Playing with Nix in adverse HPC environments

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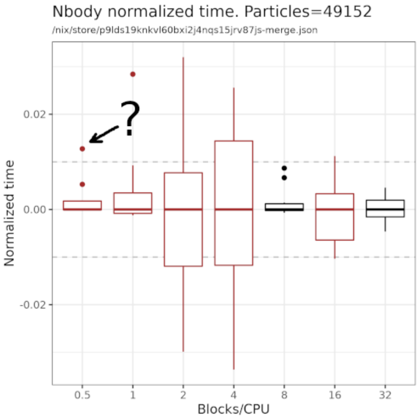
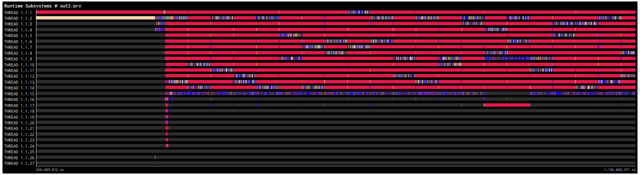
What do we do

- We develop a concurrent task-based runtime for High Performance Computing (HPC)
- LLVM-based compiler to interpret the `#pragma` directives (like OpenMP)
- Performance is **critical**
- We typically execute benchmarks on ~1000 CPUs

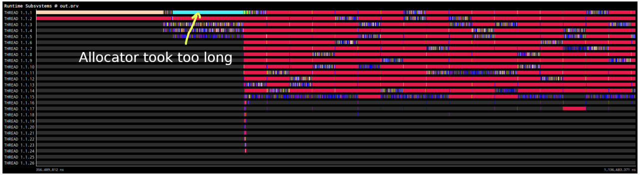
Example of a performance problem



Good case (normal):



Bad case (outlier):



Typical HPC scenario

- Login + compute nodes controlled by SLURM
- No root permission in any node
- Old LTS kernels 4.4 and software stack (**5 years old**)
- `LD_LIBRARY_PATH` used to change versions of libraries
- Hard to reproduce results after 1 year in the same machine

Question: Can we benefit from Nix?

- Up-to-date package versions, including glibc (finally)
- Explicit control over all build configuration options
- No more `LD_LIBRARY_PATH` evil dance
- Traceability: What library version did you use for experiment X?

Question: Can we benefit from Nix?

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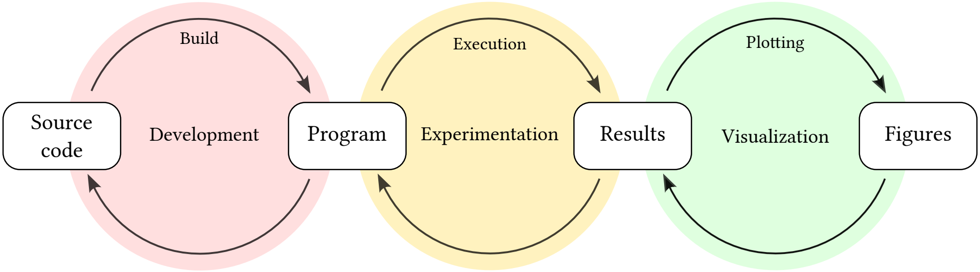
- Traceability: What library version did you use for experiment X?
- Problem: Root daemon **is not allowed** (considered unsafe, refused to install by sysadmin)

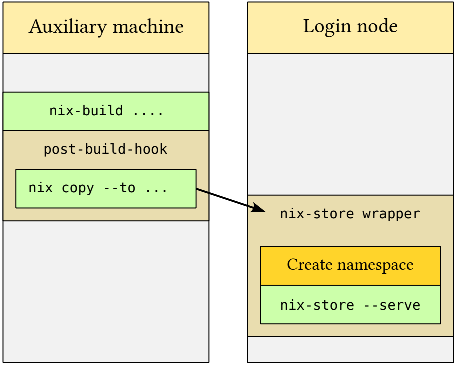
The big picture



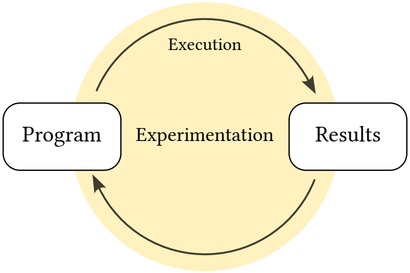
- Typically go back an forth between cycles
- Each iteration must be fast (i.e. cached builds)
- We'll focus on the **Development** and **Execution** cycles

