Nix as HPC package management system

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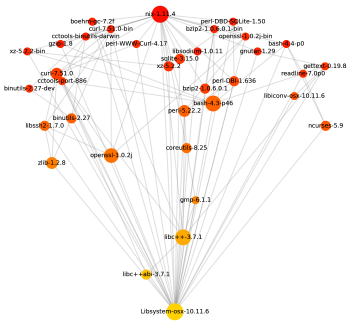
Overview

Packaging and HPC

Maintenance Reproducibility Portability



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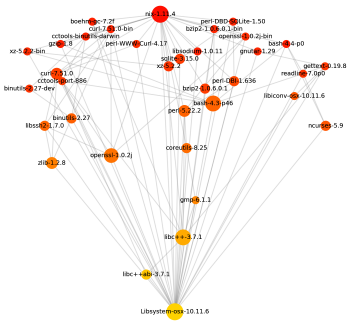

In HPC: Multi-User, Custom/Community/Private packages, many build options, OS independent.

Existing solutions

	Module	easybuild	Spack
Multi-user	✓	✓	✓
Multiple version	✓	✓	✓
Build Dependencies	✗	✓	✓
Community	✗	✓	✓
Reproducibility	✗ ✗	✗	✗ / ✓
Binary packages	✗	✗	✗
Isolated build env.	✗	✗	✗
Isolated runtime env	✗	✗	✗

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The Nix Ecosystem

https://nixos.org

Nix Ecosystem

Nix - The Expression Language

Nix - The Nix package manager

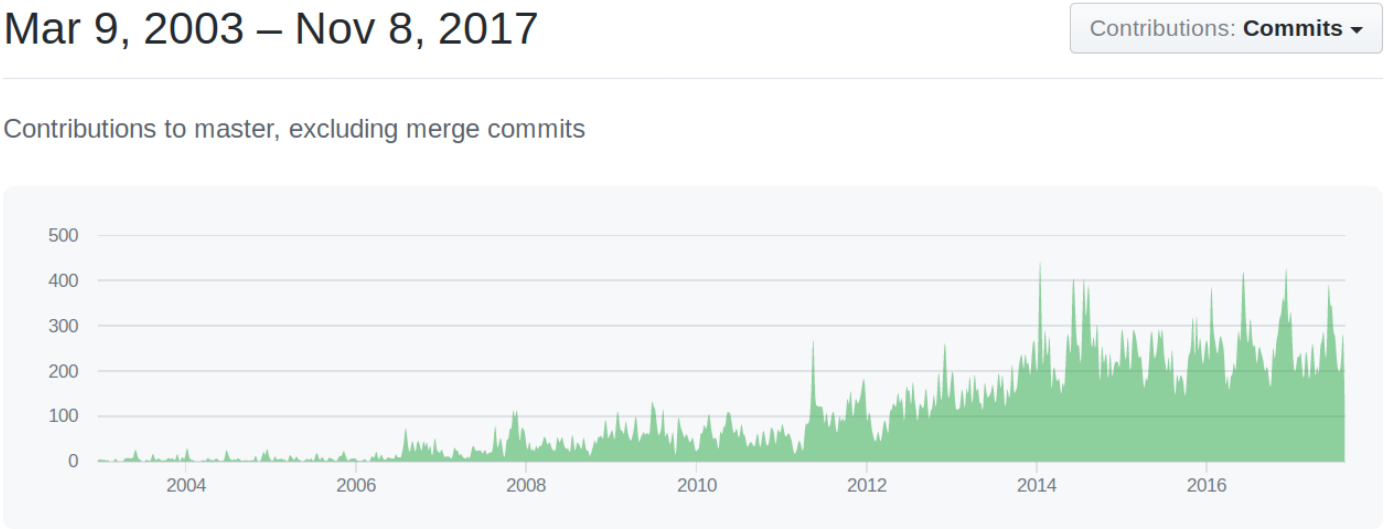
Hydra - Nix-based continuous build system

NixOS - The Purely Functional Linux Distribution

NixOps - The NixOS Deployment Tool

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

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



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.

