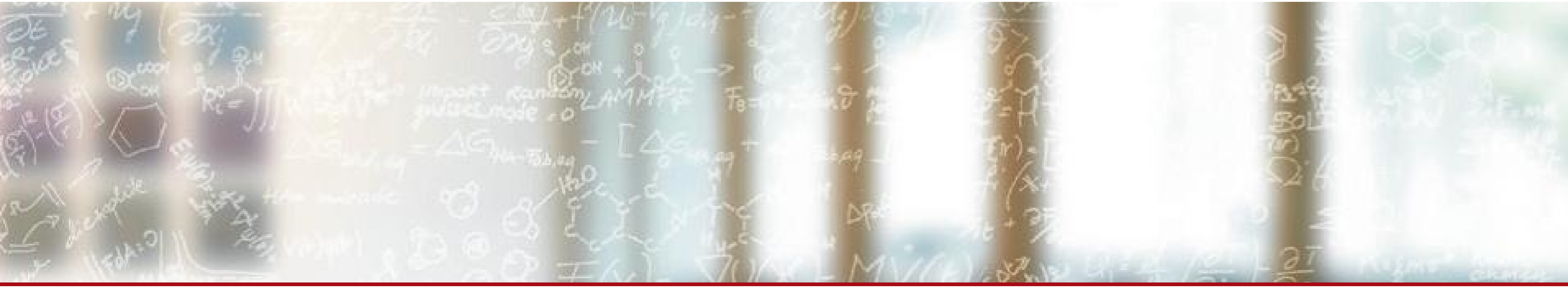
CSCS
Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

ETH zürich



Shifter: Fast and consistent HPC workflows using containers

CUG 2017, Redmond, Washington

Lucas Benedicic, **Felipe A. Cruz**, Thomas C. Schulthess - CSCS
May 11, 2017

Outline

Overview

CSCS / Piz Daint

Location:
Swiss National Supercomputing Center

Name:
Piz Daint

Model:
Cray **XC50**/XC40

Node:
Intel Xeon E5-2690, Nvidia Tesla **P100**,
Aries interconnect

TOP500:
8th in the world

Green500:
2nd in the world

Motivation

- Bring Docker containers to production on Piz Daint.
  - Docker: flexible and self-contained execution environments.
  - Tool that enable workflows for some users.
  - Part of an ecosystem that provides value to users.
- SI group focus on enhancing Shifter’s container runtime.
  - Usability.
  - Robustness.
  - High-performance.

Talk in a nutshell

- Production workflows with Docker and Shifter on Piz Daint

1. Build and test containers with **Docker** on a **Laptop**.
2. Run with high-performance with **Shifter** on **Piz Daint**.

About Docker

- Motto: “Build, Ship, and Run Any App, Anywhere”
  - Portability and convenience first
  - Target: web applications.
- Creation
  - Creates semi-isolated “containers”.
  - Packages all application requirements.
- Management
  - Easy-to-use recipe file.
  - Version-control driven image creation.
- Share
  - Push and Pull images from a community-driven Hub (i.e., DockerHub)

docker

About Shifter (1)

- A lean runtime that enables the deployment of Docker-like Linux containers in HPC systems.
  - From NERSC by D. Jacobsen and S. Canon

