Distributed HPC Applications with Unprivileged Containers

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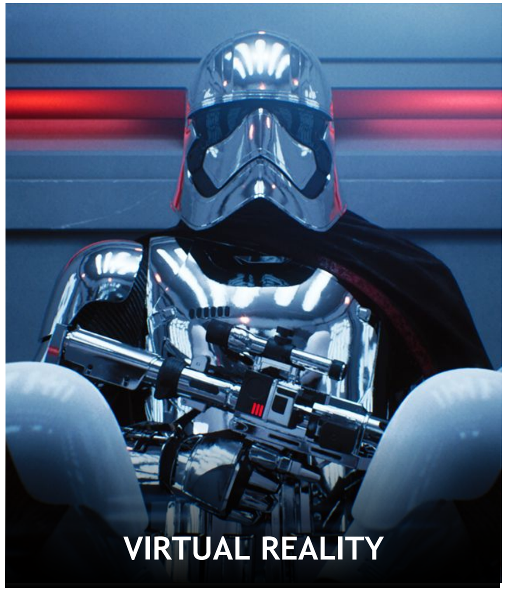
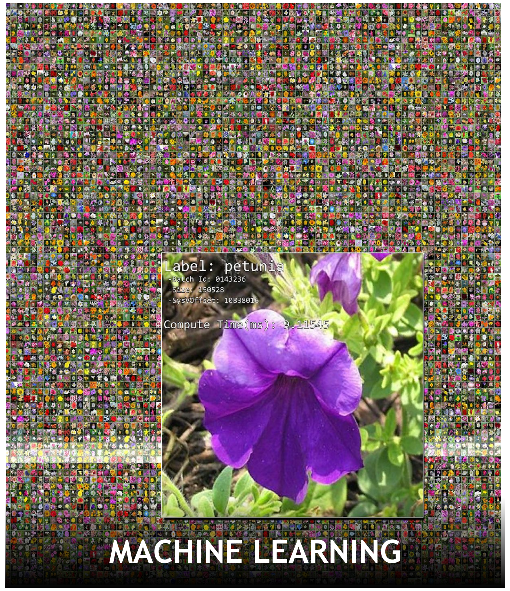
GPU Computing

Beyond video games





```
Label: petunia
 -Batch Id: 0143236
 -Size: 150528
 -SysVOffset: 10838016

Compute Time(ms): 9.11545
```

GPU COMPUTING

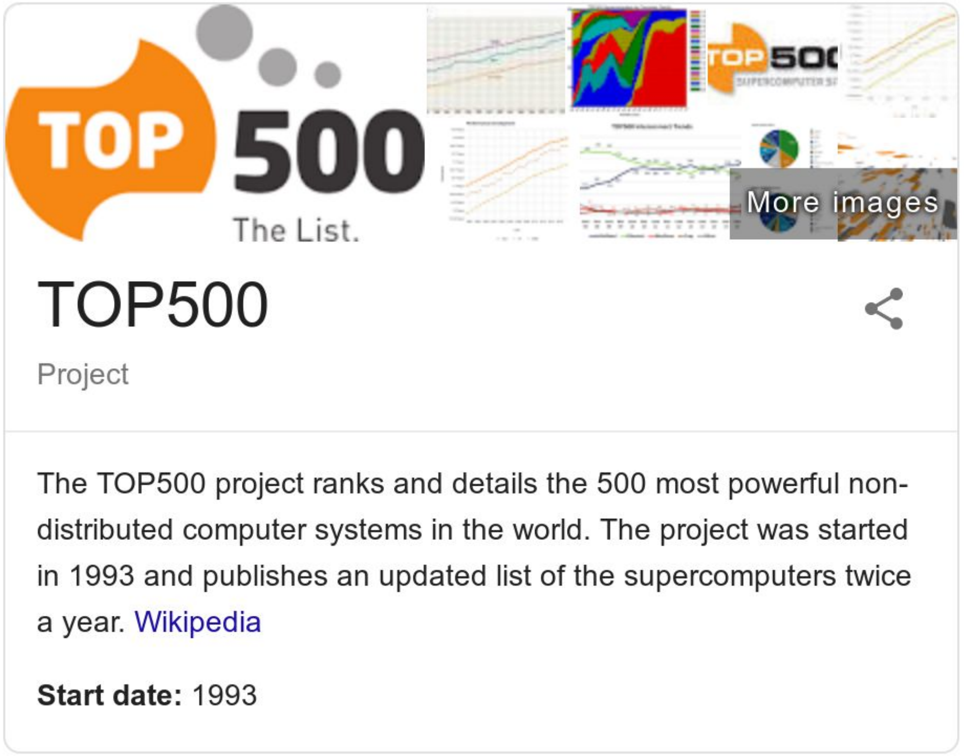
Infrastructure at NVIDIA

DGX SuperPOD GPU cluster (Top500 #20)

