Software Stack Provisioning for HPC

Build Install Configure Run

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Why Can't We Install Softwares?

Problem statement

Shared Resources, Shared State

- High Performance Computers (HPC) are **shared resources**
- Each HPC machine is a **shared software environment**

HPC users requirements

- Need to **bring there own software**
- They want **reproducibility of results**

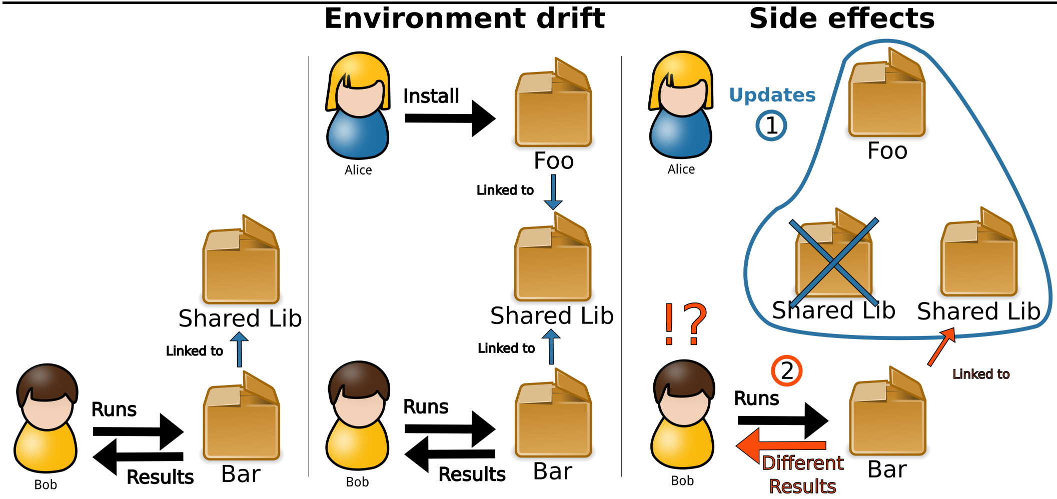
Package Managers are modifying a **shared state**

If users have permissions to install:

- **side-effects** (See Alice and Bob story)
- Drift of the environment: Operator don't know what is running

Alice and Bob Story

The Update problem



Classical Package Manager (YUM, APT, ...)

Or Why Using Shared Libraries

Heavily use **shared libraries** <= **Shared state**

Why Shared libraries?

- Loading libraries once in memory
- Storing libraries once on disk
- Can update **without re-compilation**

Static libraries: glibc in Debian

- 37% of the package depends of **glibc** in Debian Stable
- 19579 packages out of 51831
- 3 updates in Debian Stable (≈ 1 year)

=> **58737 to recompile instead of 3**

Software Provisioning Process

Build Install Configure Run

Build

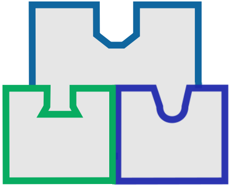
Requirements and Constraints

Reproducibility

- Bitwise reproducibility of the binaries
- Logging of the build build process with all parameters
- Changing any build parameters => explicit new version

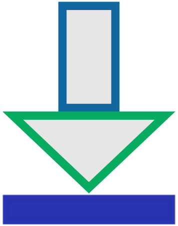
Combinatorial explosion of parameters

- Architecture (x86_64, ARM64, ...)
- Platform (Linux, Cray, ...)
- Compilers (GCC-6, GCC-7, Clang, Intel, ...)
- MPI libraries (OpenMPI-1, OpenMPI-2, mvapich, IntelMPI, ...)
- Other libraries (OpenBLAS, OpenMP, ...)
- Compilation flags (-debug, -O, ...)



Install

Requirements and Constraints



For Users

- Have permission to install!
- From source (build)
- From binary (provided by any tiers)
- Have multiple version of the same software
- Have distinct environments for development/test/run

For Operators

- Provides easy to install packages for users
- Possibility to push (security) updates to users
- Save resources by sharing libraries between users
- Keep track of what is installed and where
- Possibility to rollback to previous version if needed

Configure

Requirements and Constraints

Portability

- no pointers to user's home :)

Traceability

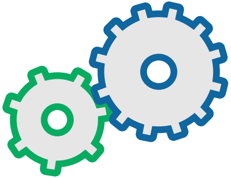
- Every configuration versions are kept
- Sharing software with configuration attached automatically

Ease of use

- Operator provides sane defaults depending on the platform
- Users are able to change configuration of software AND operating system
- Possibility to have multiple configuration for the same software (and switch easily)

Combinatorial explosion

Hadoop (Yarn/MapReduce/HDFS) have 1346 configuration properties!

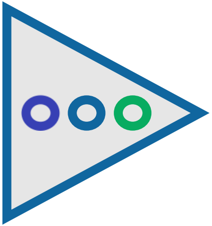


Run

Requirements and Constraints

The goal of provisioning

The final step that depends on the others



Avoid divergence between build time and run time

- Be sure to link to shared libraries used for build
- Or ABI-compatible ones with security patch

Traceability

- Have warranties that the right software is running
- Be sure that the right configuration is used

Containers don't solve the problem

Or the Unwanted Isolation

Containers Resource ans Job Managment Systems (OAR, Slurm, ...) already provides resources isolation Other types of isolations are not wanted: Mount: prevent to load and share files (where is my CSV?) special hardware support is problematic (need drivers and libraries on the host) Process ID: prevent to find other local process Net: bad network performances Inter Process Communication: No shared memory between process User ID: Give you what you have if you where not isolated A good solution for services: ensure a configuration is used (using entrypoints)

Spack and EasyBuild

Spack **Build Install Configure Run** Patch binaries to force the RPATH

Nix and Guix

TODO

Conclusion

TODO

Thanks!

Questions?

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