Multi-user nix store with auxiliary machine

- Individual user installation can be done with user namespaces.
- We can use an auxiliary machine to do the builds
- Use `post-build-hook` script to issue `nix copy`
- Use a wrapper in the login node to mount the namespace
- Then run the `nix-store --serve` to receive the derivation
- Limited success with patching nix-daemon to run as a normal user (no systemd user services allowed)



Experimentation cycle



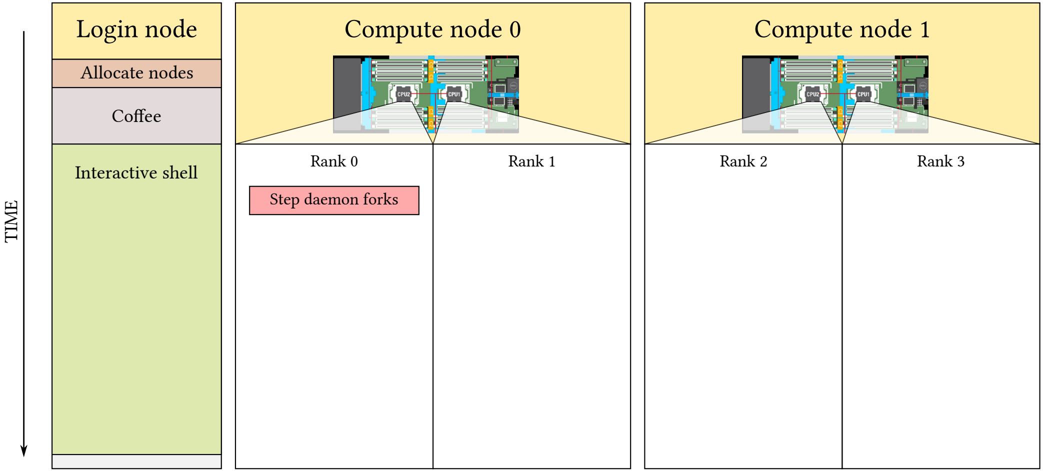
Requirement 1: safe execution environment

- Assume the program is **already built** with `nix-build` in a sandboxed environment.
- At runtime, the program may **load other libraries** (outside the nix store) with `LD_LIBRARY_PATH` or `dlopen()`
- We can create a safe execution environment similarly to the sandbox in `nix-builds` that **prevents** accesses to dangerous paths like `/usr` and `/opt`
- It needs to work with SLURM too.

Requirement 2: fast MPI intra-node communication

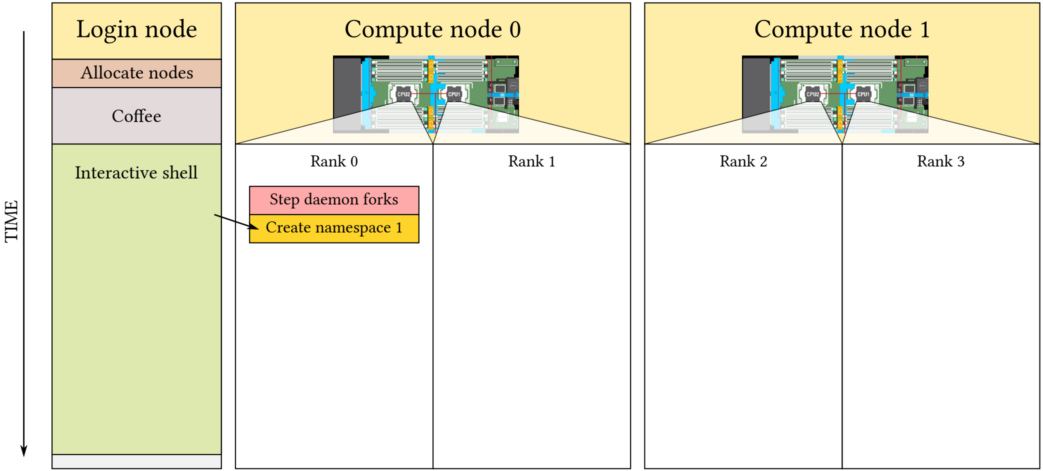
- Intra-node communication uses the `process_vm_readv()` system call.
- It only works if both processes are in the **same namespace**.
- Reenter the same namespace in the node if exists, otherwise create a new one.

