Chair of Aerodynamics
and Fluid Mechanics
Department of Mechanical Engineering

TUM

Interdisciplinary Project (IDP) / Term paper / Master's Thesis / ...   08.02.2021

Containerization of (Computational Fluid Dynamics) Workflows on High-performance Computing Systems

Part of good scientific practice, is ensuring reproducibility of conducted research. For numerical simulations on high-performance computing (HPC) systems this is challenging not only due to (computational) cost, but also to the unique software and hardware stack. Containerization might be a tool to overcome these challenges. However, standard approaches in container orchestration cannot be directly translated to an HPC-environements. For performance and security reasons.

In this work, the workflow of a computational fluid dynamics simulation from compilation over parallel execution to post-processing is moved into a container-based equivalent. The containered setup is analyzed for practicability and performance on the compute resources provided by the Leibniz Supercomputing Centre (LRZ).

Tasks:
- Familiarization with a typical container-less HPC workflow
- Familiarization with LRZ Linux-Cluster[1] and Charliecloud[2]
- Development of containers to model the workflow
- Development of scripts for container orchestration

Requirements:
- Knowledge of containers, preferential Docker
- Ability to work independently
- Experience with HPC-clusters or Charliecloud, beneficial

Take-away:
- Experience with state-of-the art container concepts
- Experience with HPC-clusters
- Project management skills

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1   https://doku.lrz.de/display/PUBLIC/Linux+Cluster
2   https://github.com/hpc/charliecloud
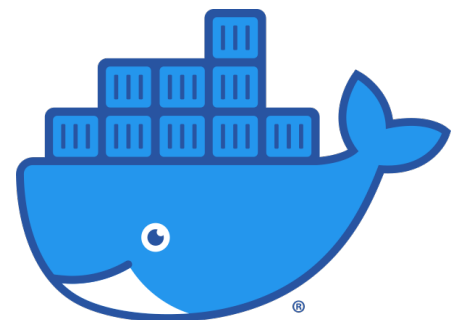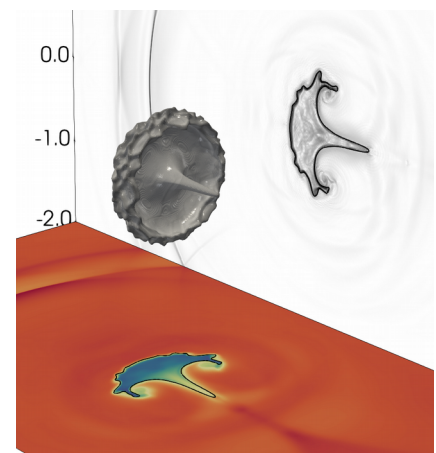
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