CSCS
Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

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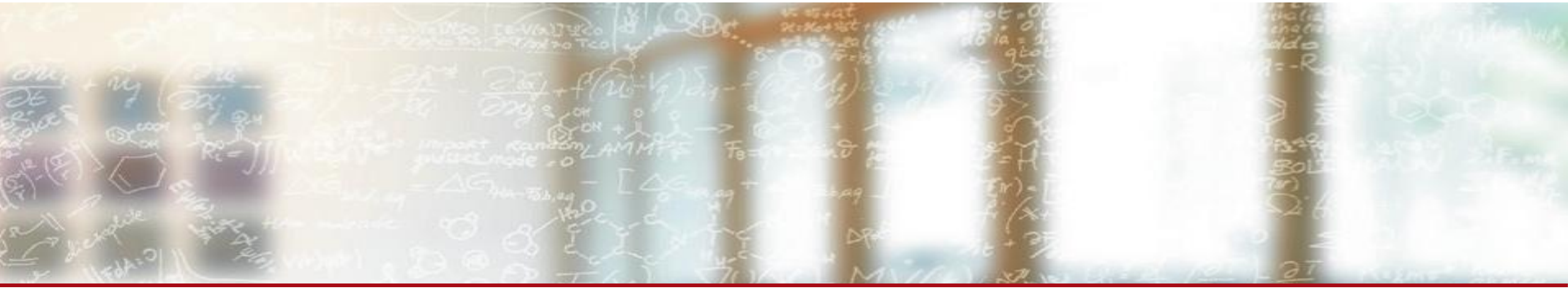

Onboarding SDSC users at CSCS

Workshop

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CSCS

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Structure of the day

Morning

- Alps overview
- MFA access
- SSH configuration:
  - Daint login nodes and compute nodes
  - Login with VS code
- Running jobs using sbatch
- Conda environment
  - create custom jupyter-kernel
    - shared between Jupyter service, IDE and shell
    - finish by running python script through sbatch

Afternoon

- Running containers with Sarus on Piz Daint
  - …using NGC containers for single node and distributed deep learning
  - Large scale training on Piz Daint in MLPerf

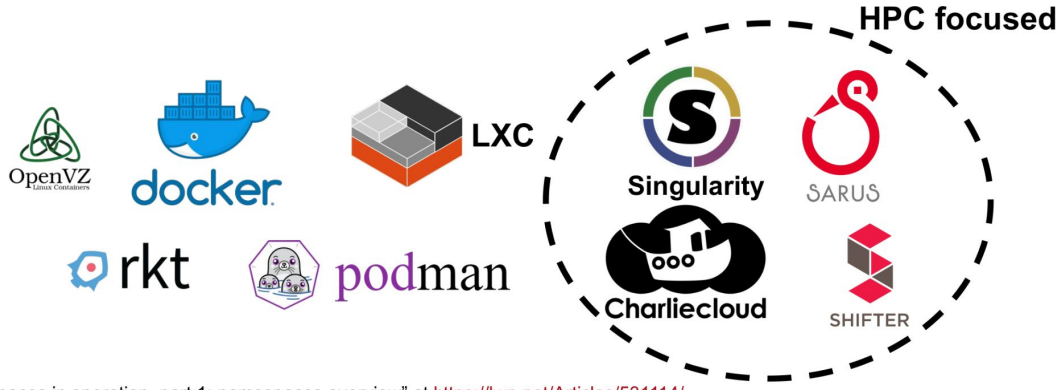
- Outlook on Alps
  - New container engine
  - FirecREST for automated workflows
  - High-performance data science with RAPIDS on Clariden

Containers - key concepts

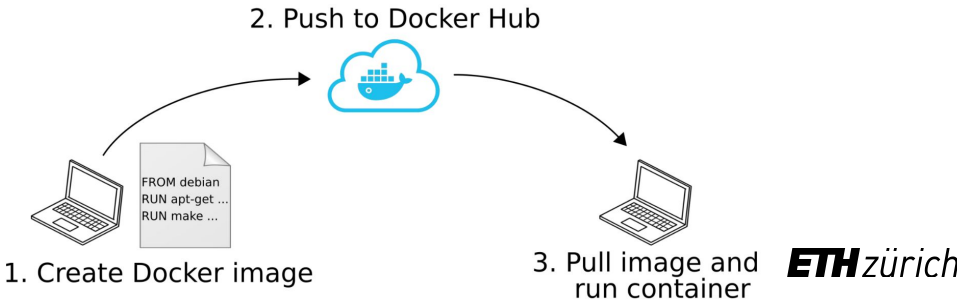
- **Isolated environments** to run applications/services
- **Images** include all software dependencies
  - standalone, executable package including code, runtime libraries, configuration files of an application
  - provides the filesystem and metadata (e.g. environment variables, initial working directory) for a container
- **Container** : a process isolated from the rest of the system through abstractions created by the OS.
  - The level of isolation can be controlled, allowing access to host resources.
  - Its filesystem content comes from an image.
  - “runtime instance” of an image: what the image becomes in memory when executed.
- **Reproducible** (explicit dependencies, consistent environment, immutable infrastructure, host-isol.), **portable, easy to build, quick to test & deploy**