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

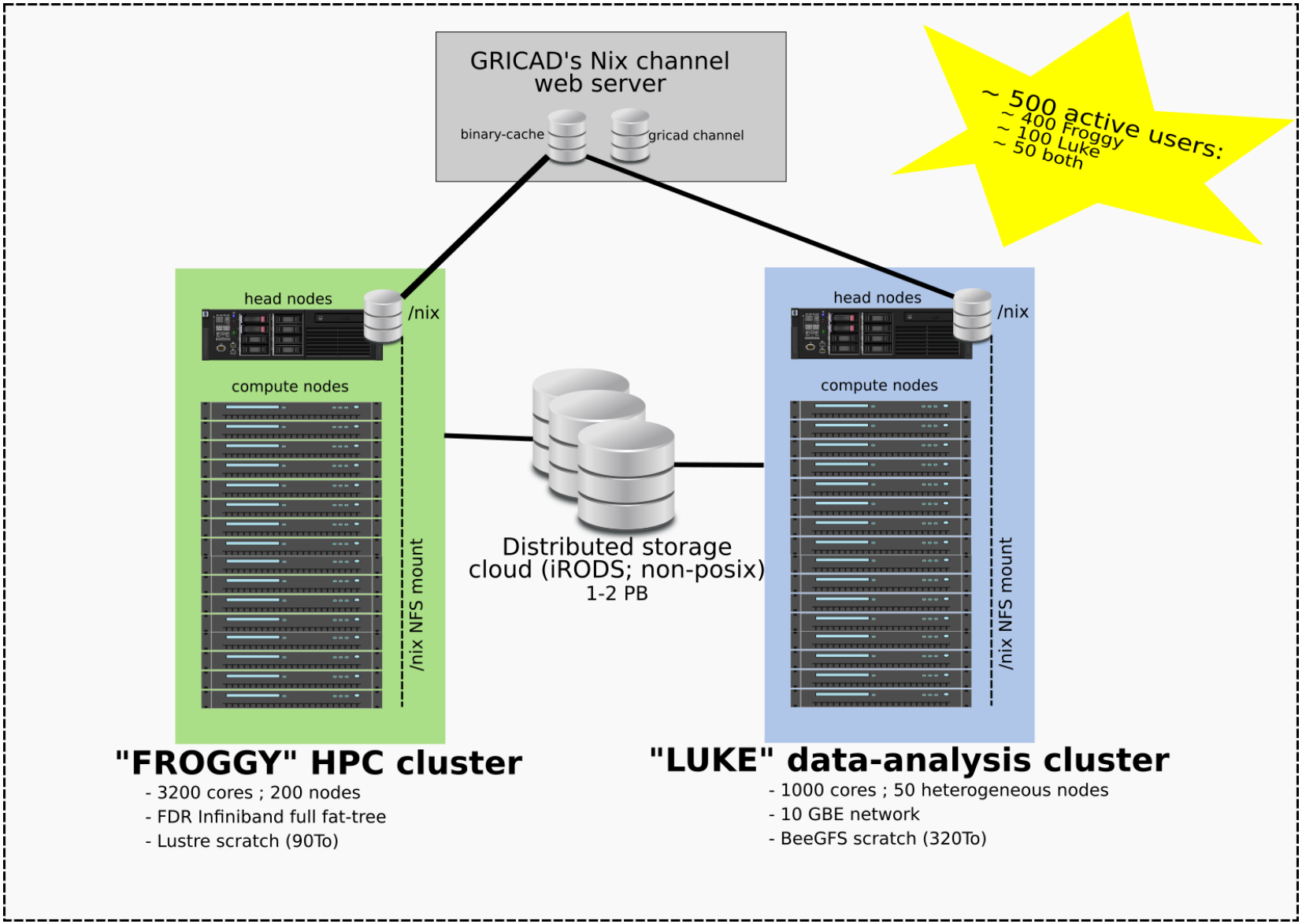
Installation of a `gromacs` application version

```
$ 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
```