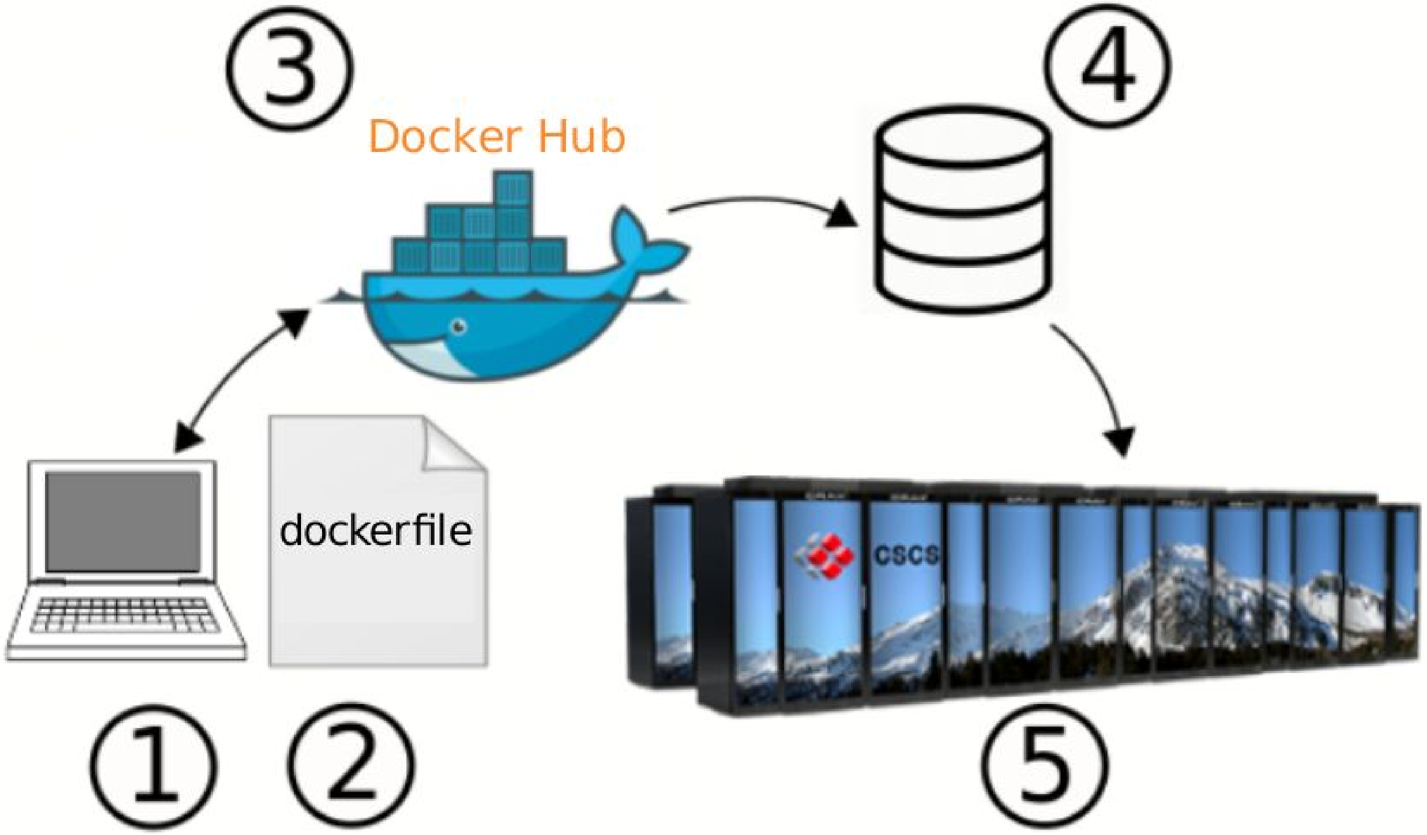
- Objectives:
  - HPC environments.
  - **Performance**.
  - **Security**.

About Shifter (2)

- **Flexibility for users**
  - Enable complex software stacks using different Linux flavors
  - Develop on your laptop and run it on an HPC system
- **Integration with HPC resources**
  - Availability of shared resources (e.g., parallel filesystems, accelerator devices and network interfaces)
- **Distribution and reproducibility**
  - Integration with public image repositories, e.g., DockerHub
  - Improving result reproducibility

Workflow (From a Laptop to Piz Daint)

- **Docker**: Ease of use and convenience (1, 2, 3).
- **Shifter**: Performance and security (4, 5).
- 1) Build container
- 2) Test container
- 3) Push to registry
- 4) Pull container
- 5) Run on Piz Daint



About Docker and Shifter

- Containers are **hardware-** and **platform-agnostic** by design
  - How do we go about **accessing specialized hardware** like GPUs?

- 1) CSCS and NVIDIA co-designed a solution that provides:
  - **direct access to the GPU** device characters;
  - automatic discovery of the required libraries at runtime;
  - NVIDIA's DGX-1 software stack is based on this solution

- 2) CSCS extended design to the MPI stack
  - Supports different versions MPICH-based implementations

- Let's look at use cases to illustrate the workflows.

