VSB TECHNICAL UNIVERSITY OF OSTRAVA | IT4INNOVATIONS NATIONAL SUPERCOMPUTING CENTER

INTRODUCTION TO HIGH PERFORMANCE COMPUTING

PART 3
HPC @ IT4INNOVATIONS
BUILDING CODE ON THE CLUSTER

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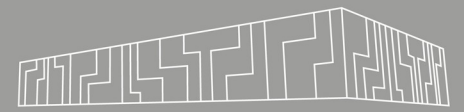
EUROPEAN UNION
European Structural and Investment Funds
Operational Programme Research,
Development and Education

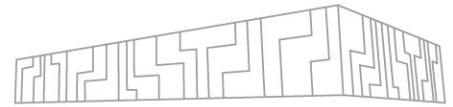
MINISTRY OF EDUCATION, YOUTH AND SPORTS

OUTLINE



- Modules
- Available software on clusters
- Common toolchains (C/C++, Python)
- MPI, distributed computing, NUMA
- Containerization
- Gitlab, CI

BUILDING CODE AND DEPENDENCIES



- You must compile your program and its dependencies for your target cluster
  - e.g. Salomon runs on CentOS 7
- You DO NOT have admin privileges on the cluster
  - Standard package managers (like `yum`) cannot be used

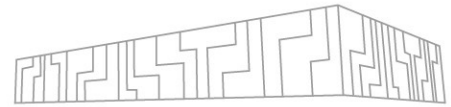
You have several options how to compile your code and its dependencies

- Use the available pre-installed modules
- Compile your code and all its dependencies from scratch
- Use Singularity containers
- Use Spack (HPC package manager)

All further command examples will assume execution on a login node

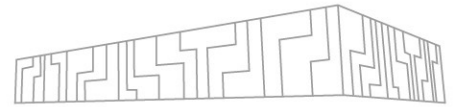
You can find more information here

REMOTE DEVELOPMENT



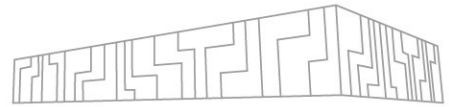
- IDEs like VSCode or Clion offer remote development over SSH
  - The server compiles code on the cluster, but the UI runs on your PC
- You can also use `sshfs` to treat the remote filesystem as a local one

USING LMOD MODULES



- Each IT4I cluster has its own set of pre-installed modules available for immediate use
- Module
  - Is a set of binaries, libraries, header files, …
  - Has a set of modules that it depends on
  - Might have several available versions (`Python/2.7.9` vs `Python/3.6.1`)
  - Might have a specific toolchain (GCC vs Intel toolchain)
- To use a module, you have to load it
  - Loading a module modifies environment variables (`PATH`, `LD_LIBRARY_PATH`)
  - This enables executing module binaries and linking to module libraries
- Lmod is used to load modules
- You can also create your own modules or ask support to install new modules for you
  - Modules are defined using EasyBuild
- If you find a module that is not working, contact support

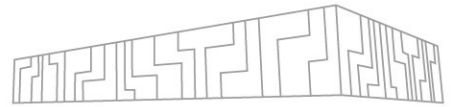
AVAILABLE MODULES



- Language toolchains (Python, Java, C#, …)
- C/C++ compilers (GCC, Clang, Intel C++ compiler, CUDA nvcc, …)
- Communication libraries (MPI, GPI-2, …)
- Parallel debuggers and profilers (Allinea Forge, VTune, PAPI, Scalasca, Score-P, Vampir, …)
- Parallelized libraries (FFTW, PETSc, Trilinos, Octave, …)
- Specialized software for chemistry, bioinformatics, physics, visualization, 3D rendering, …
  - GROMACS, Gaussian, Molpro, NWChem, Orca, Phono3py, OpenFOAM, ParaView, …

ⓘ Full list of modules available at IT4I clusters is located here

USING LMOD



```
# show available modules
$ ml av

# load a module with its dependencies
$ module load Python/3.6.8

# list loaded modules
$ module list
Currently loaded modules:
1) GCC/6.3.0 2) Python/3.6.8
$ python --version
Python 3.6.8

# unload all loaded modules
$ ml purge
$ python --version
Python 2.7.5
```

