



CSCS

Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

ETH zürich



Workshop on Exploiting Supercomputers and Containers for Data Science

Tim Robinson, ETH Zurich / CSCS

13.06.2018

Internet Access / Lunch

- **Eduroam** is the preferred choice
- If you cannot access eduroam:
 - Connect with WiFi to the SSID **public-5** or **public**
 - Login: **containers-cscs**
 - Password: **DataScience_2018**
 - If no landing page appears go to <https://enter.ethz.ch/welcome>
- **Lunch from 12:20 – ground floor by the large turbine**
 - Turn left out of this room and it's three floors down

Agenda: Wednesday 13 June 2018

- 12:00 – 13:00 *Lunch and Registration*
- 13:00 – 13:15 **Welcome and Workshop Overview** (*Tim Robinson, CSCS*)
- 13:15 – 14:30 **Short Presentations by Participants** (*All*)
- 14:30 – 15:00 **Keynote: LHC on Cray** (*Maxime Martinasso, CSCS*)
- 15:00 – 15:30 *Coffee Break*
- 15:30 – 18:00 **Tutorial: Introduction to Creating and Using Containers** (*Alberto Madonna, CSCS*)

Agenda: Thursday 14 June 2018

- 09:00 – 10:30 **Introduction to Shifter** (*Alberto Madonna, CSCS*)
- 10:30 – 11:00 *Coffee Break*
- 11:00 – 12:30 **Tutorial: Analytics and AI on Cray Systems, Part I**
 (*James Maltby, Charles Siegel, and Alessandro Rigazzi, Cray Inc.*)
 - Introduction to Urika-XC, a Container-based AI Environment
 - Python, Anaconda, and Dask
 - Deep Learning with TensorFlow
- 12:30 – 13:30 *Lunch Break*
- 13:30 – 15:00 **Tutorial: Analytics and AI on Cray Systems, Part II**
 - Scaling Deep Learning with the Cray PE Machine Learning Plugin
 - HPC, AI, and Analytics with R and pdbR
- 15:00 – 15:45 **Keynote: ABCpy** (*Ritabrata Dutta, USI*)
- 15:45 – 16:00 *Coffee Break*
- 16:00 – 17:30 **Tutorial: Analytics and AI on Cray Systems, Part III**
 - Spark and Alchemist
 - BigDL

Agenda: Friday 15 June 2018

- 09:00 - 10:30 **Tutorial: Analytics and AI on Cray Systems, Part IV**
(Maltby, Siegel, and Rigazzi, Cray Inc.)
 - Cray Graph Engine
 - Urika-XC Success Stories
- 10:30 – 11:00 *Coffee Break*
- 11:00 – 12:00 **Keynote: Pipeline Interoperability for Biomedical Use Cases Using Docker and Singularity** *(Balazs Laurenczy, ETH Zurich)*
- 12:00 – 13:00 *Lunch Break*
- 13:00 – 15:00 **NVIDIA Containers and Solutions for Data Science**
(Peter Messmer and Vishal Mehta, NVIDIA)
- 15:00 – 15:15 *Coffee Break*
- 15:15 – 17:30 **Hands-On with Participants' Use Cases** *(All)*



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Flash Presentations from Participants

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- Scientific domain or research area
- Use cases
- Software tools/techniques/interfaces that you currently make use of – or want to use in the future
- Your expectations for the course

Accessing Piz Daint

- Take a sheet of paper from the back of the room with a course account username and login, and sign the terms of usage
- **ssh -X ela.cscs.ch -l <course_account>**
- Enter your course account password
- **ssh -X daint.cscs.ch**

- To launch an session asking for one (GPU-based) compute node
- **salloc -N 1 -C gpu --res=hpccrs02**

- To close the session
- **exit**

CSCS in a Nutshell

- A unit of the Swiss Federal Institute of Technology in Zurich (ETH Zurich)
 - Founded in 1991 in Manno, Ticino
 - Relocated to Lugano in 2012
- Develops and promotes technical and scientific services for the Swiss research community in the field of high-performance computing
- Enables world-class scientific research by pioneering, operating and supporting leading-edge supercomputing technologies

CSCS User Community

- Academic users can access computing resources for free
 - Production projects; development projects; preparatory projects
 - Proposals are assessed by international experts
 - 43.4 million node hours were consumed in 2017
 - 116 projects, 1213 users
- CSCS operates third party systems/services for paying customers
 - MeteoSwiss for the numerical weather forecasting service
 - The Blue Brain 4, an IBM Blue Gene/Q acquired from the Blue Brain Project (EPFL Lausanne)
 - ETH Zurich professors from various fields
 - Archival of scientific data for PSI
- CSCS2go
 - Paid service: currently offered only to researchers employed by a Swiss University
 - Fast access, no peer review process