Reproducible bioinformatics software environments with GNU Guix

Compromise

System Admins
prefer **mature** software, no variants, only apply unavoidable updates

Users
want **fresh** software, multiple variants, latest tools, **flexibility**

Use stable software for systems; let users manage their software stack on their own. This often leads to environments with following properties:

ad-hoc There is no way to **reproduce** the environment, even on the same machine at a different point in time.

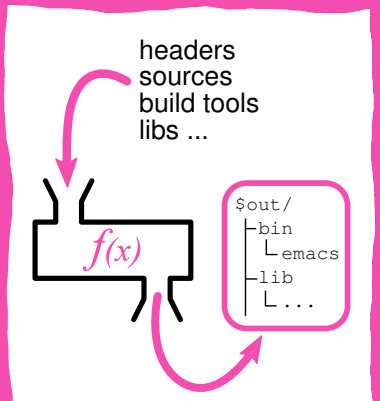
volatile Due to a **lack of isolation**, the environment will change or break when the host system changes.

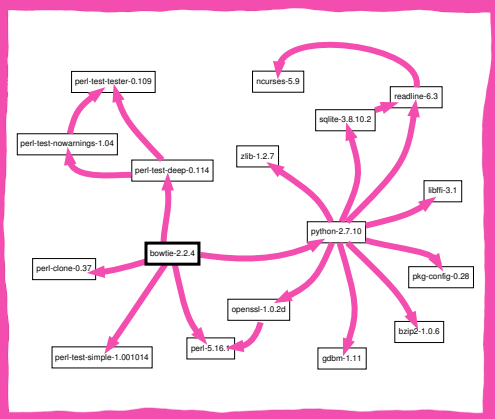
primitive **No safe upgrades** or **roll-backs**. No separation for different workflows. **Unportable**.

Functional package management

The package build is seen as a **function** in the mathematical sense, taking **inputs** (build scripts, compiler, libraries, sources), and **returning an installed package**.

As a **pure function** its result depends **solely** on its inputs; there is **no global state**. Just like the result of a pure function can be cached, the package output directory is cached in the **store**.

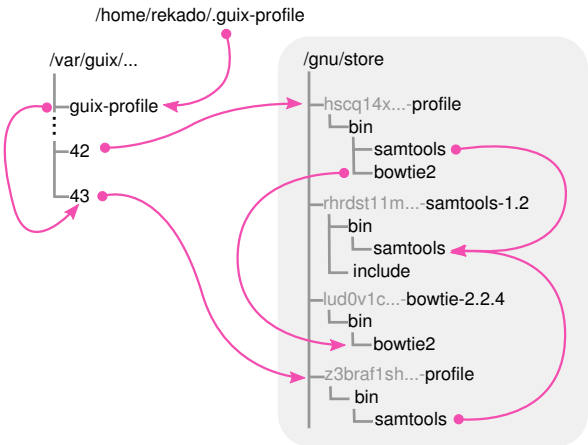




Software profiles

The name of each output directory is **unique** as it is derived from **all** inputs. A **software environment** can be built by creating the **union** of the output directories of all desired packages.

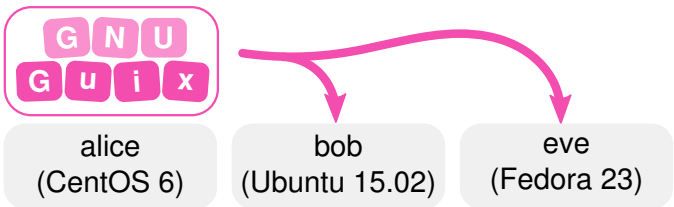
These software **profiles** can be **independently** managed **by users** with Guix. A profile is just a forest of symbolic links to items in the shared store. This enables a user to **roll-back** to previous versions of the environment, and to install **different variants** of applications and libraries using **separate** profiles.



Towards reproducible research

As each package **captures the complete dependency graph**, down to the kernel headers, all dependencies are immutable and are satisfied by the store. There are no dependencies on the host system, enabling the **sharing of well-defined software environments** across machines, aiding reproducible research.

See http://arxiv.org/abs/1506.02822v2 for more information.



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