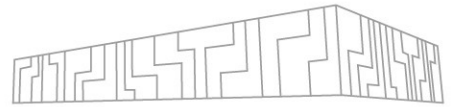
Useful hints

- Always load specific versions of modules to avoid surprises
  - `ml GCC/6.3.0` ✓
  - `ml GCC` ✗
- Module load order matters (because of conflicting dependencies)
  - `ml A B` might produce different results than `ml B A`
- Save module combinations that you commonly use into *collections*

```
$ ml purge
$ ml GCC/6.3.0 Python/3.6.8 MPICH/3.2.1-GCC-6.3.0-2.27
$ ml save mpienv1 # save current modules under name mpienv1
# ... later
$ ml restore mpienv1 # restore modules from collection mpienv1
```

- Filtering modules
  - `$ ml spider <package>`
  - `ml` command also provides tab completion
- `ml` command is case sensitive
- Match module toolchains (GCC vs Intel)
- Do not forget to load correct modules in your PBS job script!

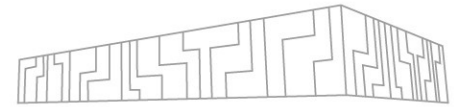
COMPILING C/C++ PROGRAMS



1. Load necessary modules
   - Compiler (e.g. `GCC/6.3.0`)
   - Dependencies (e.g. `MPICH/3.2.1-GCC-6.3.0-2.27`)
   - Build system (e.g. `CMake/3.16.2`)
2. Build your program on a login node
   - Once your binary is built, it can be accessed by all cluster nodes using the shared filesystem
   - You usually cannot "install" (e.g. `make install`) your program into the default (global) location
     - Use `CMAKE_INSTALL_PREFIX` or similar to change installation path
     - You can also modify your `PATH`/`LD_LIBRARY_PATH` or other environment variables manually
       - PATH – directories where binaries are located
       - LD_LIBRARY_PATH – directories where shared dynamic libraries are located

ⓘ If a dependency is not available as a module, you must compile it yourself

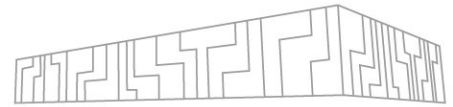
C/C++ COMPILATION FLAGS AND TIPS (GCC)



- Make use of optimizations and available instruction sets
  - Karolina has AVX2 (256-bit vectorization)
  - Barbora has AVX-512 (512-bit vectorization)
- Useful flags
  - Optimizations: `-O2`, `-O3`
    - Benchmark what works best for your code
  - Use native instruction set: `-march=native`
  - Fast floating point math (at the cost of precision): `-ffast-math`
  - Link-time optimization: `-flto`
  - Profile-guided optimization: `-fprofile-generate`, `-fprofile-use`
  - Enable OpenMP: `-fopenmp`

- General tips
  - Check generated assembly at godbolt.org
  - Use Intel accelerated libraries where possible (Barbora) - Intel MKL modules are available

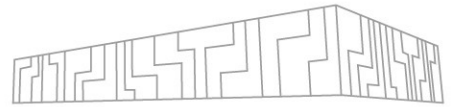
COMMON C/C++ BUILD SYSTEMS



- Makefile
  - Simply run `make` in the project directory
- CMake
  1. Load CMake module
  2. Create build files inside a build directory
  3. Invoke Make (or other build system, e.g. Ninja) to build the project

```
$ ml CMake/3.13.1
$ mkdir build
$ cd build
$ cmake -DCMAKE_BUILD_TYPE=Release ..
$ make -j16
```

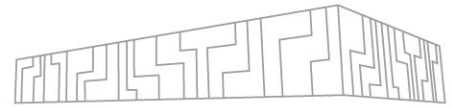
PYTHON (USAGE)



- Works mostly out-of-the-box on all clusters
- Make sure to load the same Python version module
  - When setting up your environment
  - Inside PBS jobs
- Avoid using system/user Python, use virtual environments instead
  - Puts all your dependencies inside a single directory
  - Make sure to load the same Python as is inside the virtual environment!
  - `venv` usage example

```
$ python3 -m venv venv
$ source venv/bin/activate
(venv) $ pip install -U pip setuptools wheel
(venv) $ pip install <my-package>
```

PYTHON (PERFORMANCE)



