Containers in HPC – Pyxis

UManitoba Fall 2025
High-Performance Computing And Cloud Workshop

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October 15, 2025

About me

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Software Developer and DevOps Specialist since 2017

Linux User/Admin since 2005

What is a container

From Wikipedia (Containerization):

> *Containerization is operating-system–level virtualization or application-level virtualization so that softwares can run in isolated user spaces called "containers" in any cloud or non-cloud environment, regardless of type or vendor.*

Properties of containers

- Each container is a fully functional and portable computing environment surrounding the application and keeping it independent of other environments running in parallel
- Each container simulates a different software application and runs isolated processes (including configurations, libraries, and dependencies)
- Multiple containers share a common operating system kernel (operative system)

Terminology

Image	Archive (or number of archives – i.e. “layers”) of a filesystem tree along with metadata
Containerfile	Recipe for building an image, including OS and software within the image (e.g. *Dockerfile*)
Container	A running instance of an image (can be a computing process, or a service daemon)
Container Runtime	Lower level component responsible for reading the image and communicating with the host kernel to start containerized processes (e.g. *runc*, *crun*)
OCI (Open Container Initiative)	Open governance structure that creates open industry standards for container formats and runtimes
Registry	An online storage area for images (e.g. *DockerHub*, *Quay.io*)

Focusing On Pyxis

What is Pyxis

From GitHub (NVIDIA/pyxis):

> *Pyxis is a SPANK plugin for the Slurm Workload Manager. It allows unprivileged cluster users to run containerized tasks.*
>
> *A pyxis is an ancient small box or container.*

Features

Pyxis is currently only available on Grex, providing the following benefits:

- Seamlessly execute Slurm jobs in unprivileged containers
- Simple command-line interface
- Support for OCI image registries
- Support for layers caching and layers sharing across nodes
- Supports multi-node MPI jobs through PMI2 or PMIx
- Allows users to install packages inside the container

Command line options

Pyxis introduces some new command line options to the Slurm default job submission tools (i.e. *salloc*, *sbatch*, *srun*):

`--container-image=IMAGE[:TAG]`	Image to use for the container filesystem
`--container-mounts=SRC:DST[:OPTS][,SRC:DST]`	Bind mount(s) directories inside the container
`--container-workdir=PATH`	Working directory inside the container
`--container-remap-root`	Ask to be remapped to root inside the container
`--container-entrypoint`	Execute the entrypoint from the container image
`--container-env=NAME[,NAME]`	Names of environment variables to override with the host environment

The full list of options can be printed using the "`--help`" flag.

Example

Using `salloc`

To submit a test job using “`salloc`” and Pyxis, it is enough to specify the “`--container-image`” option:

```
salloc --partition=skylake --container-image=debian:stable-slim
```

When using Pyxis through “`salloc`”, Slurm will start an interactive job and return a shell from inside the container.

Example

Using sbatch

```
#!/bin/bash

#SBATCH --partition=lgpu
#SBATCH --nodes=1
#SBATCH --gpus=2
#SBATCH --ntasks=4
#SBATCH --cpus-per-task=8
#SBATCH --mem-per-cpu=8G
#SBATCH --container-image=nvcr.io/hpc/gromacs:2023.2
#SBATCH --container-mounts=/PATH/TO/INPUT:/host_pwd
#SBATCH --container-workdir=/host_pwd
#SBATCH --container-entrypoint

gmx mdrun -ntmpi 4 -ntomp 8 -nb gpu -pme gpu -npme 1 -update gpu -bonded gpu \
    -nsteps 100000 -resetstep 90000 -noconfout -dlb no -nstlist 300 -pin on \
    -v -gpu_id 01
```

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Demo

Running a GROMACS benchmark with Pyxis

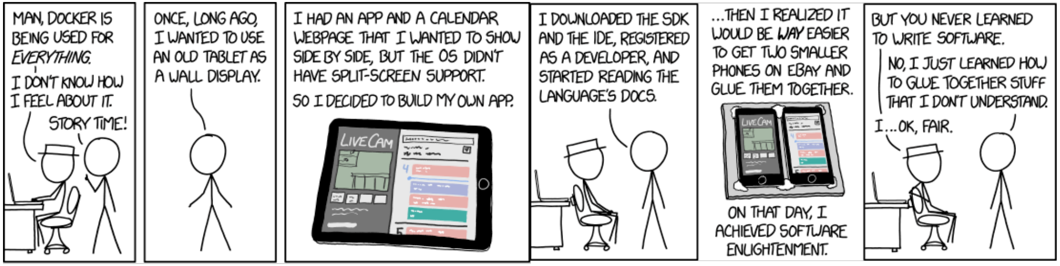
Running a GROMACS benchmark with Pyxis

Specifications

Container Engine	⇒	Pyxis/Enroot (on Grex)
Image	⇒	nvcr.io/hpc/gromacs:2023.2 (from the nVidia NGC Catalog)
Software	⇒	GROMACS
Benchmark	⇒	STMV

Is Pyxis a silver bullet?

- Always check if the same software is already provided via modules-based HPC software stack
- It requires *well-built* images
  - Making or finding a suitable image is a bit of work
  - Bleeding-edge versions of programs could be poorly maintained/tested (including their images)
- Useful to encapsulate software and sometimes data to reduce number of files (e.g. python or conda based programs)


MAN, DOCKER IS BEING USED FOR *EVERYTHING*.
I DON'T KNOW HOW I FEEL ABOUT IT.
STORY TIME!
ONCE, LONG AGO, I WANTED TO USE AN OLD TABLET AS A WALL DISPLAY.
I HAD AN APP AND A CALENDAR WEBPAGE THAT I WANTED TO SHOW SIDE BY SIDE, BUT THE OS DIDN'T HAVE SPLIT-SCREEN SUPPORT.
SO I DECIDED TO BUILD MY OWN APP.
LIVE CAM
I DOWNLOADED THE SDK AND THE IDE, REGISTERED AS A DEVELOPER, AND STARTED READING THE LANGUAGE'S DOCS.
...THEN I REALIZED IT WOULD BE *WAY* EASIER TO GET TWO SMALLER PHONES ON EBAY AND GLUE THEM TOGETHER.
ON THAT DAY, I ACHIEVED SOFTWARE ENLIGHTENMENT.
BUT YOU NEVER LEARNED TO WRITE SOFTWARE.
NO, I JUST LEARNED HOW TO GLUE TOGETHER STUFF THAT I DON'T UNDERSTAND.
I...OK, FAIR.

XKCD [1988]

Questions?

Thank you

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