HPC user software environment management with Nix

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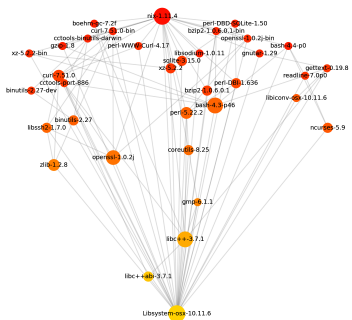
3rd Easybuild User Group, January 29, 2018

Overview

Software Packaging in HPC

Maintenance Reproducibility Portability



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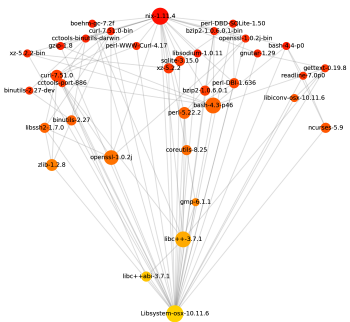


HPC Specific needs..

- Advanced rights management (user envirenments, community-specific packages, licenses)
- Automated development workflow: custom packages, automated rebuilds, HPC machine vs laptop
- Advanced build option access
- OS independent

Existing solutions

Package-based solutions


Nix

Container-based solutions


Singularity

udocker

Charliecloud

Shifter

The Jungle

	easybuild	Spack	/ GuixHPC
Build Reproducibility	up to system libs	up to system libs	almost binary
User Environments	module-based	module-based	pure, isolated
Runtime env	module/os-based	module/os-based	static deps
Portability	no	no	yes
Packaging Language	Python/Easyconfig/tcl	Python	Nix
Multiple versions	yes	yes	rebuild/grafts
Binary packages	no	yes	yes
Isolated build env.	no	no	yes
External/Legacy Modules	yes	?	no
Who packages	anyone?	no	anyone
Who builds	admin and user?	admin or user	admin and user on head (daemon+store)
Community/Doc	HPC	HPC	large
Custom Packages	?	?	source-based

The Nix Ecosystem. https://nixos.org

Nix Ecosystem

Nix - The Expression Language

Nix - The Nix package manager

Hydra - Nix-based continuous build system

NixOS - The Purely Functional Linux Distribution

NixOps - The NixOS Deployment Tool

Nix - The Expression Language

What?

- Functional, Turing complete language.
- Typed. int, bool, path, string, set, list, lambda.
- Large built-in and standard lib. `stdenv`, `fetchTarball`, `fromJson`, `fromGitHub`, `assert`, `test`..

Nix - The Expression Language

Why?

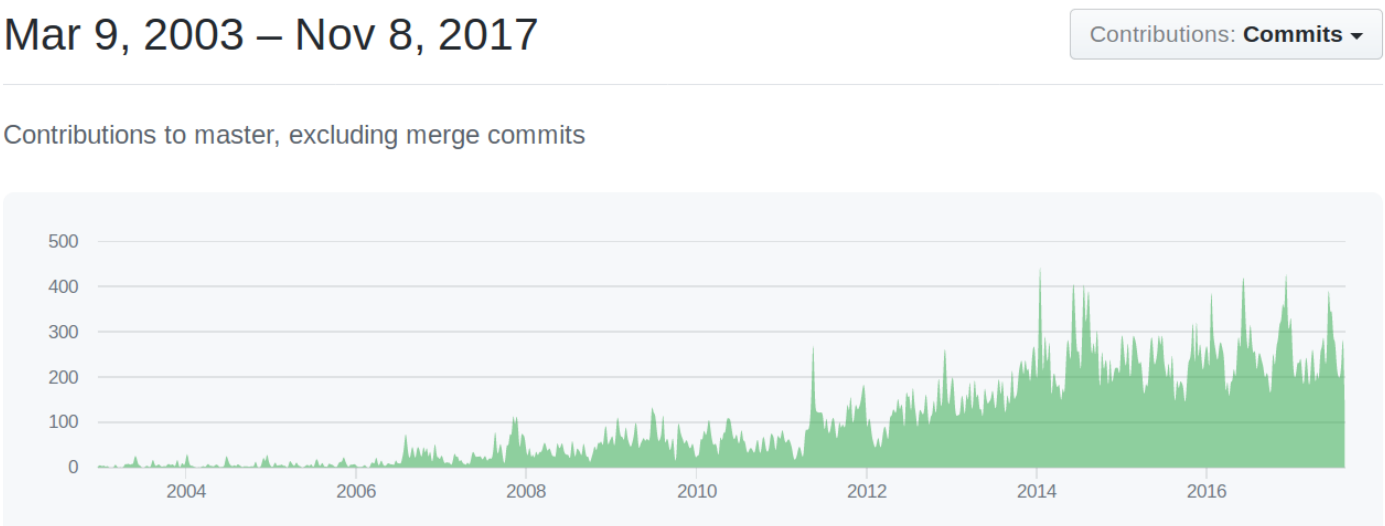
- Packaging is complex.
- Abstraction layers.
- Better reusability, factorization.
- (Readable and Mantainable)