Reentering the mount namespace



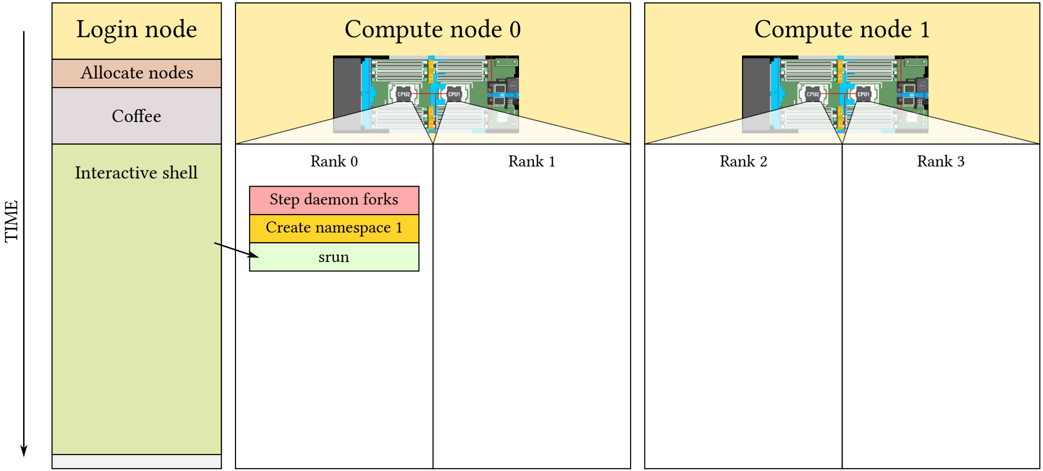
SLURM will allocate the nodes and fork a process in the first rank.

Reentering the mount namespace



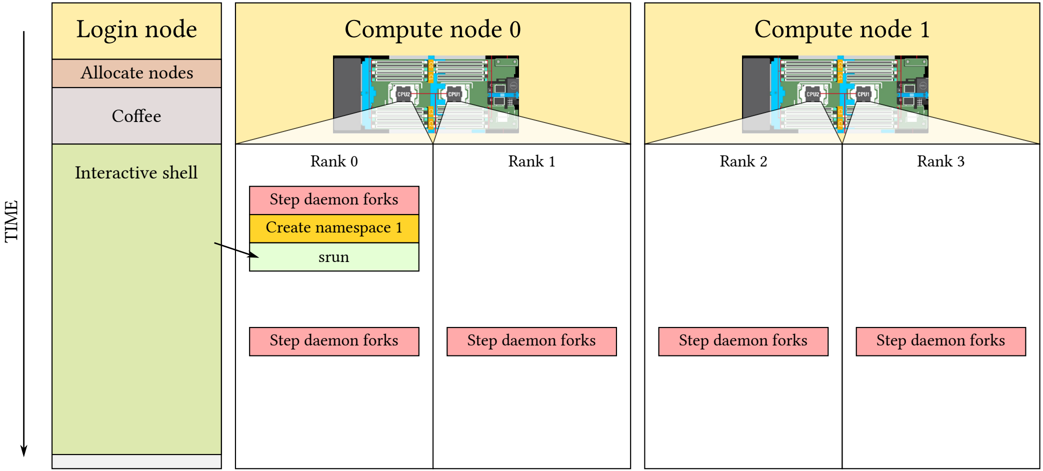
We enter the namespace from the first compute node to load `/nix`.

Reentering the mount namespace



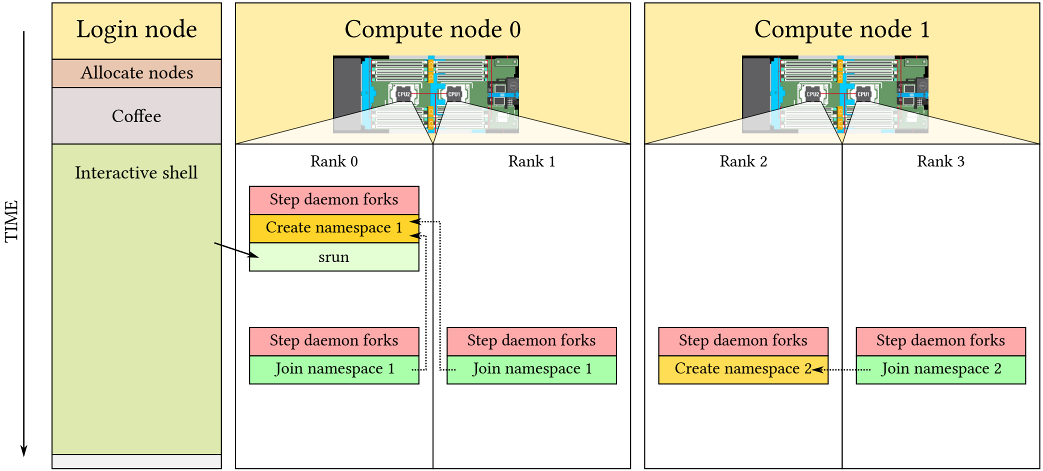
Run `srun` from nix store so we can link MPI against the same PMI2 version.