SYSTEM SPECIFICATIONS

GPUs	16X NVIDIA® Tesla V100
GPU Memory	512GB total
Performance	2.1 petaFLOPS
NVIDIA CUDA® Cores	81920
NVIDIA Tensor Cores	10240
NVSwitches	12
Maximum Power Usage	12kW
CPU	Intel® Xeon® Platinum 8174 CPU @3.10GHz, 24 cores per CPU
System Memory	1.5TB
Network	8X 100Gb/sec Infiniband/100GigE Dual 10/25/40/50/100GbE
Storage	OS: 2X 960GB NVME SSDs Internal Storage: 30TB (8X 3.84TB) NVME SSDs
Software	Ubuntu Linux OS

x96



TOP500

Project

The TOP500 project ranks and details the 500 most powerful non-distributed computer systems in the world. The project was started in 1993 and publishes an updated list of the supercomputers twice a year. Wikipedia

Start date: 1993

NVIDIA Containers

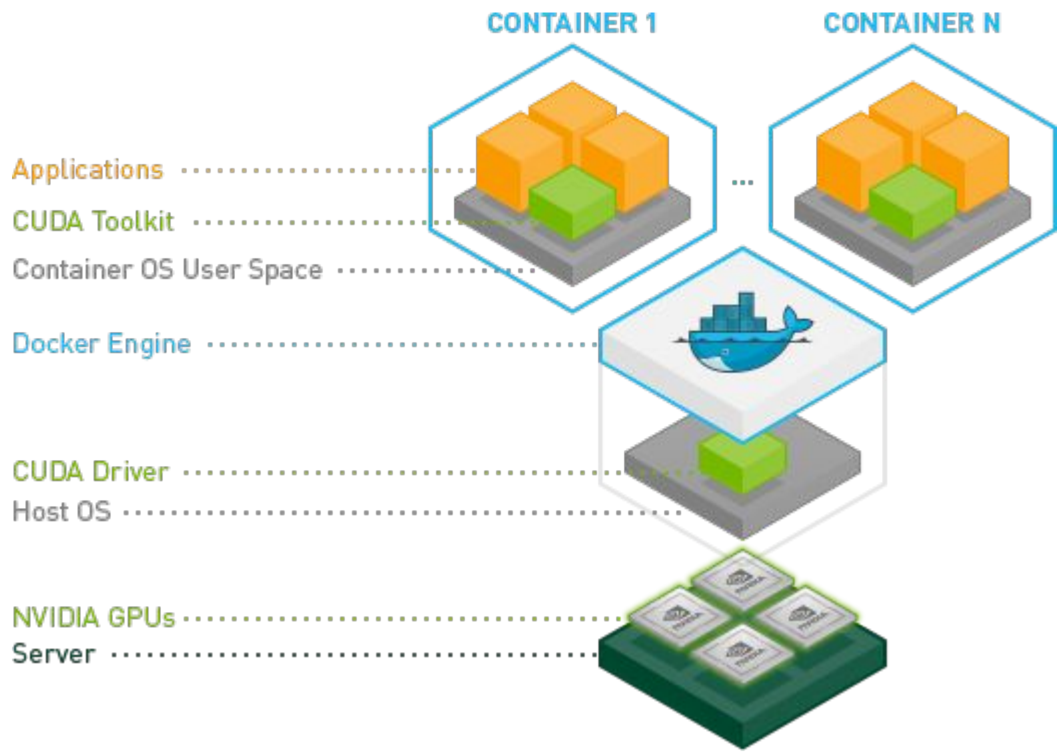
Supports all major container runtimes

We built libnvidia-container to make it easy to run CUDA applications inside containers

We release optimized container images for each of the major Deep Learning frameworks every month

We use containers for everything on our HPC clusters - R&D, official benchmarks, etc

Containers give us portable software stacks without sacrificing performance



Typical cloud deployment

e.g. Kubernetes

Hundreds/thousands of small nodes

All applications are containerized, for security reasons

Many small applications running per node (e.g. microservices)

Traffic to/from the outside world

Not used for interactive applications or development

Advanced features: rolling updates with rollback, load balancing, service discovery

GPU Computing at NVIDIA

HPC-like

10-100 very large nodes

“Trusted” users

Not all applications are containerized

Few applications per node (often just a single one)

Large multi-node jobs with checkpointing (e.g. Deep Learning training)

Little traffic to the outside world, or air-gapped

Internal traffic is mostly RDMA

Slurm Workload Manager

https://slurm.schedmd.com/slurm.html

Advanced scheduling algorithms (fair-share, backfill, preemption, hierarchical quotas)

Gang scheduling: scheduling and starting all processes of a multi-node job simultaneously

Low runtime overhead

Topology-aware (NUMA/PCIe) job scheduling for better performance

Simple CLI with jobs as bash scripts

GPUs are a first-class resource

Supports interactive jobs

Slurm does not support containers out of the box… but is extensible through plugins

Containers for HPC

What do we need?

