



CSCS

Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

ETH zürich



Overview of User Lab services

CSCS User Lab Day

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Overview of User Lab services

- Support (help@cscs.ch)
 - Proposal submission
 - Benchmarking
 - Debugging
- Scientific Computing
 - Scientific applications
 - Data Science libraries
 - Visualisation
 - Code compilation
 - Code analysis
- Training
 - Webinars
 - Courses
- Documentation
 - User Portal
- Data Transfer
- Containers
- Continuous Integration
- Interactive Supercomputing
- Regression testing

Scientific Computing

- Popular codes (used by several user communities) are officially supported
 - Installed and maintained by CSCS
- Requests from individual projects are treated case by case
 - CSCS can support users on the installation of software
 - Either by providing build instructions or automated build recipes (EasyBuild)
 - Reminder: all software requirements should be explicitly mentioned in the project proposals
- All build recipes made by CSCS are publicly available on Github
 - <https://github.com/eth-cscs/production/>

Tools -> Containers (Shifter)

- Shifter allows running container workloads on HPC systems, addressing the unique needs of high-performance environments
- It is compatible with Docker images
- Main use cases are applications that:
 - Require specific OS version
 - Are already available as docker images
 - Have many dependencies and that are updated very frequently
 - Such as the most popular data analytics frameworks
- Current limitations
 - Usage of licensed software not yet supported (for example, Cray CCE and PE)
 - Cray Aries high speed interconnect can only be used with MPICH ABI compatibility
 - Such as MVAPICH and Intel MPI
 - OpenMPI is not supported

Tools -> Continuous Integration (Jenkins)

- CSCS has recently deployed a multi-user CI service
- Any project doing active development on Piz Daint can apply for the service
- CSCS offers support for integrating Piz Daint into your CI workflow



Tools -> High-Throughput Scheduler (Greasy)

- CSCS provides the GREASY meta scheduler to manage high throughput simulations on Piz Daint
- Slurm currently cannot handle HTC workloads properly
 - **Massive submission of Slurm jobs cause disruptions to other users**
- GREASY currently supports the following types of workload
 - Serial tasks
 - Multithreaded tasks +OpenMP
 - MPI
 - MPI + OpenMP

Tools -> Interactive Supercomputing (JupyterHub)

- CSCS supports the use of Jupyter Notebooks for interactive supercomputing
 - powered by JupyterHub
- The initial design allows two kinds of workload
 - Single node jobs (with resources dedicated to JupyterHub)
 - Regular multi-node jobs (that are submitted as a regular job to the normal queue)
- Python environment should be prepared before launching the notebook
 - And should be activated ".jupyterhub.env"

Libs -> SIRIUS library

- SIRIUS is a domain specific library for electronic structure calculations developed at CSCS. The aim of SIRIUS project is to create a robust and reusable solution for porting plane-wave based electronic structure codes to novel architectures
- SIRIUS-enabled Quantum ESPRESSO code is provided through the EasyBuild infrastructure
- Compiling the code:

```
module load daint-gpu EasyBuild-custom/cscs  
eb QuantumESPRESSO-SIRIUS-6.3-CrayIntel-17.08-cuda-8.0.eb -r
```
- Running Sirius

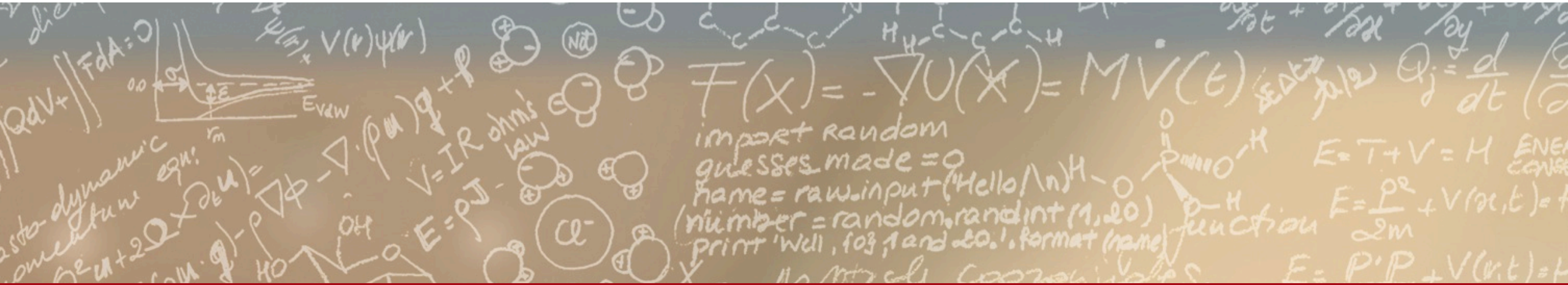
```
module load daint-gpu  
module use $HOME/easybuild/daint/haswell/modules/all  
module load QuantumESPRESSO-SIRIUS-6.3-CrayIntel-17.08-cuda-8.0.eb  
export MKL_NUM_THREADS=12  
export OMP_NUM_THREADS=12  
srun -n 10 --hint=nomultithread -c 12 pw.x -i pw.in -ndiag 1 -npool 10 -sirius
```




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Thank you for your attention.