Reentering the mount namespace



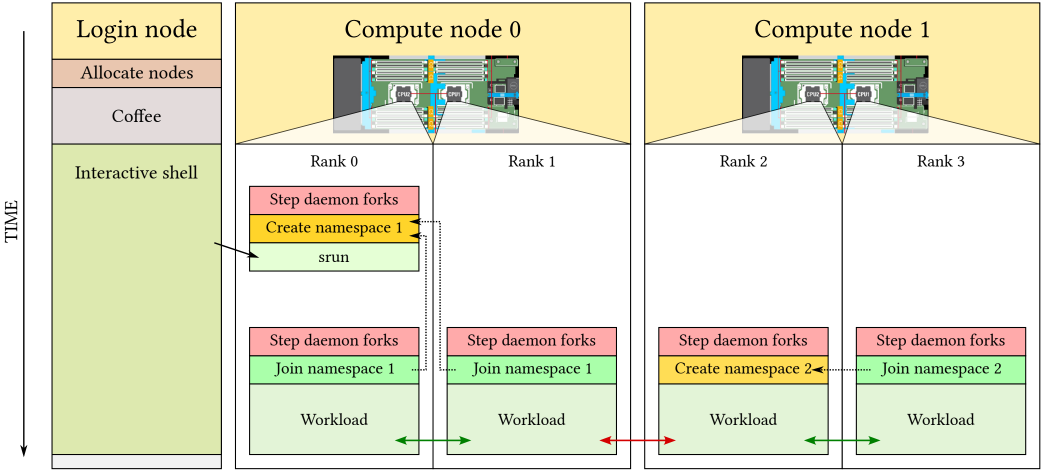
SLURM will fork a step process **outside** the safe environment.

Reentering the mount namespace



We reenter the namespace or create a new one if it doesn't exist.

Reentering the mount namespace



Finally, we can safely run the workload in parallel using **one** user namespace per node.

Requirement 3: custom software[1]

- We provide an overlay with our custom packages extending `nixpkgs`.
- Sometimes we need to add patches or specific versions to upstream packages.
- Avoid rebuilding other packages keeping the scope inside an attribute set with a custom `callPackage`.

```
last: prev:
with last.lib;
let
  inherit (last.lib) callPackageWith;
  inherit (last.lib) callPackagesWith;

  _custom = makeExtensible (custom:
    let
      callPackage = callPackageWith (last // custom);
    in
    {
      inherit callPackage;
      xyz = callPackage ./custom/xyz/default.nix { };
      mpi = custom.mpich; # Select default MPI library
      mpich = callPackage ./custom/mpich/default.nix { };
      mpichDebug = custom.mpich.override {
        enableDebug = true;
      };
      ...
    }
  );
in
  { custom = _custom; }
```