Use case: deviceQuery (GPU)

deviceQuery (1): building a simple image

- Start with an image: nvidia image + deviceQuery
  - ethcscs/dockerfiles:cudasamples8.0

```
FROM nvidia/cuda:8.0

RUN apt-get update && apt-get install -y --no-install-recommends \
        cuda-samples-$CUDA_PKG_VERSION && \
    rm -rf /var/lib/apt/lists/*

RUN (cd /usr/local/cuda/samples/1_Utilities/deviceQuery && make)
RUN (cd /usr/local/cuda/samples/5_Simulations/nbody && make)
```

deviceQuery (2): Testing on a Laptop

- Let’s start with Docker on the laptop

```
$ nvidia-docker build -t "ethcscs/dockerfiles:cudasamples8.0" .

$ nvidia-docker run ethcscs/dockerfiles:cudasamples8.0 ./deviceQuery

$ nvidia-docker push ethcscs/dockerfiles:cudasamples8.0
```

```
./deviceQuery Starting...

 CUDA Device Query (Runtime API) version (CUDART static linking)

Detected 1 CUDA Capable device(s)

Device 0: "GeForce 940MX"
  CUDA Driver Version / Runtime Version          8.0 / 8.0
  [...]
deviceQuery, CUDA Driver = CUDART, CUDA Driver Version = 8.0, CUDA Runtime Version = 8.0,
NumDevs = 1, Device0 = GeForce 940MX
Result = PASS
```

deviceQuery (3): Running on a Piz Daint

- Running the container on Piz Daint

```
$ shifterimg pull ethcscs/dockerfiles:cudasamples8.0

$ salloc -N 1 -C gpu
$ srun shifter --image=ethcscs/dockerfiles:cudasamples8.0 ./deviceQuery
```

```
./deviceQuery Starting...

 CUDA Device Query (Runtime API) version (CUDART static linking)

Detected 1 CUDA Capable device(s)

Device 0: "Tesla P100-PCIE-16GB"
  CUDA Driver Version / Runtime Version          8.0 / 8.0
  [...]
deviceQuery, CUDA Driver = CUDART, CUDA Driver Version = 8.0, CUDA Runtime Version = 8.0,
NumDevs = 1, Device0 = Tesla P100-PCIE-16GB
Result = PASS
```

Use case: Nbody (GPU)

Nbody: same image

- N-body double-precision calculation using 200k bodies, single node.
- GPU-accelerated runs using the **official** CUDA image from DockerHub.
- Relative GFLOP/s performance when comparing Laptop and Piz Daint.

	Laptop	Piz Daint (P100)
Native	**18.34** [GFLOP/s]	**149.01**x
Container*	**18.34** [GFLOP/s]	**149.04**x

*Laptop run using **nvidia-docker,** Piz Daint uses **Shifter**

Use case: TensorFlow (GPU / Third party container)

TensorFlow

- Software library capable of building and training neural networks uses CUDA.
- **Official** TensorFlow image from DockerHub (not modified).
- TensorFlow has a **rapid release cycle** (Once a week new build available!).
- **Ready to run** containers.
- Performance relative to the Laptop wall-clock time of image classification tests: MNIST.

Test case	Laptop*	Piz Daint (P100)
MNIST, TF tutorial	**613** [seconds]	**17.17**x

*Laptop run using **nvidia-docker**

Note on MPI-stack support

- Based on the **MPICH**, Application Binary Interface (**ABI**) **compatibility**
  - MPICH v3.1 (released February 2014)
  - IBM MPI v2.1 (released December 2014)
  - Intel MPI Library v5.0 (released June 2014)
  - CRAY MPT v7.0.0 (released June 2014)
  - MVAPICH2 v2.0 (released June 2014)

```
$ srun -n 2 shifter --mpi --image=osu-benchmarks-image ./osu_latency
```

- MPI library from the container is **swapped** by Shifter at run time.
- ABI-compatible MPI from the **host** system is checked.
  - **Hardware acceleration is enabled**.

Use case: OSU benchmark (MPI)

OSU Benchmark

```
$ srun -n 2 shifter --mpi --image=osu-benchmarks-image ./osu_latency
```

- Host MPI:
  - Cray MPT 7.5.0
  - Cray aries Interconnect
- Container MPI:
  - MPICH v3.1 (A)
  - MVAPICH2 2.1 (B)
  - Intel MPI Library (C)
- Native performance!

