Bioconda Recipes

meta.yaml build.sh post-link.sh

Limitations

Supported OSs:

- Linux & MacOS

Supported Repositories:

- as-yet-unbuilt recipes in the repo but that will be included in the PR
- conda-forge channel
- bioconda channel
- default Anaconda channel

Limitations

Supported Python versions:

- 2.7, 3.6, 3.7, 3.8 (development)

Supported Languages (other than Python):

- R
- Java
- Perl
- C/C++
- Haskell
- Fortran (Not listed)

meta.yaml

- Template Jinja2 template language over yaml

Preprocessing selectors are also replaced before installation

meta.yaml: Jinja2

```
{% set name = "biobb_md" %}
{% set version = "3.5.1" %}
{% set file_ext = "tar.gz" %}
{% set hash_type = "sha256" %}
{% set hash_value = "20112124ccda9f95f708bd98a8b34b539b0390778b07adfcf93d59655340706e" %}
package:
  name: '{{ name|lower }}'
  version: '{{ version }}'
source:
  url: https://pypi.io/packages/source/{{ name[0] }}/{{ name }}-{{ version }}.{{ file_ext }}
  '{{ hash_type }}': '{{ hash_value }}'
```

meta.yaml: Preprocessing Selectors

```
requirements:

host:

python ==3.7.*

setuptools

tensorflow ==2.3.0 # [linux]

tensorflow ==2.0.0 # [osx]

run:

python ==3.7.*

tensorflow ==2.3.0 # [linux]

tensorflow ==2.3.0 # [linux]
```

meta.yaml: Sections

- package
- source
- build
- requirements
- test
- outputs
- about
- app
- extra

meta.yaml: package section

```
package:
    name: name_of_your_project (no quotes needed, no spaces)
    version: "x.x.x" (ie. "3.5.1")
                  {% set name = "biobb_md" %}
                  {% set version = "3.5.1" %}
                  {% set file_ext = "tar.gz" %}
                  {% set hash_type = "sha256" %}
                  {% set hash_value = "20112124ccda9f95f708
                 package:
                    name: '{{ name|Lower }}'
                    version: '{{ version }}'
```

meta.yaml: source section

source:

```
url: https://... (it can be a git repo, pypi or file in server)
md5: xxxxxxxxxx (use one of the following: md5, sha1, sha256)

source:
   - url: http://packages.seqan.de/yara/yara-{{ version }}-Mac-x86_64.zip # [osx]
   sha256: d519e797c1c66252331146b63f0cb6edba9c1a6a9e7b342fd60e7344b29baf36 # [osx]
   - url: http://packages.seqan.de/yara/yara-{{ version }}-Linux-x86_64_sse4.tar.bz2 # [linux]
```

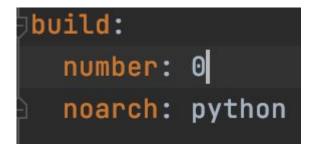
[linux]

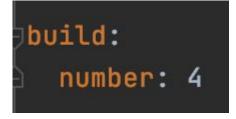
sha256: 4f68552fbb4e4002fc4320bdd60b76c678e17d087bd3f893bf179387b1668b40

meta.yaml: build section

build:

```
number: X (integer 0, 1, 2... it's like a version of the recipe)
noarch: python (for pure python and platform independent packages)
skip: True # [osx] (conda will skip the build of this recipe, for platform dependent)
```





meta.yaml: requirements section

requirements:

build: build from build.sh dependencies (compilers not listed anywhere)

host: same as build section in case the build and the host platform are not the same

run: packages required in runtime

```
requirements:
  build:
    - {{ compiler('c') }}
    - {{ compiler('cxx') }}
    - {{ compiler('fortran') }}
    - make
  host:
  run:
```

```
requirements:
  host:
    - python ==3.7.*
    setuptools
    - biobb_common ==3.5.1
    - gromacs ==2019.1
  run:
    - python ==3.7.*
    - biobb common ==3.5.1
    - gromacs ==2019.1
```

meta.yaml: test section

test:

commands: for command line tools tests if exit code is 0. import: for python packages tests if it is possible to import a package

```
imports:
    - biobb_md
    - biobb_md.gromacs
    - biobb_md.gromacs_extra
```

```
test:
commands:
commands:
```

meta.yaml: about section

```
about:
    home: ...
    license: ...
    license_family: ...
    license_file: ...
    summary: ...
    description: ...
```

```
home: https://github.com/bioexcel/biobb_md
license: Apache Software License
license_family: APACHE
license_file: LICENSE
summary: Biobb_md is the Biobb module collection to perfo
description: "Biobb_md is the Biobb module collection to
doc_url: http://biobb_md.readthedocs.io/en/latest/
dev_url: https://github.com/bioexcel/biobb_md
```

```
home: http://mmb.irbbarcelona.org/gitlab/gelpi/CMIP
license: Apache Software License
license_family: APACHE
summary: CMIP Classical Molecular Interaction Potentials
description: "The latest version of the classical molecula
```

meta.yaml: about section

```
about:
    home: ...
    license: ...
    license_family: ...
    license_file: ...
    summary: ...
    description: ...
```

```
home: https://github.com/bioexcel/biobb_md
license: Apache Software License
license_family: APACHE
license_file: LICENSE
summary: Biobb_md is the Biobb module collection to perfo
description: "Biobb_md is the Biobb module collection to
doc_url: http://biobb_md.readthedocs.io/en/latest/
dev_url: https://github.com/bioexcel/biobb_md
```

```
home: http://mmb.irbbarcelona.org/gitlab/gelpi/CMIP
license: Apache Software License
license_family: APACHE
summary: CMIP Classical Molecular Interaction Potentials
description: "The latest version of the classical molecula
```

meta.yaml: extra section

Schema-free section

```
extra:
    any kind: ...
    of: ...
    extra information: ...
```

```
extra:
recipe-maintainers: PauAndrio
```

build.sh: Bash style installation script

Provided env vars:

- **\$PREFIX** The install prefix (the root directory of the new environment)
- \$PKG_NAME The name of the package
- \$PKG_VERSION The version of the package
- \$PKG_BUILDNUM The build number of the package
- \$SP_DIR Site-packages directory of the new environment (not listed)

Provided compiler vars:

- \${FC} Fortran 77 compiler (not listed)
- \${cxx} C++ compiler (not listed)
- \${c} C compiler (not listed)

post-link.sh: Print messages after installation

- Not working for messages (does not respect break lines)
- Everything done here is not translated to the container