Containers in HPC – Podman

UManitoba Fall 2026
High-Performance Computing And Cloud
Workshop

Stefano Ansaloni

University of Manitoba

October 22, 2026



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Digital Research Alliance of Canada

Stefano Ansaloni

Cloud Computing Specialist at University of Manitoba

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.*

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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)

Wikipedia [Containerization]

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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*)

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Focusing On Podman



What is Podman

From Wikipedia (Podman):

> *Podman (pod manager) is an open source OCI-compliant container management tool from Red Hat used for handling containers, images, volumes, and pods; offering APIs for the lifecycle management of those components (the API is identical to the Docker API).*

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Why not Docker

Podman aims to provide a more secure and lightweight alternative to Docker:

- Daemonless ⇒ Don't rely on a process with root privileges to run containers
- Rootless containers ⇒ Run containers as regular users, without interacting with a root-owned daemon
- User namespaces ⇒ Careful use of kernel capabilities

Red Hat [What is Podman]
Better Stack [Exploring Podman]

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Compatibility with Docker

For most use cases, Podman can be used as a “drop-in” replacement for Docker:

- Podman CLI syntax is almost the same as Docker’s one
- Podman can use the same images as Docker
- Podman can use the same registries as Docker

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Podman on HPC – Disclaimer

Podman is considered an advanced tool to be used only by experienced users when their workloads cannot be run using standard HPC programs/modules, or through Singularity/Apptainer (i.e. Podman should be the very last resort).

In any case, Podman must **NOT** be used:

- on login nodes
- to execute long-running services (e.g. daemons, databases, ...)

Podman on HPC

Podman is available as a module on national clusters and UManitoba HPC cluster (Grex).

HPC System	Command	Current version
National Clusters	`module load StdEnv/2023 podman`	5.7.1
Grex	`module load podman`	5.8.9

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Podman on Grex

When on Grex, it is important to use the local version of Podman:

- local proxy cache for registries
- better default configuration
- newer version

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Basic commands

Print version	`podman version`
Pull image	`podman pull <REGISTRY>/<NAME>:<TAG>`
Delete image	`podman image rm <IMG>`
List images	`podman image ls`
Create and start a container	`podman run [OPTS] <IMG> [CMD [ARGS]]`
Execute command inside a running container	`podman exec [OPTS] <CNT> [CMD [ARGS]]`
Stop a running container	`podman stop <CNT>`
Start a stopped container	`podman start <CNT>`
Delete a container	`podman rm <CNT>`
List containers	`podman ps [-a]`

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Getting an image

From a registry

The "`pull`" subcommand can be used to download an image from an online registry (e.g. *DockerHub*) into a local (temporary) registry, that is available only on the node where the *pull* has been performed and will be deleted when the job ends.

```
podman pull docker.io/alpine
```


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Getting an image

Building your own

If it becomes necessary to build a custom image, it can be accomplished with the "`build`" subcommand.

By default the built image will be saved into a local (temporary) registry, that is available only on the node where the *build* has been performed and will be deleted when the job ends.

To overcome this problem, the "`--tag`"/"`-t`" option can be specified using "`docker-archive:`" as the *tag* prefix.

```
podman build -t docker-archive:/path/to/custom.image \
             -f /path/to/Containerfile
```


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Binding host directories

To let containers access data on the host (e.g. the user home directory), the "`--volume`" / "`-v`" option can be specified (multiple times) using the format "`HOST_DIR:CNT_DIR`".

```
podman run -v $HOME:$HOME docker.io/alpine ls $HOME
```

When binding directories, the container will be able to read and write the content of those directories (if the user has the correct filesystem permissions).

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Setting environment variables

The option "--env" / "-e" can be specified (multiple times) to set environment variables inside the container.

```
podman run -e V1="hi" -e V2="$USER" docker.io/alpine sh -c 'echo $V1 $V2'
```

If the value is not specified, Podman will map the host variable value into the container.

```
podman run -e USER docker.io/alpine sh -c 'echo $USER'
```


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Demo

Running a GROMACS benchmark with Podman



Running a GROMACS benchmark with Podman

Specifications

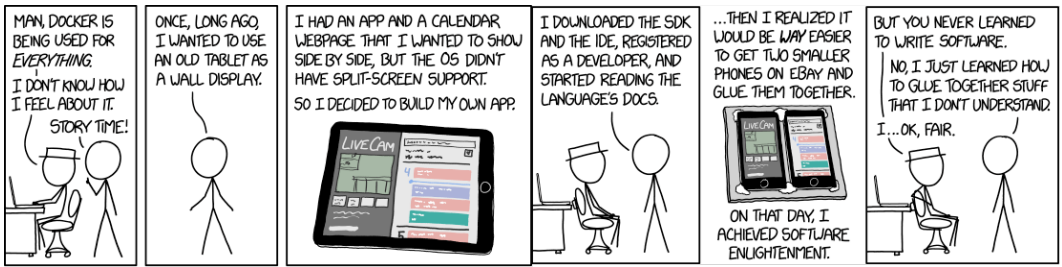
Container Engine	⇒	Podman (on Grex)
Image	⇒	nvcr.io/nvidia/gromacs:v2026.2 (from the nVidia NGC Catalog)
Software	⇒	GROMACS
Benchmark	⇒	STMV

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Is Podman 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)

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XKCD [1988]

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Questions?

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Thank you