		Shifter MPI support *Enabled*			Shifter MPI support *Disabled*		
Size	Native	A	B	C	A	B	C
32	1.1	1.00	1.00	1.00	4.35	6.17	4.41
128	1.1	1.00	1.00	1.00	4.36	6.15	4.51
512	1.1	1.00	1.00	1.00	4.47	6.22	4.56
2K	1.6	1.06	1.00	1.06	4.66	5.03	4.04
8K	4.1	1.00	1.02	1.02	2.17	2.02	1.86
32K	6.5	1.03	1.03	1.03	2.10	2.17	1.91
128K	16.4	1.01	1.01	1.01	2.63	2.84	1.95
512K	56.1	1.00	1.01	1.01	2.23	1.78	1.67
2M	215.7	1.00	1.00	1.00	2.02	1.41	1.37

Table 4: Results from `OSU_latency` on Piz Daint: Native runs use Cray MPT 7.5.0 over Cray Aries interconnect; relative performance against native is reported for containers with (A) MPICH 3.1.4, (B) MVAPICH2 2.2, and (C) Intel MPI library using Shifter with MPI support *enabled* and *disabled*.

Use case: PyFR (CUDA + MPI / Complex build)

PyFR

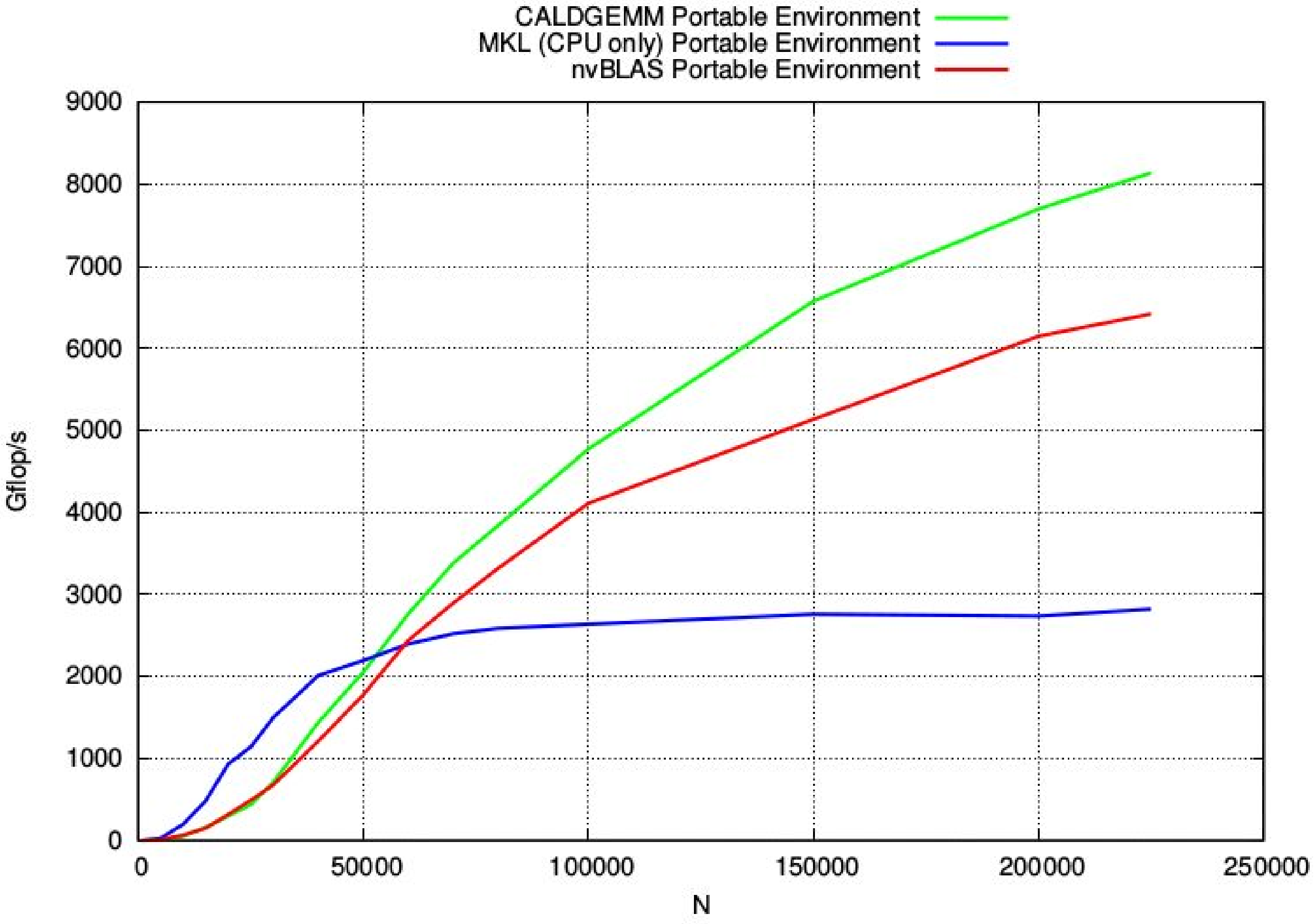
- **Python** based framework for solving advection-diffusion type problems on streaming architectures. 2016 **Gordon Bell** Prize finalist (Highly scalable).
- **GPU-** and **MPI-accelerated** runs using containers.
- Complex build (100 lines dockerfile) and test on Laptop.
- Production-like run on Piz Daint.
- Parallel efficiency for a 10-GB test case on different systems (4 node setup).