Linux containers ecosystem

- Linux containers rely on abstraction features (namespaces[1]) provided by the kernel
- Different design decisions and use cases gave rise to several solutions:



[1] “Namespaces in operation, part 1: namespaces overview” at https://lwn.net/Articles/531114/



Using NVIDIA GPUs in Docker

GPU-accelerated application

- Included/built in the image, along with its runtime dependencies
- NVIDIA provides base images for CUDA, featuring compilers, runtime and accelerated libraries: https://hub.docker.com/r/nvidia/cuda
- Quickest way to get a Dockerfile going:
  `FROM nvcr.io/nvidia/cuda`

GPU driver

- It is tied to the hardware: cannot be part of a portable image!
- Has to be imported upon container creation
- NVIDIA Container Toolkit to the rescue!
  https://github.com/NVIDIA/nvidia-docker
- Docker >= 19.03 has native support:
  `docker run --gpus all nvcr.io/nvidia/cuda nvidia-smi`

Docker and HPC: not a good fit

- Security model assumes root privileges
- No integration with workload managers
- Missing support for diskless compute nodes
- Very limited support for kernel bypassing devices (e.g. accelerators and NICs)
- No adequate parallel storage driver

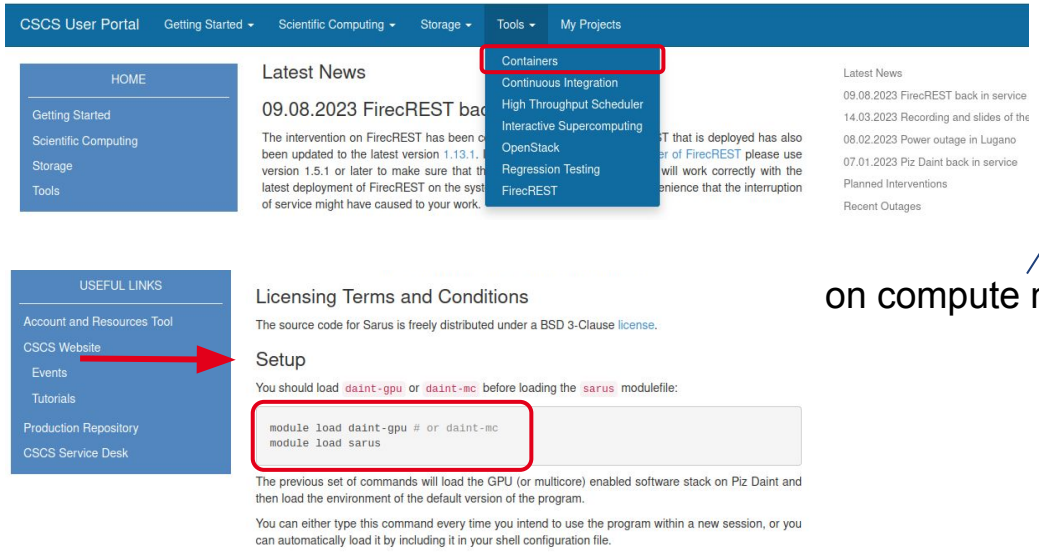
The Sarus container engine

- Security oriented to HPC systems
- SLURM-aware
- Integrates with HPC infrastructure and software
- OCI-compliant runtime that customizes containers through OCI hooks
  - HW can achieve native performance
- Pulls regular Docker images (e.g. from Docker Hub etc.) and provides Docker-like CLI

→ combines container portability with native HPC performance

Sarus resources

- user.cscs.ch→Containers→Sarus→Setup



- Comprehensive user guide
- Unofficial cheat sheet by Tomas Aliaga
- More materials at eth-cscs/containers-hands-on by Alberto Madonna

on compute node

Basic Commands	
help	List **commands** and *options*
version	Print sarus semantic version
--debug	Make commands output debug logs
--verbose	Make commands output info logs

Sarus is driven by its *sarus.json* configuration file, typically located at */opt/sarus/<version-number>/etc/sarus.json*.

