]
pyct : 0.4.6 (keep) [49, 31]
colorcet : 2.0.2 (keep) [49, 32]
path : 13.1.0 (keep) [49, 33]
path.py : 12.4.0 (keep) [49, 34]
pyviz-comms : 0.7.3 (keep) [49, 35]
holoviews : 1.12.7 (keep) [49, 36]
typing-extensions : 3.7.4.1 (keep) [49, 37]
MarkupSafe : 1.1.1 (keep) [49, 38]
Pillow : 7.0.0 (keep) [49, 39]
Jinja2 : 2.10.3 (keep) [49, 40]
tornado : 6.0.3 (keep) [49, 41]
bokeh : 1.4.0 (keep) [49, 42]
hvplot : 0.5.2 (keep) [49, 43]
scplot : 0.0.15 (keep) [49, 44]
seaborn : 0.10.0 (keep) [49, 45]
umap-learn : 0.3.10 (keep) [49, 46]
XlsxWriter : 1.2.7 (keep) [49, 47]
pegasuspy : 0.16.6 (keep) [49, 48]
POT : 0.6.0 (keep) [49, 49]
wot : 1.0.8 (keep) [49, 50]
```

Updated Packages: 1

New Packages: 1

Dropped Packages: 0

Fred Hutch EasyBuild Environment

Using Docker containers for building EasyConfigs

Base container with EasyBuild, toolchain and Lmod

No Build or development tools in the container

Each easyconfig is built in a clean environment

Releases of New Toolchains

Release new R for toolchains - R dependences

Start bounty program to accelerate package building

Thank you



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My Questions

Adding Imod environment to container

Installing EasyBuild with Python 3.7

My keys for –new-pr are broken

Index of external site EasyConfigs

Reproducible Science

Issues – Scientific software with no tag/release