[1] https://pm.bsc.es/gitlab/rarias/bscpkgs

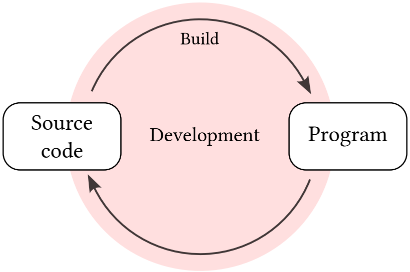
Requirement 4: custom compilers

- We need to use several compilers to build our benchmarks
- Custom LLVM compiler added with the `wrapCCWith` mechanism and setup hooks
- We also packaged some proprietary compilers with the help of `rpmextract`, `autoPatchelfHook` and *some* patience.

```
wrapCCWith {
  cc = clangOmpss2Unwrapped;
  extraBuildCommands = ''
    ...
    # Set the runtime in the wrapper to avoid rebuilds
    echo "export NANOS6_HOME=${nanos6}" >> \
      $out/nix-support/setup-hook
  '';
}
```

```
  buildInputs = [ rpmextract autoPatchelfHook ... ];
  installPhase = ''
    rpmextract rpm/intel-icc-*.rpm
    rpmextract rpm/intel-comp-*.rpm
    rpmextract rpm/intel-c-comp-*.rpm
    rpmextract rpm/intel-openmp*.rpm
    rpmextract rpm/intel-ifort*.rpm
    mkdir -p $out/{bin,lib,include}
    pushd ./opt/intel/${composer_xe_dir}/linux/
      cp -a bin/intel64/* $out/bin/
      cp -a compiler/include/* $out/include/
      cp -a compiler/lib/intel64_lin/* $out/lib/
      ln -s lib $out/lib_lin
      rm $out/lib/*.dbg
    popd
  '';
```

Development cycle



Requirement 1: fast development cycle

Issuing a full nix-build:

```
~ $ time -p nix-build llvm..
...
real 645.33
user 35119.64
```

Issuing a full nix-build + ccache:

```
~ $ time -p nix-build llvm..
...
real 102.86
user 1618.21
```

Reusing the previous build:

```
~/llvm $ vim src/...
~/llvm $ time -p ninja
...
real 8.03
user 57.01
```

- Developer wants to do fast changes and recompile without building the whole application again.
- Rebuilding the entire project with `nix-build` takes a lot of time in each cycle.
- Reuse the current source and configuration without copying to the nix store
- Cache previous builds with `make`

Requirement 2: prevent accesses to /opt or /usr

```
find_program(
  HIP_HIPCC_EXECUTABLE
  ...
  ENV HIP_PATH
  /opt/rocm /opt/rocm/hip
  PATH_SUFFIXES bin
  NO_DEFAULT_PATH
)
```

```
$ grep /opt CMakeOutput.log
Found HIP installation: /opt/rocm
```

- The `nix-shell` environment is **not isolated**
- Assume that software always tries to find software in the system
- Silent contamination with system software is not easy to detect (it builds and runs fine)
- Patching every package is doable but very time consuming
- We need to provide an **isolated development environment** without access to the system software.

Isolated development shell

Create a isolated mount namespace

```
~ $ nix-wrap
wrap ~ $ ls /usr
not found
wrap ~ $ nix-build -E '(import <nixpkgs> {}).\
  runCommand "test" {} "ls /"'
...
bin  build  dev  etc  nix  proc  tmp
```

Enter a development `nix-shell`:

```
wrap ~/llvm $ nix-shell
nix-shell ~/llvm $ vim src/...
nix-shell ~/llvm $ time -p ninja
real 10.43
user 54.68
```

Test a compiled application:

```
nix-shell ~/apps/bin $ srun nix-wrap ./app1
```

- The `nix-wrap` script uses **bubblewrap** to create the user namespace with isolated mount (no /usr or /opt)
- The nix-build command can create a **nested namespace** to perform the build in a sandbox.
- Use nix-shell with extra development packages.
- Configure phase cannot access to /opt or /usr

Requirement 3: tune for specific CPUs

- We need to build **only a subset** of packages tuned for the target CPU
- Hand crafted arguments to `-march`, *native* doesn't even work (non-reproducible too)
- Build a stdenv with the proper `hostPlatform`
- Prevent massive rebuild with stdenv inside our custom scope only

```
gccDetails = {
  arch = "armv8.2-a+crypto+fp16fml";
  tune = "tsv110";
  cpu = "tsv110";
};

stdenvNoCC = self.stdenvNoCC // rec {
  hostPlatform = self.stdenvNoCC.hostPlatform // {
    gcc = gccDetails;
  };
  targetPlatform = hostPlatform;
};

gcc11' = self.gcc11.override {
  stdenvNoCC = custom.stdenvNoCC;
};

stdenv = self.overrideCC self.stdenv custom.gcc11';
```

Conclusions

- We can benefit from the properties provided by Nix but with some drawbacks.
- Development and experimentation cycles can still be done **quickly**.
- A rootless nix daemon with a shared nix store will solve most of the problems among trusted peers in HPC.

Conclusions

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- Development and experimentation cycles can still be done **quickly**.
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Thank you!