Images		
images	`sarus images`	List local images
pull	`sarus pull python:alpine`	Pull image from DockerHub
load	`sarus load ./debian.tar my_debian`	Loads tarball as image
rmi	`sarus rmi centos:7`	Deletes image

Runtime	
run	`sarus run alpine cat /etc/os-release`
--tty	Allocate a pseudo-TTY in the container
--entrypoint echo hi	Overwrite the default ENTRYPOINT of the image
--mount=type=bind, src=HD,dst=CD	Mount custom host directories HD into the container at CD
--mpi	Enable MPI support
--ssh	Enable SSH in the container
--centralized-repository	Use centralized repository instead of the local one

You need to **pull** the image before you can **run** the container.

Useful Links	
documentation	https://sarus.readthedocs.io
</> code	https://github.com/eth-cscs/sarus/
download	https://github.com/eth-cscs/sarus/releases

on compute node (prev. salloc)

Examples on Localhost

```
GPU    sarus run ethcscs/cudasamples:9.2
nbody  /usr/local/cuda/samples/bin/x86_64/linux/release/nbody
       -benchmark -fp64 -numbodies=2000
```

on login node, through SLURM

Examples on HPC

```
GPU    srun -C gpu -N1 -t1 sarus run
nbody  ethcscs/cudasamples:9.2
       /usr/local/cuda/samples/bin/x86_64/linux/release/nbody
       -benchmark -fp64 -numbodies=200000
MC     srun -C gpu -N2 -t2 sarus run --mpi
all2all ethcscs/osu-mb:5.3.2-mpich3.1.4 ./osu_latency
```

Find more examples in the Sarus Cookbook.

Practical part - developing with Sarus on Piz Daint

Go to https://github.com/lukasgd/SDSC-user-onboarding

Distributed Training

Instructions for Horovod (alternative to DDP):

- user.cscs.ch→ Data Science → PyTorch

Large-scale distributed training comes in different flavors

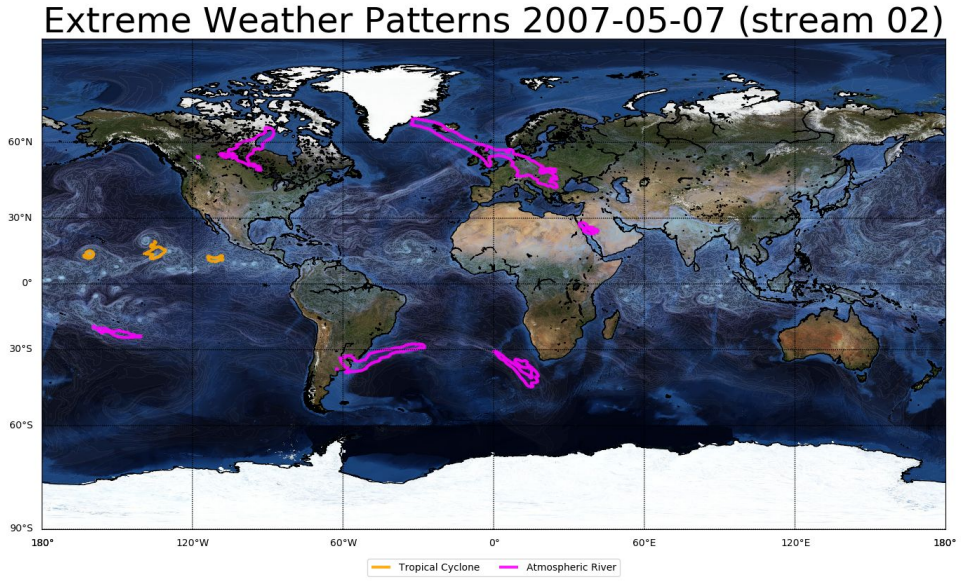
- data-parallel is most accessible
- pipeline-, model-parallel more advanced
- Experience from MLPerf HPC benchmark
  - https://mlcommons.org/en/training-hpc-07/, hpc-10/
  - significant speedups possible, e.g. DeepCAM with 9 TB requiring ~300 GPU hours converges in ~20 mins on 1000 GPUs!
  - more details presented at MLHPC SC'21

Considerations for scaling SGD with data-parallelism

- Optimize on a single GPU first
  - data loader - check GPU utilization, compare to loading synthetic data, be aware of kernel launch overhead
- Then scale horizontally
  - aim for ideal weak scaling, tune communication
- Be aware of convergence (#epochs) as a function of batch size