Number of nodes	Piz Daint (P100)
1	1.000
2	0.975
4	0.964
8	0.927
16	0.874

Use case: Portable compilation units / Linpack benchmark

Vanilla Linpack with specialized BLAS

- Some application performance depends on targeted optimization of libraries.
- Use container to pack application environment.
- Proof of concept: pack vanilla Linpack, compile specialized BLAS before run.
- Two stage: compile first (link against host libs), then run.

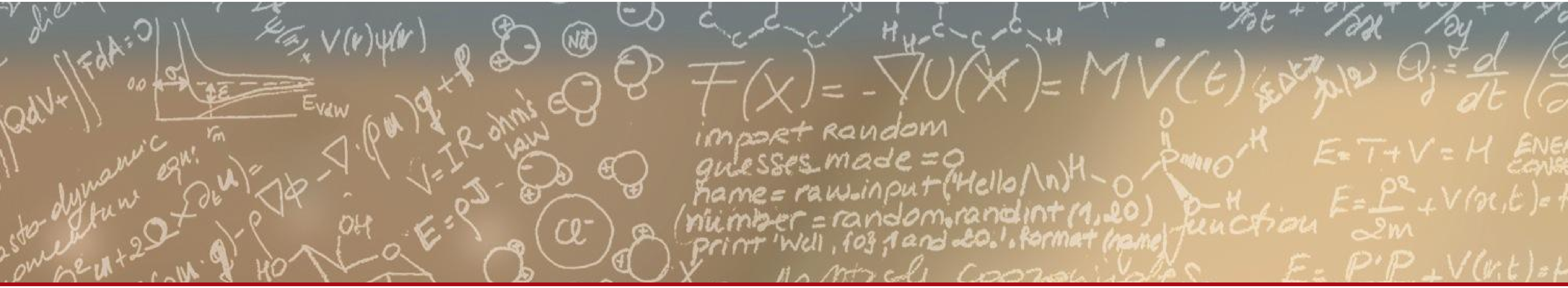


Conclusion

Conclusion

- The Docker-Shifter combo towards production on Piz Daint:
  - Portability
  - Scalability
  - High-performance.

- The showed use cases highlighted:
  - Pull and run containers;
  - high-performance containers;
  - access to hardware accelerators like GPUs;
  - use of high-speed interconnect through MPI;
  - portable compilation environment.



Thank you for your attention

GPU device access (3)

- On the GPU device numbering
  - Must-have for application portability
  - A containerized application will consistently access the GPUs starting from ID 0 (zero)

```
$ export CUDA_VISIBLE_DEVICES=0
$ srun shifter --image=ethcscs/dockerfiles:cudasamples8.0 ./deviceQuery
[...]
Detected 1 CUDA Capable device(s)
Device 0: "Tesla K40m"
[...]

$ export CUDA_VISIBLE_DEVICES=2
$ srun shifter --image=ethcscs/dockerfiles:cudasamples8.0 ./deviceQuery
[...]
Detected 1 CUDA Capable device(s)
Device 0: "Tesla K80"
[...]
```

GPU device access (4)