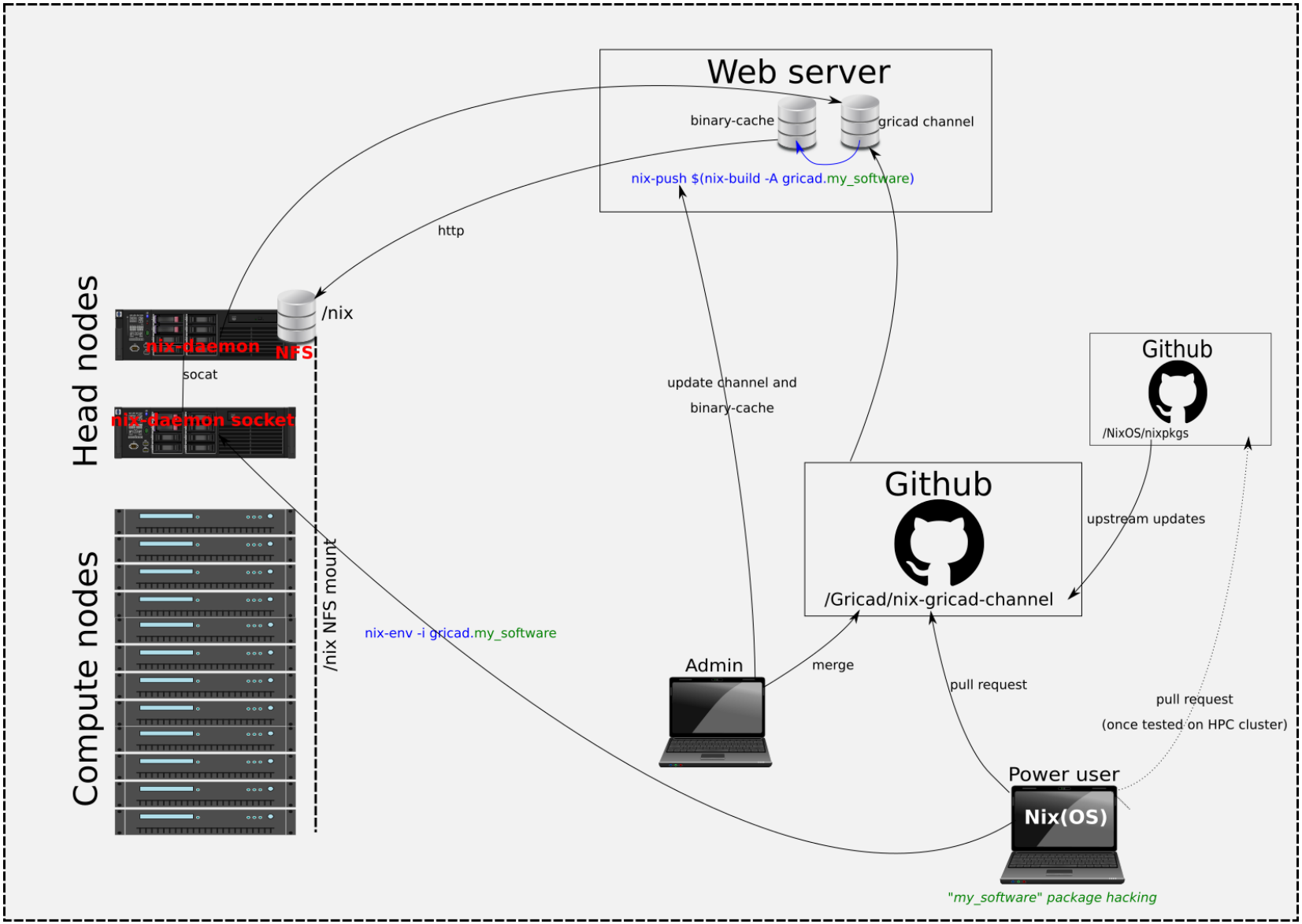
Legend: `attribute`

Nix at GRICAD

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

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