High performance

Support for Docker images

Soft cluster multi-tenancy

Exposing NVIDIA GPUs and Mellanox InfiniBand cards inside containers

Resources (CPU/Mem/GPUs/HCAs) isolation through cgroups

Launching multi-node jobs

Development workflow: interactive jobs, installing packages, debugging

No existing container runtime fulfilled all our requirements, so we built our own

Unprivileged runtime

aka “rootless”

Writing a **secure** privileged container runtime is **very hard** (see the latest runc CVEs)
Watch "*Securing Container Runtimes -- How Hard Can It Be?*" - Aleksa Sarai (LCA 2020)

Even when trusting users to not actively exploit the runtime, we don’t want real root:

- users could break the system, or corrupt shared filesystems
- users won’t be able to delete files created from the container
- users won’t be able to gdb/strace applications running inside the container

ENROOT

Overview

Fully unprivileged “chroot”

Standalone

Little isolation, no overhead

Docker image support

Simple image format

Composable and extensible

Simple and easy to use

Advanced features

User namespaces

root outside container != root inside container

We use “user namespaces” with **optional** remapping to UID 0

```
root@superpod-01:/root# cat /proc/self/uid_map
         0       1000          1

felix@superpod-01:/home/felix$ cat /proc/self/uid_map
      1000       1000          1
```

Some applications refuse to run as UID 0

Convenient to have the same username and $HOME inside and outside the container

runc-based container runtimes always remap you to UID 0 inside the container

Subordinate UIDs/GIDs

/etc/subuid and /etc/subgid

We run application containers, we don’t need UID separation

Installing packages requires to be UID 0, **plus additional UIDs**

Difficult to maintain subordinate UIDs across multiple nodes

Permissions issues for files you created while assuming a subordinate UID

We use a seccomp filter to trap all setuid-related syscalls, to make them succeed

Standalone runtime

Low overhead and ephemeral

No persistent spawning daemon

Inherits cgroups from the job as opposed to Docker

The runtime prepares the container and then executes the application

runc and docker (containerd-shim) have “supervisor” processes

Minimal isolation

Containers for packaging applications, not sandboxing

We don’t need an IP for each container, nor need to bind “privileged” ports

A PID namespace requires careful handling for the PID 1 process and tend to confuse programs

We want only 2 namespaces: mount and user

Resource isolation (cgroups) is handled by the scheduler (e.g. Slurm)

Having minimal isolation simplifies the runtime and improves performance

Impact on performance

Container isolation is bad for performance

Using a network namespace adds overhead (bridge, NAT, overlay…)

Seccomp and LSMs (AppArmor, SELinux) have an overhead

We need a shared IPC namespace (and `/dev/shm`) for fast intra-node communications

Rlimits might not be adapted to certain workloads (e.g. Docker memlock)

Seccomp triggers Spectre mitigation on most distributions:

```
$ docker run ubuntu grep 'Speculation_Store_Bypass' /proc/self/status
Speculation_Store_Bypass:       thread force mitigated
```

Message Passing Interface

The HPC industry standard

We use MPI for intra/inter nodes communications of distributed jobs

PID/IPC namespaces confuses MPI for intra-node communications

CMA (`process_vm_writev`) requires ptrace access between processes

We use PMI/PMIx for coordination and need pass file descriptors from Slurm to the application

Importing Docker images

Speeding up the pull

The hardest part of the container runtime: authentication, OCI manifests, AUFS whiteouts

Rely on overlayfs rather than sequential extraction (e.g. docker, umoci)

Pipelines like "`parallel curl|pigz|tar`" tend to be faster than Golang alternatives

The "`vfs`" format has a huge storage cost (each layer copies the full rootfs)

Layers are usually uncompressed and not shared across users

Enroot shares layers across users, and they are compressed with `zstd`

We have helper binaries with capabilities to convert AUFS to overlayfs and to create a squashfs image of all the layers

Image format

KISS and Unixy

Standard squashfs file and configuration files:

```
ENTRYPOINT=/etc/rc        ENV=/etc/environment        VOLUME=/etc/fstab
```

