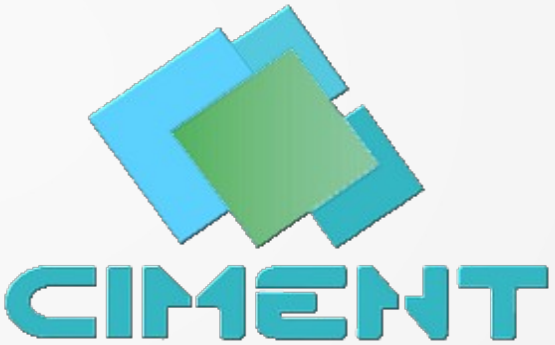
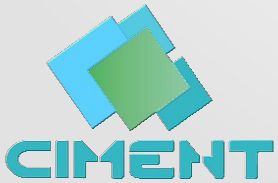
My operating system is old but I don't care :

I'm using NIX !



B.Bzeznik
BUX meeting , Vilnius
22/03/2016



UNIVERSITÉ Grenoble Alpes

CIMENT is the computing center of the University of Grenoble

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CIMENT computing platforms

132Tflops (88 BullX)

HPC platform	**Data processing platform**	**Other thematic platforms**
Froggy	*Luke*	*r2d2,foehn,ceciccluster,digitalis,...*
3200 Xeon E5 cores @2.6Ghz +18 GPUS K20m **BullX DLC** **SCS4 AE R3**	~400 cores – heterogeneous systems and continuously evolving	~3000 cores heterogeneous systems federated from 10 clusters of member laboratories
High performance distributed storage (Lustre): 90 TB	Local scratches on nodes : 450 TB	NFS filesystems: a few TB per cluster
Infiniband FDR network	10 GE network	Infiniband QDR networks

Common storage (IRODS) : 1 PB

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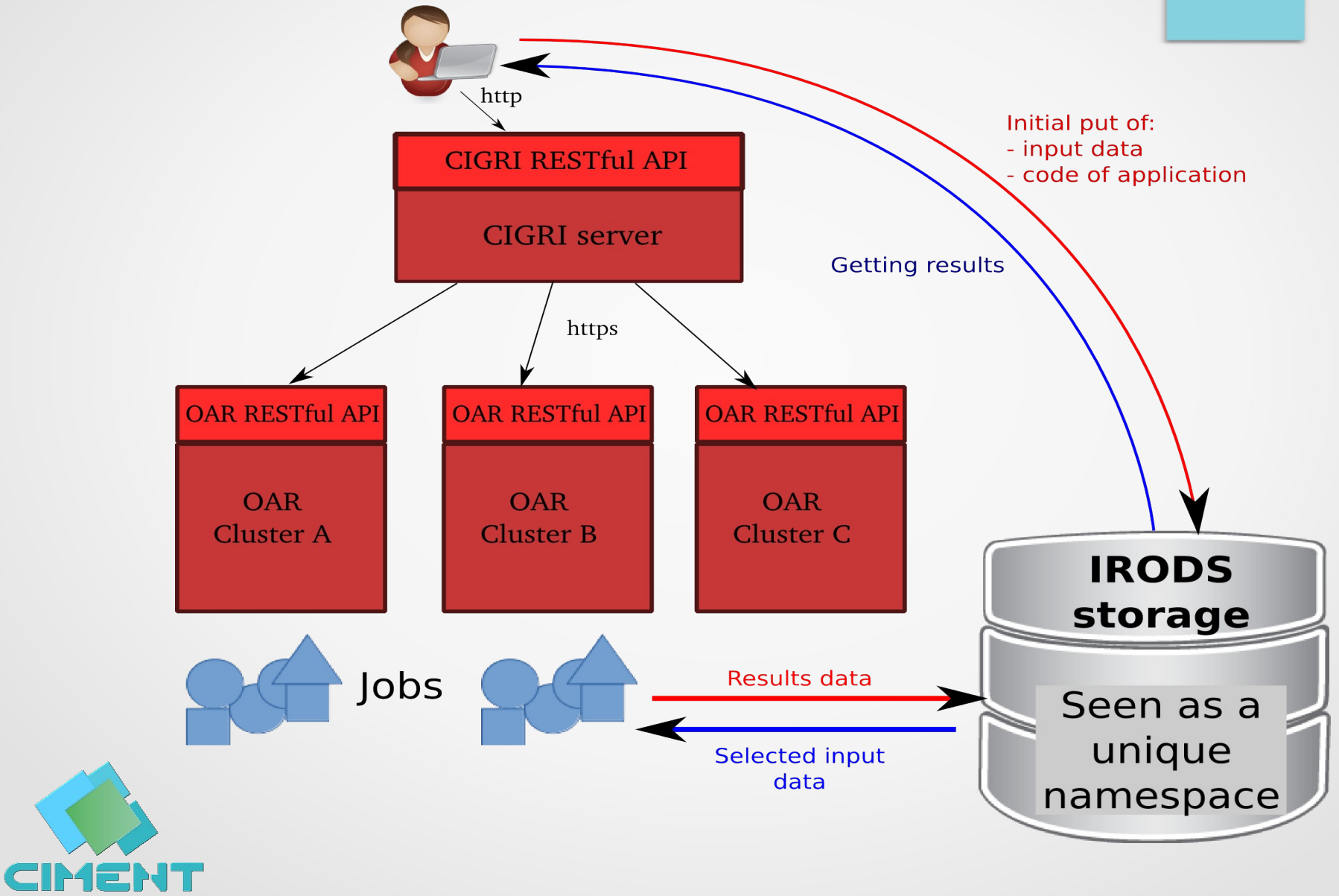
CIMENT computing GRID



