

## ***Thesis / Interdisciplinary Project (IDP) / Research Practice / Study Project***

to assist with the

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

for TUM-students within

### ***Informatics, Aerospace, Mechanical Engineering, Data Science or similar***

Part of good scientific practice, is ensuring reproducibility of conducted research. In this work, the workflow of a CFD simulation from compilation over parallel execution to post-processing is moved into a container-based equivalent. The containerized setup is analyzed for practicability and performance on the compute resources provided by the Leibniz Supercomputing Centre (LRZ), Jülich Supercomputing Centre (JSC) and High-Performance Computing Center Stuttgart (HLRS).

#### **Tasks**

- Familiarization with HPC workflows
- Familiarization with JUWELS supercomputer (possibly also HLRS)
- Familiarization with container software (Apptainer)
- Container setup and performance improvement
- Documentation



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#### **Requirements**

- Knowledge of Python or C++
- Knowledge of Linux-CL
- Knowledge of GPU computing
- Knowledge of containers (e.g. Docker or Apptainer)
- Experience with HPC-clusters (beneficial)



#### **Benefits**

- Flexible working hours, mostly remote work
- Recognition within your study program (thesis / internships / projects etc.)
- Exclusive experience with tier-0 HPC-clusters
- Experience with state-of-the art container concepts
- Insight into a nationwide research project

#### **Links**

- GPU Computing at JSC: <https://apps.fz-juelich.de/jsc/hps/juwels/gpu-computing.html>
- Container Runtime at JSC: <https://apps.fz-juelich.de/jsc/hps/juwels/container-runtime.html>
- GitLab "Containerization": <https://gitlab.lrz.de/nfdi4ing/containerization>
- NFDI4Ing research group: <https://www.epc.ed.tum.de/en/aer/research-groups/nfdi4ing/>

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