Nix - The Package Manager

- Packages are defined in Nix expressions
- Independent of the system.
- Atomic upgrades and rollbacks
- Several version of the same package on the same system
- Unprivileged package installation
- Provides isolated build & runtime environments
- Reproducible build from source
- Binary Cache
- Garbage collection
- Declarative & Imperative use.

Nixpkgs - https://github.com/NixOS/nixpkgs

- >**10 000** packages
- >**1 400** contributors
- >**110 000** commits



Derivations

```
  { stdenv, fetchurl, cmake, fftw, openmpi
  singlePrec ? true,
  mpiEnabled ? false,
  }:
  stdenv.mkDerivation {
    name = "gromacs-4.6.7";
  src = fetchurl {
    url = "ftp://ftp.gromacs.org/pub/gromacs/gromacs-4.6.7.tar.gz";
  sha256 = "6afb1837e363192043de34b188ca3cf83db6bd189601f2001a1fc5b0b2a214d9";
};
  buildInputs = [cmake fftw]
  ++ (stdenv.lib.optionals mpiEnabled [ openmpi ]);
  cmakeFlags = ''
  ${if singlePrec then "-DGMX_DOUBLE=OFF" else "-DGMX_DOUBLE=ON -DGMX_DEFAULT_SUFFIX=OFF"}
  ${if mpiEnabled then "-DGMX_MPI:BOOL=TRUE
  -DGMX_CPU_ACCELERATION:STRING=SSE4.1
  -DGMX_OPENMP:BOOL=TRUE
  -DGMX_THREAD_MPI:BOOL=FALSE"
  else "-DGMX_MPI:BOOL=FALSE" }
  '';
  meta = ...
}
```

Store

Packages are stored in the nix store: `/nix/store`.
They are identified with a sha-256 hash of the source nix file and its "inputs".
`/nix/store/an9dli66ng2jzvqf13b2i230mm9fq7qk-cdo-1.7.2`
changing a flag alters the inputs produce new packages:
`/nix/store/srf6grrfy9vkc9fsplk8xk292lm8jvz5-cdo-1.7.2`

Profiles

Users have profiles. Profiles :

- are independent.
- are unlimited.
- can be rolled back.

Channels, binary caches

Channels:

- `nixpkgs-unstable`
- `nixos-YY.MM` (NixOS-users)
- `ciment-channel` (The GRICAD channel)

Example: `openmpi` installation

```
$ nix-env -i -A nixpkgs-unstable.openmpi
```

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Binary caches

Installing a package:

1. Check if exists in the `binary-cache`
2. Else, building from sources & deps

Attributes

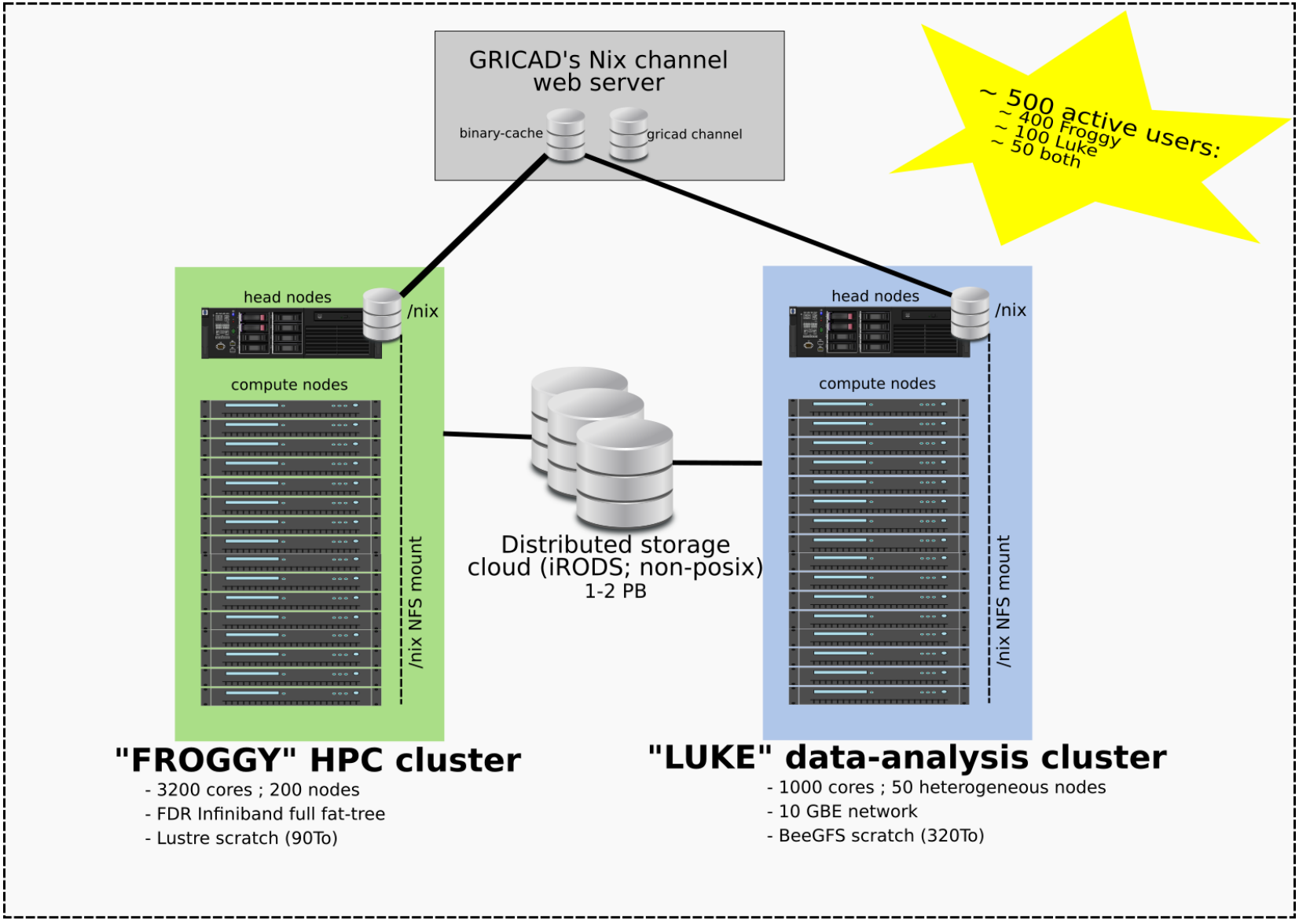
Installation of a `gromacs` application version

```
$ nox gromacs Refreshing cache
1 gromacs-4.6.7 (ciment-channel.gromacs)
Molecular dynamics software package
2 gromacs-4.6.7 (ciment-channel.gromacsDouble)
Molecular dynamics software package
3 gromacs-4.6.7 (ciment-channel.gromacsDoubleMpi)
Molecular dynamics software package
4 gromacs-4.6.7 (ciment-channel.gromacsMpi)
Molecular dynamics software package
```