- Many useful cluster/HPC frameworks exist
  - Parallelize computation or put it on GPU with a few lines of codes
  - Distributing computation: Dask, Ray, PySpark, HyperLoom
  - GPU-acceleration: RAPIDS (cuDF, cupy), numba

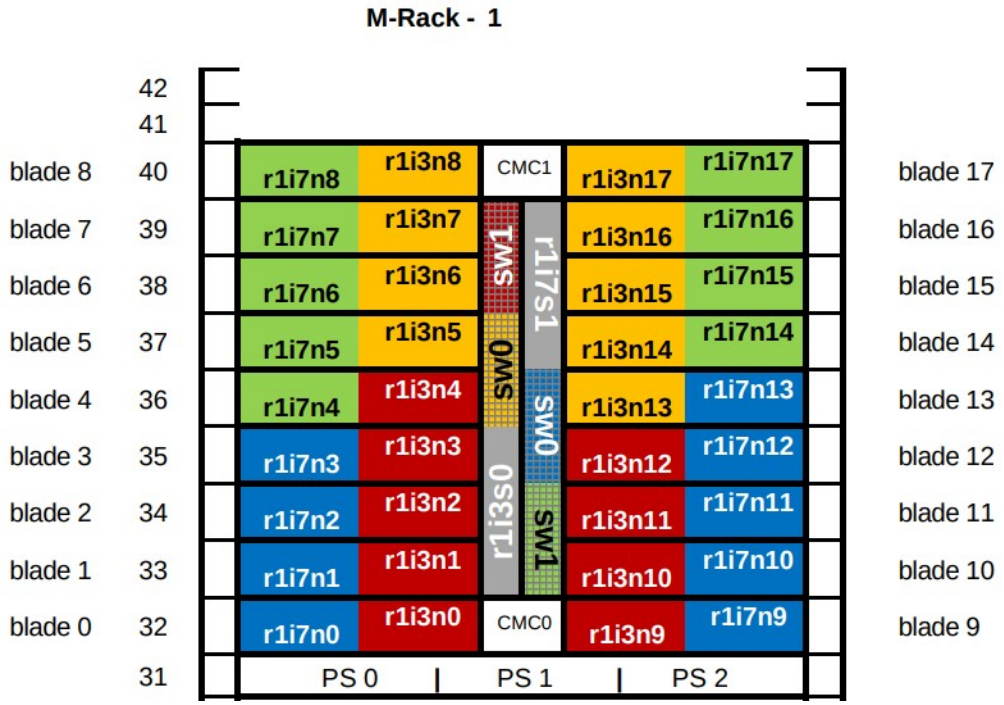
```
import dask.dataframe as dd

df = dd.read_csv("2015-*-*.csv")
df.groupby(df.user_id).value.mean().compute()
```

```
import dask

@dask.delayed
def inc(x):
  return x + 1

output = []
for x in (1, 2, 3, 4, 5):
  output.append(inc(x))

print(dask.delayed(sum)(output))
```

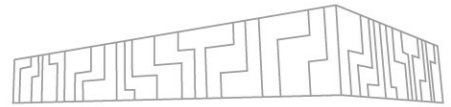
- Python compute bound programs can be accelerated by PyPy or Cython
- Profile performance using py-spy or Scalene

NETWORKING

- Computing nodes are connected using InfiniBand
  - Barbora
    - Fat tree topology, 100 Gbit/s
  - Karolina
    - Fat tree topology, 100/200 Gbit/s
- Node name is an address in network topology
- Computation vs communication ratio

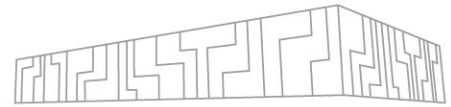


DISTRIBUTED COMPUTING



- List of nodes inside a job available in PBS_NODEFILE
  - SSH can be used to connect to them
- Check used network interface
  - Usually auto-detected correctly, but not always
  - InfiniBand (`ib`) vs TCP (`eth`)

