Prof. Dr. Jens Vogelgesang · CSH Study Program Director · j.vogelgesang@uni-hohenheim.de

Registration now open for the

CSH Spring School 2024
Reproducible Science with Containerization on High Performance Computing Infrastructure

with Dr. Daniela Bendel, Dr. Konstantin Kuck & Dr. Johannes Bleher
May 21 – May 23, 2024 – 9h00 - 17h30
HS 36, Fruwirthstr. 47, Kavaliershaus 1

Overview

Has your friend ever had difficulties running your code from an old research project of yours? Or, his code did not run on another computer? Or, your friend's code did not work on the HPC cluster, since not all library dependencies were met? Increasing complexity of code dependencies and rapidly changing statistical programming environments like R and Python are challenging. We all have that friend.

This CSH Spring School 2024 is for your friend – and you.

Reproducibility of data analysis workflows in scientific research promote scientific integrity and form a pilar on which trust in scientific results rests. Containerization provides a flexible approach to reproducibility. It allows to bundle software independently from the underlying operating system and its libraries. Containerization, allows to build and operate completely separate environments (e.g., with different version of the same library) for different research projects on the same computer. Containerization also facilitates the migration of software environments to HPC clusters.

Join us in the CSH Spring School 2024.

You will learn how computational workflows can be containerized using the flexible Docker system.

On day 1, we cover the fundamental tools in scientific computing and the command line interface, before discussing in detail the concept of containerization. We focus on the building process and show how containers created on one computer can be run on another.

Day 2 is devoted to composing several containers to building small webapps, data pipelines and a short introduction to Singularity and Enroot, alternative containerizarion environments popular on cluster systems.

On day 3, we briefly introduce high-performance computing, using the state-funded bwUniCluster 2.0 in Baden-Württemberg as an example. We discuss the fundamentals of cluster computing like login, file transfer and job management. Finally, we demonstrate how software containers created locally can be run on a cluster computer, greatly facilitating the migration process. Live coding examples and practical exercises strengthen the understanding.

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The schedule

(HS 36, Fruwirthstr. 47, Kavaliershaus 1)

Day 1: May 21, 2024, 9h00 – 17h30:

9h00 - 12h00	–	Linux, SSH, Git	*Konstantin Kuck*
12h00 - 13h00	–	Lunch Break	
13h00 - 15h30	–	Introduction to Docker	*Daniela Bendel*
15h30 - 16h00	–	Coffee Break	
16h00 - 17h30	–	Docker-Compose	*Johannes Bleher*

Day 2: May 22, 2024, 9h00 – 17h30:

9h00 - 12h00	–	Containerization of a ShinyApp	*Johannes Bleher*
12h00 - 13h00	–	Lunch Break	
13h00 - 15h30	–	Containerized Data Pipelines	*Johannes Bleher*
15h30 - 16h00	–	Coffee Break	
16h00 - 17h30	–	Singularity	*Konstantin Kuck*

Day 3: May 23, 2024, 9h00 – 17h30:

9h00 - 12h00	–	Introduction to HPC Clusters	*Konstantin Kuck*
12h00 - 13h00	–	Lunch Break	
13h00 - 15h30	–	SLURM Jobs in Applications	*Daniela Bendel*
15h30 - 16h00	–	Coffee Break	
16h00 - 17h30	–	Using Containerzation on the Cluster	*Konstantin Kuck*

Target Audience

The course mainly aims at researchers in the early stages of their career who want to work with reproducible workflows. As such, the course is also open to Master's students with sufficient knowledge in R and Python. By attending, participants receive a certificate of participation. No ECTS points can be earned.

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Fees, Devices and Credits

Interested participants can register via weiterbildung.uni-hohenheim.de for the workshop until May 1, 2024.

For external participants the following tuition fee structure applies:

Group	Through April 2 (prices in EUR)	After April 2 (prices in EUR)
Students	50.00	100.00
PhD students / Staff Members	120.00	150.00
PostDocs	200.00	240.00
Professors and Others	240.00	300.00

Outstanding fees have to be wired as indicated in the payment instructions. An email with detailed payment instructions will be send to participants after registration and before the workshop. Registration is binding. Fees transferred are non-refundable.

Participants should bring their own laptop (incl. charger). Participants should have installed GIT. Windows users should make sure that they have GIT bash installed as well.

At the conclusion of the Spring School, participants will receive a certificate for the number of hours attended.

Contact

For any further information please contact

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