CIMENT libraries repository

- Like everybody in the HPC world, we use environment modules
- Each computing cluster has it's “site” modules that we compile “by hand”
- For the grid, we created an environment which holds it's own glibc to have a uniform set of modules on every clusters

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CIMENT libraries repository

- PROBLEMS:
  - Hard to maintain
  - Not very easy to link against our libraries
  - A lot of dependencies, more and more complicated to build as the operating system becomes old
  - Recompilation at system change (or not, but...)
  - Jobs are not reproducible in the “sites” environments as soon as we upgrade the system
  - A feeling of doing something that could be more effective if we share our work

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Solutions

- lmod
  https://www.tacc.utexas.edu/research-development/tacc-projects/lmod
  Lua replacement for “modules”, with hierarchical support
- Easybuild https://hpcugent.github.io/easybuild
  User level automatic building
- Spack https://github.com/LLNL/spack
  User level automatic building
- Nix https://nixos.org/nix/
  A packaging system that allows user-level installs
- Guix https://www.gnu.org/software/guix
  A packaging system that allows user-level installs (the GNU one)

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NIX packaging system

- Nix is a free packaging system
- Packages are described with a functional language (the Nix language) → *derivations*
- Nix packages can be installed at the user level, into a shared /nix store
- Each package version is stored into a unique directory of /nix/store, starting by a hash
- Glibc is embedded, so Nix can run on top of almost every Linux flavour

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NIX profiles

- Each user can have many profiles, allowing installation of different versions of a given package
- Rollback at a given version of a profile is very easy
- Administrator can set up system wide default profiles
- A profile is a set of symbolic links into `~/.nix-profile`
- The PATH of the user contains `~/.nix-profile/bin`
- switch profile:

```
$ nix-env -switch-profile $NIX_USER_PROFILE_DIR/my_test_profile
```