Editing configuration from within the container is straightforward

Squashfs images, can be stored on parallel filesystems as a single file

Avoids thundering herd problems on multi-node jobs

Useful for air gapped systems, admins can control the applications you can run

Can be mounted as a block device and lazily fetched (e.g. over NFS)

Simple and Extensible

Accommodates heterogeneous clusters

The runtime is a simple shell script consisting of ~500 LoC

Uses a set of basic Linux utilities for unprivileged users

System wide and user-specific configurations to control the container environment, mounts and (prestart) hooks

Admins and users can customize the runtime, including tweaking builtins features (e.g. cgroups, shadow DB, GPU/HCA support)

ENROOT

Basic usage

```
# Convert a Docker image to squashfs file
$ enroot import docker://nvcr.io#nvidia/tensorflow:19.08-py3
$ ls nvidia+tensorflow+19.08-py3.sqsh

# Extract a squashfs to a rootfs
$ enroot create --name tensorflow nvidia+tensorflow+19.08-py3.sqsh
$ ls -d ${XDG_DATA_PATH}/enroot/tensorflow

# Start the container with optional root remapping and read/write rootfs
$ enroot start tensorflow nvidia-smi -L
$ enroot start --root --rw tensorflow apt update && apt install …
```

ENROOT

Advanced usage

```
# Run an in-memory container from a squashfs image through fuse
$ enroot start ubuntu.sqsh

# Build a self-extracting TensorFlow bundle (image + runtime) and run it like you
# would run any executable
$ enroot bundle --output tensorflow.run nvidia+tensorflow+19.05-py3.sqsh
$ ./tensorflow.run python -c 'import tensorflow as tf; print(tf.__version__)'
```

ENROOT

Advanced Linux utilities

`enroot-unshare`	similar to `unshare(1)` and `nsenter(1)`
`enroot-mount`	similar to `mount(8)`
`enroot-switchroot`	similar to `pivot_root(8)` and `login(1)`
`enroot-aufs2ovlfs`	converts AUFS whiteouts to OverlayFS
`enroot-mksquashovlfs`	`mksquashfs(1)` on top of OverlayFS

ENROOT

“Container” from scratch

```
$ curl https://cdimage.ubuntu.com/[...]/ubuntu-base-16.04-core-amd64.tar.gz | tar -C ubuntu -xz

$ enroot-nsenter --user --mount bash

$ cat << EOF | enroot-mount --root ubuntu -
  ubuntu      /         none bind,rprivate
  /proc       /proc     none rbind
  /dev        /dev      none rbind
  /sys        /sys      none rbind
EOF

$ exec enroot-switchroot ubuntu bash
```

Slurm plugin

100% YAML-free

Our plugin adds new arguments to the Slurm CLI:

```
# Bare-metal application
$ srun python train.py

# Containerized application
$ srun --container-image=tensorflow/tensorflow python train.py
```

The container image is imported and the container is started in the background

Before Slurm execs `python train.py`, the plugin joins the running container:

- `setns(container_userns_fd, CLONE_NEWUSER)`
- `setns(container_mntns_fd, CLONE_NEWNS)`
- `import /proc/container_pid/environ`
- `chdir(container_workdir)`

Slurm example 1

Interactive single-node job

```
# You can start a container by importing an image from Docker Hub
$ srun --container-name=pytorch --container-image=pytorch/pytorch apt install -y vmtouch

# We can reuse the existing container and execute our new binary on the dataset
$ srun --container-name=pytorch --container-mounts=/mnt/datasets:/datasets vmtouch /datasets

# Now we can start an interactive session inside the container, for development/debugging:
$ srun --container-name=pytorch --container-mounts=/mnt/datasets:/datasets --pty bash
root@superpod-01:/workspace#
```

Slurm example 2

Batch multi-node jobs

```
$ cat job.sh
#!/bin/bash

# You can start a container on each node from a shared squashfs file
srun --nodes=64 --ntasks-per-node=16 --mpi=pmix \
     --container-image=/mnt/apps/tensorflow.sqsh --container-mounts=/mnt/datasets:/datasets \
     python train.py /datasets/cats
# The container rootfs get automatically cleaned up at the end of the script
echo "Training complete!"

# Submitting the job is done through the command-line too
$ sbatch --nodes=64 --output=tensorflow_training.log job.sh
```

Conclusion

We built a new container runtime for our use case

a. Unprivileged
b. Lightweight, without excessive isolation
c. Flexible plugins, including support for NVIDIA and Mellanox devices

http://github.com/nvidia/enroot

http://github.com/nvidia/pyxis (Slurm plugin)

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