- Same image on an multi-GPU system with Shifter

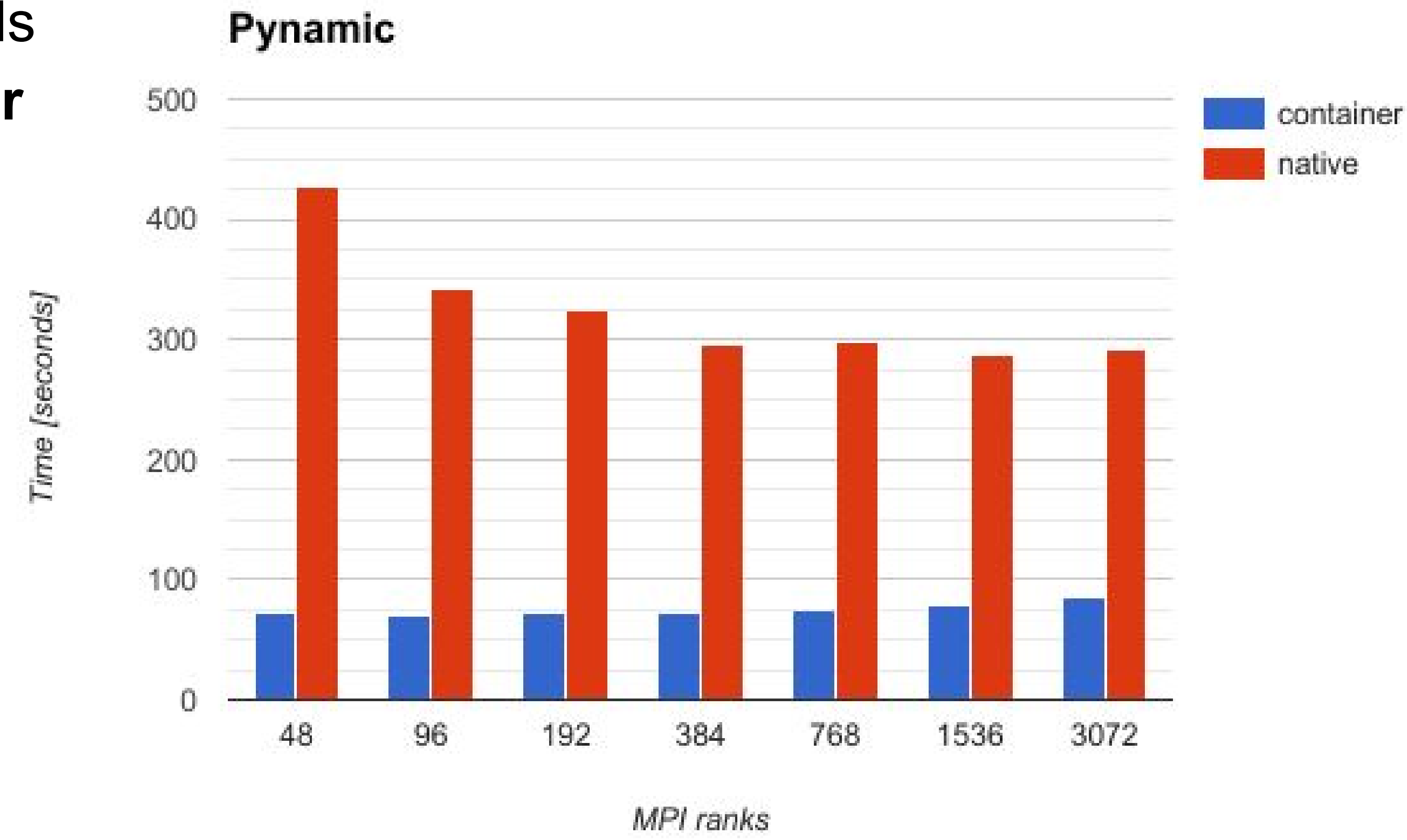
```
$ shifterimg pull ethcscs/dockerfiles:cudasamples8.0

$ export CUDA_VISIBLE_DEVICES=0,2
$ srun shifter --image=ethcscs/dockerfiles:cudasamples8.0 ./deviceQuery
```

```
/usr/local/cuda/samples/bin/x86_64/linux/release/deviceQuery Starting...

 CUDA Device Query (Runtime API) version (CUDART static linking)

Detected 2 CUDA Capable device(s)

Device 0: "Tesla K40m"
  [...]
Device 1: "Tesla K80"
  [...]
deviceQuery, CUDA Driver = CUDART, CUDA Driver Version = 8.0, CUDA Runtime Version = 8.0,
NumDevs = 2, Device0 = Tesla K40m, Device1 = Tesla K80
Result = PASS
```

Use case: deploy at scale

Pynamic*

- Test startup time of workloads by simulating **DLL behaviour of Python** applications.
- Compare wall-clock time for **container vs native**.
- Over +**3000** MPI processes.



*Pynamic parameters: 495 shared object files; 1950 avg. functions per object; 215 math like library files; 1950 avg. math functions; function name lenght ~100 characters.