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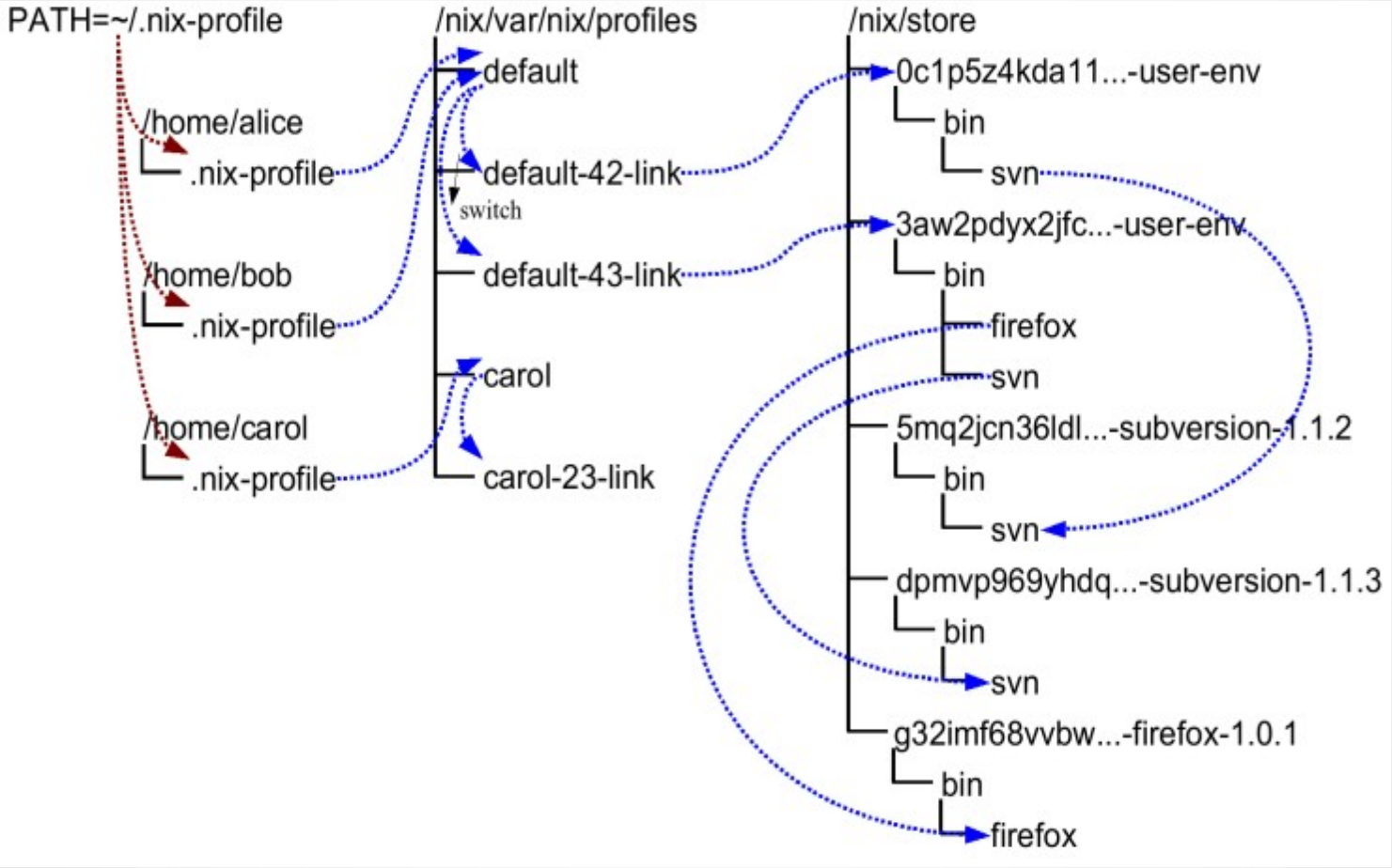
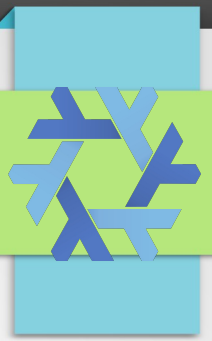
NIX profiles



(abstract from the Nix manual: https://nixos.org/nix/manual/)

NIX packages: nixpkgs



- Nixpkgs is a set of more than 10k packages
- To get all the latest derivations at once:
  `$ git clone git://github.com/NixOS/nixpkgs.git`
- install a package:
  `$ nix-env -i -A gromacsMPI`
  It will install the MPI variant of the gromacs package. If not already in the binary cache, it will be automatically compiled and be available for the other users directly as a binary
- remove a package:
  `$ nix-env -e gromacs`

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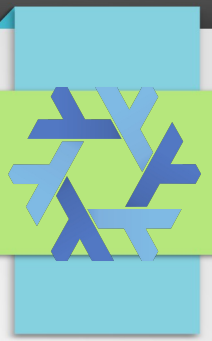
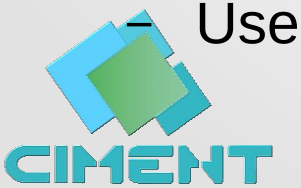
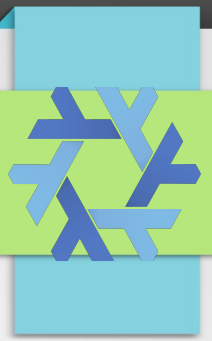
NIX