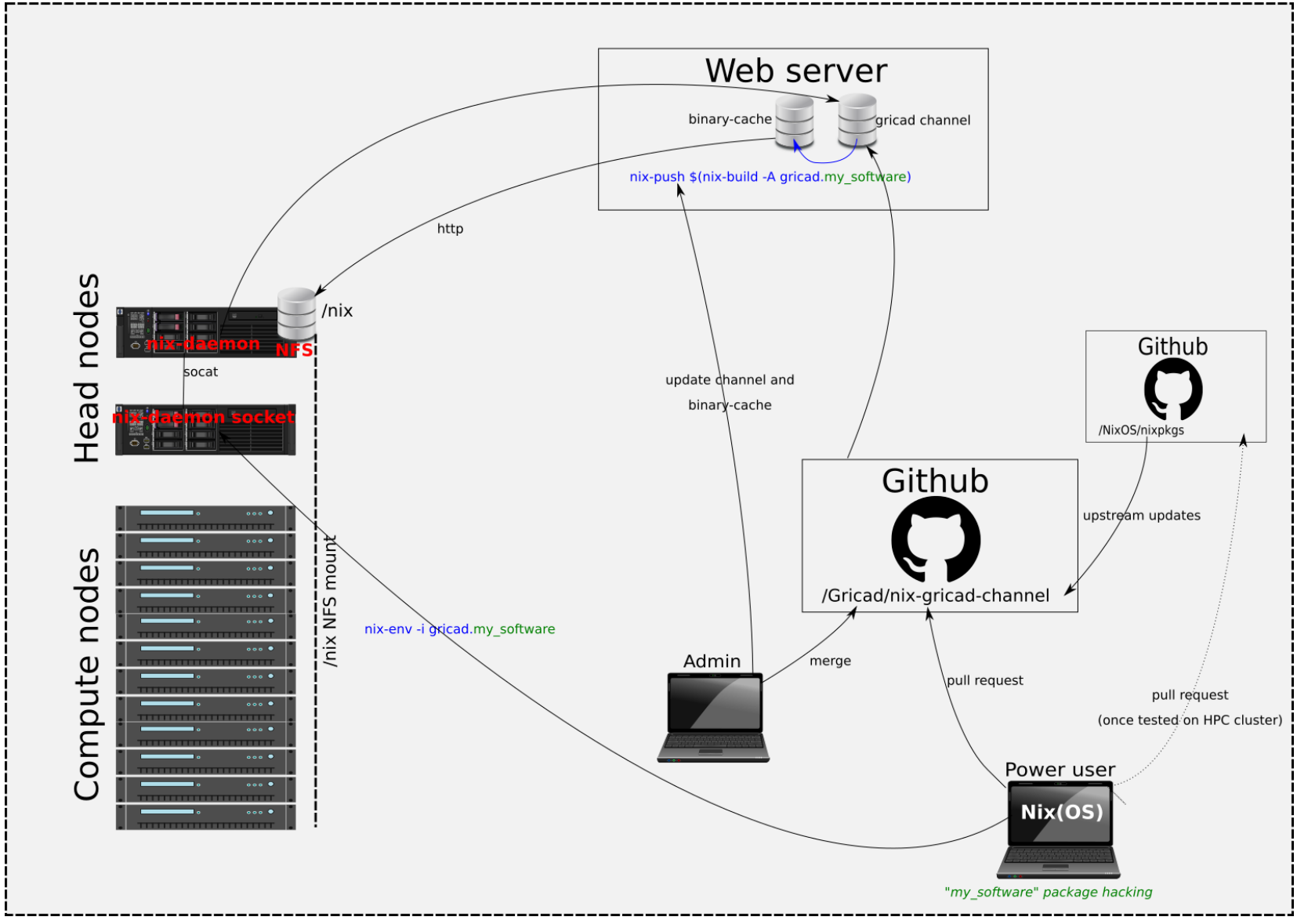
Legend: `attribute` → Multiple concurrent versions of one particular application 

Nix at the GRICAD HPC center

The GRICAD HPC center



The Nix setup



User feedback

12 month experiment. Nix at GRICAD has:

- $>$ 50 users
- $>$ 100gb `/nix/store`
- $>$ 20k derivations
- $>$ 1200 generations

References

Official links

Nix: `https://nixos.org/nix/`
NixOS: `https://nixos.org/`
Nixpkgs: `https://nixos.org/nixpkgs/`

Our documentation

Blog: `https://gricad.github.io/calcul/`
Channel: `https://github.com/Gricad/nix-ciment-channel`

Thanks. Discussion Time..

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