

NUMPEX Tutorial:

How to use Guix and Spack for Application Deployment Across Supercomputers

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Challenge

Context:

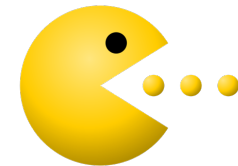
(Post-)Exascale apps are becoming increasingly **difficult to build, deploy and maintain** under the double pressure of the **growing machine complexity** and the applications' needs to combine **multiple compute and data processing paradigms (HPC+HPDA+AI)**.

At Stake:

Need for **HPC DevOps (HPCOps) methodologies and tools** to enhance **productivity** and enforce **interoperability, portability** as well as **reproducibility**.

Numpex Strategy 1/2

Empowering users beyond modules with modern **Package Managers**



Pack-Man versus Modules:

For users: more flexibility, better portability and reproducibility

For compute centers: reduced support effort

Pack-Man versus Containers:

A rich environment of user-level tools:

“virtual env”, “rollback”, “transformation”, “tune”, “test”

More flexible: can work in a containerized env or not.

Numpex Strategy 2/2

Progressive transition:

Pack-Man can produce containers:

```
guix pack -f docker mysoft
```

Pack-Man native install at compute center (with build nodes for sharing and enforced security):

```
guix install mysoft
```

Numpex supports 2 Pack-Mans:



Spack (<https://spack.io/>)

- Relaxed isolation



Guix (<https://hpc.guix.info/>)

- Strong isolation (down to libc)

NUMPEX WP3/Exa-DI Team

Exa-DI/WP3: a team dedicated to software integration

Lead: Bruno Raffin, INRIA, Benoit Martin, CEA

Part time participants: Ludovic Courtes, INRIA, Pierre Neyron, CNRS, Julien Bigot, CEA

Full-time dedicated engineers:

Romain Gabage, Bordeaux

Fernando Hayats, Grenoble

To-be-hired , Saclay

Regular contacts with national compute centers: (Idris, Cines and CCRT)

NUMPEX WP3/Exa-DI Work

Users Actions:

- Help you package your code with Guix and Spack
- Help you make Spack and Guix part of your usual tools

System Admins Actions:

- Work with compute centers to make the use of Spack and Guix as frictionless as possible

Structural Actions:

- Contribute to Spack and Guix tools and infrastructure, and key packages (MPI, compilers, etc.)

Communication Actions: at national, EU and international levels.

This Tutorial

Is about:

-How to use Guix and Spack for deployment across supercomputers

Is not about (will be the object of other tutorials):

- Learning Guix or Spack
- Learning how to package code

To reach us:

Slack: <https://numpex.slack.com/archives/C07UT051H7Y>

Mailing list: numpex-pc5-wp3@inria.fr