Sustainable Computing:
Welcome to Workshop on Containers

Juliette Alimena, Christoph Beyer, Ben Brueers, Frank Gaede, Eleanor Jones, Yves Kemp, Thomas Madlener, Tigran Mkrtchyan, Kilian Schwarz, Christoph Wissing

FH Sustainable Computing Workshop

March 28, 2025

Sustainable Computing: What and Why

- Experimental high energy physics is a **computationally intensive field**
  - **Petabytes/exabytes** of data and simulation
  - Large CPU and GPU demands (trigger, offline)
- **Maximizing the physics potential** requires an **investment in the software** used to collect, process, and analyze the data and simulation
- **Sustainable computing** is the idea that we need to **maintain the computational ability** to perform HEP:
  - At the **rate** we want **(physics)**
  - For **as long** as we want **(reproducibility, preservation, scalability)**
  - While **minimizing the impact on the planet (efficiency, minimizing waste, reducing memory consumption)**

Sustainable Computing Workshop (I)

- This is a **1/2-day workshop** hosted by the FH Sustainability Forum and FH IT experts
- **You will learn how to use and build containers**
- Examples demonstrated with local computing clusters and **tailored to the needs of the DESY particle physics (FH) division**
- **Short talks** followed by **hands-on examples - bring your laptop! Let us know before we start if you can’t ssh to the NAF**
- In person, but with zoom available

Sustainable Computing Workshops

- We offer beginner workshops at regular intervals, so that incoming students and postdocs can profit
- Options for more advanced, topical workshops like this one - let us know if you have ideas for topics!
- **Agenda:** https://indico.desy.de/event/48241/
- **Zoom:** https://desy.zoom.us/j/65183923946 (Passcode: 550365)
- **Mattermost:** https://chat.desy.de/desy/channels/fh-sustainable-computing-workshop
- **Exercises:** https://gitlab.desy.de/fh-sustainability-forum/sustainable-coding-tutorial
- At the end of the workshop: **brief closeout survey**, similar to what you filled in when registering - please fill out!

Agenda

9:00 AM → 9:05 AM **Opening** 5m

Speaker: Juliette Alimena (DESY (CMS))

9:05 AM → 9:50 AM **Introduction to Containers** 45m

Speaker: Christoph Wissing (DESY)

Lecture.pdf

9:50 AM → 10:20 AM **Containers on the NAF** 30m

- Hands-on example
- Run a container on the NAF
- Execute a batch job in a container

Speaker: Christoph Beyer (IT (IT Systems))

10:20 AM → 10:50 AM **Coffee break** 30m

10:50 AM → 12:10 PM **Building your own container with Apptainer on the NAF** 1h 20m

- Build your own container with an analysis chain
- Exercise on CMS open data

Speaker: Ben Brueers (Z_ATUP (ATLAS-Upgrade))

12:10 PM → 12:20 PM **Stretch** 10m

12:20 PM → 12:50 PM **Building a container with GitLab CI** 30m

Speaker: Tigran Mkrtchyan (DESY-IT, Scientific Computing)

12:50 PM → 1:00 PM **Wrap Up and Closing Survey** 10m

Speaker: Juliette Alimena (DESY (CMS))

Coffee will be provided!

Ask questions! Try things out! Discuss!

Enjoy!