

Dependency management: Lessons learned

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Context

- Developing Python and/or C++ libraries and applications
- Using GitHub (or similar) with Github Actions (or similar) to:
 - Build and run tests for pull requests (PRs).
 - Build documentation.
 - Build conda packages.
 - Build PyPI wheels.

Problem

Example: scipp, scippnexus, scippneutron, ess

- Experienced issues in about 10 cases in 2021, such as:
 - Pull request builds suddenly fail for no apparent reason.
 - Documentation builds stop working.
 - Package builds don't work any more.
- ...despite previously passing Cl, issue is not a bad merge.

Previous approach

- Waste time discussing the "weird" issue at the daily standup.
- Dig through build logs: which package upgraded?
- Does older version work? Check upstream for issue, or open one.
- Pin version, restart all builds.
- Open issue as a reminder to remove the pin once upstream made a fix.
- Add pin across all projects.
- Remove pins once possible, half the time it is unclear how to reproduce.

Concrete examples from 2022

Five Six such issues in less than four months!

- February 18 Conan suddenly produces an error, caused by update of markupsafe https://github.com/pallets/markupsafe/issues/282. Lost ability to make a (patch) release until we found this and pinned the version.
 - March 24 Documentation builds stop working due to https://github.com/jupyter/nbconvert/issues/1736 causes by https://github.com/pallets/jinja/issues/1626. Lost ability to pass CI (blocking all merges) or release builds (which build and update docs).
 - April 1 We notice that navigation buttons in documentation pages have disappeared. The sphinx-book-theme 0.3.0 release causes this.
 - April 7 scikit-build releases 0.14.0, breaking our PyPI builds. Lost ability to make a (patch) release until we found this and pinned the version.
 - April 19 We notice that plots no longer show up in documentation pages, traced to an ipympl update https://github.com/matplotlib/ipympl/issues/462.
 - May 12 All Linux build broken by mamba 0.23.1 patch release https://github.com/mamba-org/mamba/issues/1669.

By continuously upgrading, we see almost every upstream issue, even if fixed within hours/days.

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Recommended reading

Approach

- Step 1: Read https://hynek.me/articles/semver-will-not-save-you/. Recommends to freeze everything, including transitive dependencies.
- Step 2: Conclude that we cannot do that because if we do that for a *library* almost no one will be able to use it.

Recommended reading

Approach

- Step 1: Read https://hynek.me/articles/semver-will-not-save-you/.
 Recommends to freeze everything, including transitive dependencies.
- Step 2: Conclude that we cannot do that because if we do that for a library almost no one will be able to use it.
- Step 3: Realize that many or most of our dependency issues are not issues that ever reach a user. Actually we can freeze for quite a few cases:
 - Building documentation.
 - Requirements need for building packages.
 - Pull-request builds.
- Step 4: Must read for more details and better understanding: https://iscinumpy.dev/post/bound-version-constraints/

Implementation

Requirement: All builds should be reproducible

Reproducible means:

- Builds for a commit that passed previously should continue passing if we re-run it later.
- Builds should fail only when there is a problem in the current source repository, not if a dependency or transitive dependency makes a release.

This requirement applies to "everything":

- Going back to much older version, e.g., to make a patch release.
- Documentation builds (Sphinx).
- Release builds (making packages for PyPI and conda).
- PR builds.
- Builds on main after merging a PR.
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Workflow

Setup (example for Python-based project with pip workflow)

- Write requirements.in file(s). Do this for *everything* that is needed for your builds.
- 2 Use pip-compile from pip-tools. See also pip-compile-multi. Resulting requirements.txt is *checked into version control*.
- Treat warnings as errors in CI, in particular DeprecationWarning
 - Avoids issues from *intentional* breaking changes, since we can take action early.

From time to time

- Re-run pip-compile, run all the builds (including release builds!) and check that things work, merge.
 - dependabot may be an alternative, but it updates individual requirements, which seems too noisy for us, with too little control.
- Make patch-releases when a dependency update causes issues for users
 - Much rarer than issues we experience in development.
 - Treating DeprecationWarning as errors should catch many issues months/years ahead.
 - Users can freeze dependency version when setting up their environment as a immediate workaround.

Status

- We (scipp and subprojects) do *not* have long term experience with this yet:
 - So far implemented in https://github.com/scipp/scippnexus and https://github.com/scipp/scipp (excluding C++ build dependencies).
 - Have not gone through update cycles (re-run of pip-compile) and do not know how many headaches this will cause.
- Our conan dependencies have been pinned since the beginning.
- conda dependencies are not pinned yet. What is best use of tools for keeing this up to date, including pins of transitive dependencies?
 - Does the conda-forge global pinning help? See https://conda-forge.org/docs/maintainer/pinning_deps.html.

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Better solution: Freeze all dependencies for PR builds to decouple the tasks

- A new contributor, Alice, opens a PR with a small bugfix. Builds pass and it gets merged. Alice is happy and may continue contributing.
- Independently, Bob notices that a new upstream release requires a fix. He re-runs pip-compile and fixes the issue in a PR. After a merge, all future PR builds will now use the new upstream version.