DeepCAM

- Gordon-Bell prize paper at SC18 (Kurth et al)
- convolutional encoder-decoder segmentation model
- identifies extreme weather phenomena: atmospheric rivers and tropical cyclones (3 per-pixel classes)
- 8.8 TB climate simulation data (HDF5), 0.25° spatial, 3h temporal resolution, shape (768, 1152, 16)
- Reference implementation in PyTorch



Outlook on Alps

Flash-based scratch FS

New container engine on Alps
- based on enroot/pyxis
- more user-friendly
  - TOML format
  - Infrastructure-as-Code
  - closer integration with SLURM

```
$ cat env.toml
image = "/iopsstor/scratch/.../.enroot/my_images/NGC-pytorch-23.09-py3.sqsh"
mounts = ["/iopsstor/scratch/cscs/lukasd:/scratch", "/users/lukasd"]
workdir = "/iopsstor/scratch/cscs/lukasd/path/to/repo"
writable = true

$ srun -ul --environment=$(pwd)/env.toml --gpus-per-task=1 bash -c '...'
```

Clariden
- Current testbed for the ML platform

Node configuration
- 128-core CPU
- > 500 GB RAM
- 4 A100 GPUs per node

Enables high-performance data science with RAPIDS:
https://github.com/lukasgd/SDSC-user-onboarding/tree/main/clariden

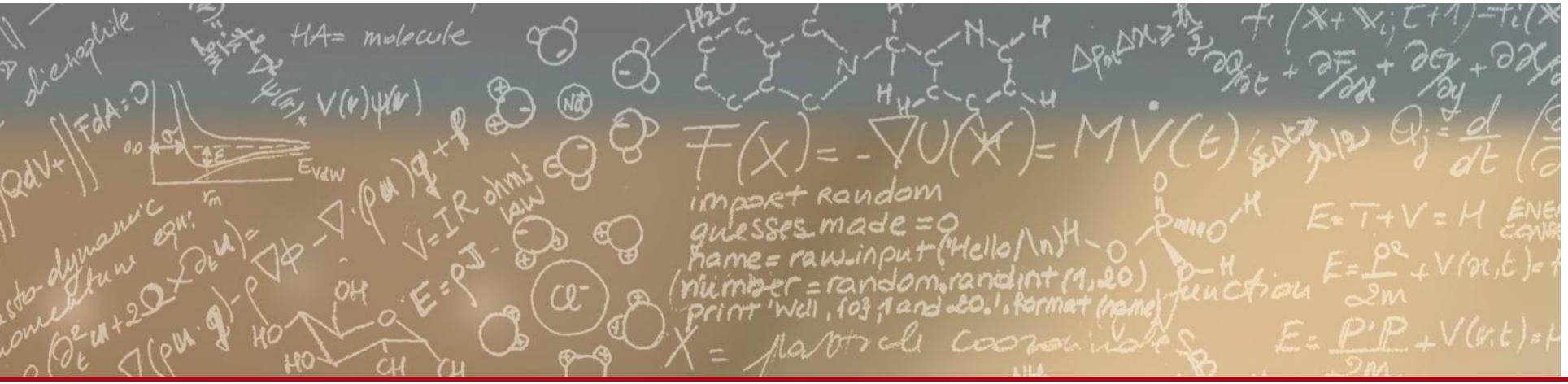
FIRECREST

REST API for HPC systems
https://firecrest-api.cscs.ch/

Take Home Messages

- It is very easy to set up persistent Conda environments on CSCS machines
  - They are reusable in the shell, IDE and the Jupyterlab service
  - Use miniconda to create custom development environments
  - It is also possible to attach IDEs (like VS Code) to compute nodes
  - Writing multi-gpu ML programs is easy, with DDP/Horovod/etc, then launch with `SBATCH` scripts
- **Sarus**, our high performance container engine allows using Docker images pushed to Dockerhub on compute nodes at CSCS
  - Start with **Nvidia NGC containers** for key packages like PyTorch/TensorFlow/etc as a basis
  - Containers are used for **CI on CSCS hardware** for development projects hosted on Git repos
- The **future ALPS platform** will be a **containers-first ecosystem** where replicating environments is designed to be seamless and user-friendly
  - **Full flash storage** for home and scratch for fast I/O
  - **Powerful CPU+GPU** hardware with **large memory** and **high bandwidths**
  - Dedicated cluster and service offering for the ML/AI user community
  - Customized workflows and services can be built with **FirecREST** (products.cscs.ch)

… also, we are just one floor away!



Thank you for your attention.