- Why is this a good solution?
  - Focuses on reproducibility
  - Offers an isolated development environment (nix-shell)
  - Already +10k packages maintained by a strong community
  - Optimized to share binaries and packages definitions among the users (multiuser mode + binary caches)
  - Ease of use
  - Ease to contribute (github pull requests)
  - Ease of hacking and sharing *derivations* (a package description that allows to rebuild the package, eventually after some modifications)
  - Users can install the same environment on their workstation



NIX



- What do you need to make it available for your users?
  - a shared **/nix** mount on all the nodes
  - **nix-daemon** on one of your head node (+'socat' if you have several head nodes)
  - a local repository (web server) if you want to setup a custom channel
    - to hold packages of non-free applications
    - to hold packages variants you've contributed to but that are not already in the official distribution
- NIXOS: the NIX operating system (nix + nixpkgs)

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CIMENT contributions

- openib support into openmpi
- mpi support into Gromacs
- netcdf support into gdal
- mlx4 support into libibverbs (not yet merged)
- new packages: libmatheval, scotch, nco, libdap,...
- Non public: Intel 2016 compilers packaging
- A lot more to come!

- You can also contribute!
- A BullX Nix channel with bullxmpi one day? :-)
- Try it! → `$ curl https://nixos.org/nix/install | sh`

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Thank you !

https://nixos.org/nix/

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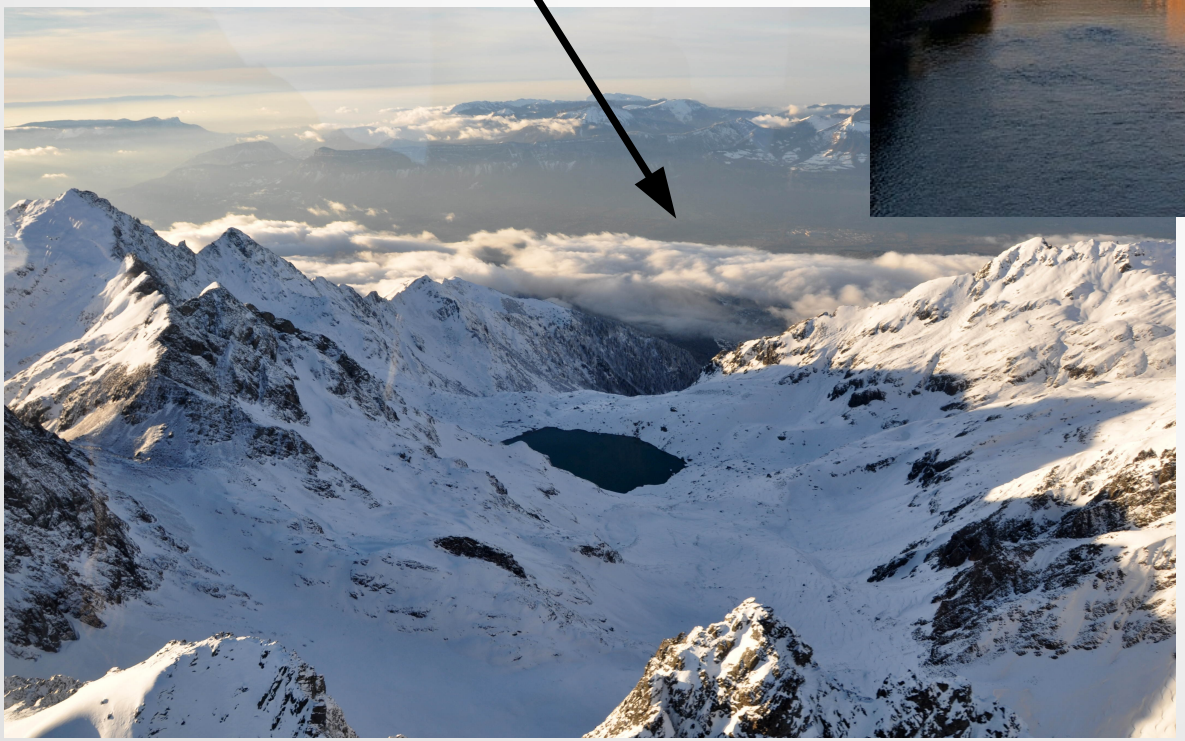
Thank you !

Grenoble