MPI

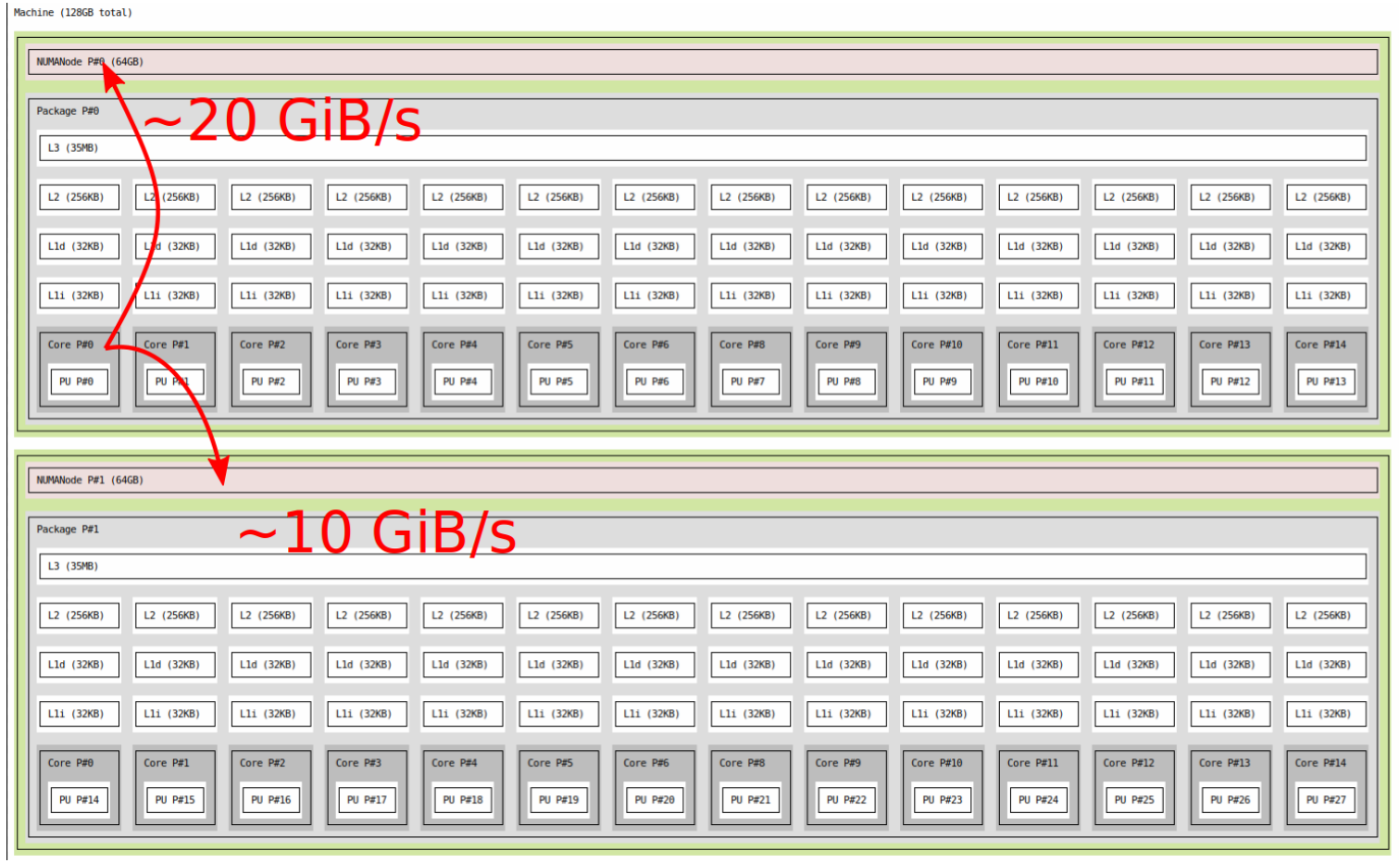


- Choose desired MPI implementation and module
  - MPICH, OpenMPI, Intel MPI (`impi`)
  - Keep the same impl. and version for compilation and execution
- Compile using `mpicc` or `mpicxx`
- Run your program
  - `$ mpirun -n 2 <program>`
- Number of MPI processes vs threads
  - `$ qsub –lselect=2:mpiprocs=2:ompthreads=16`
    - Uses 2 MPI processes per node by duplicating nodes in PBS_NODEFILE
    - Sets `OMP_NUM_THREADS=16`
  - Consider pinning threads to cores

There is also MPI4Py for Python

NUMA (NON-UNIFORM MEMORY ACCESS)

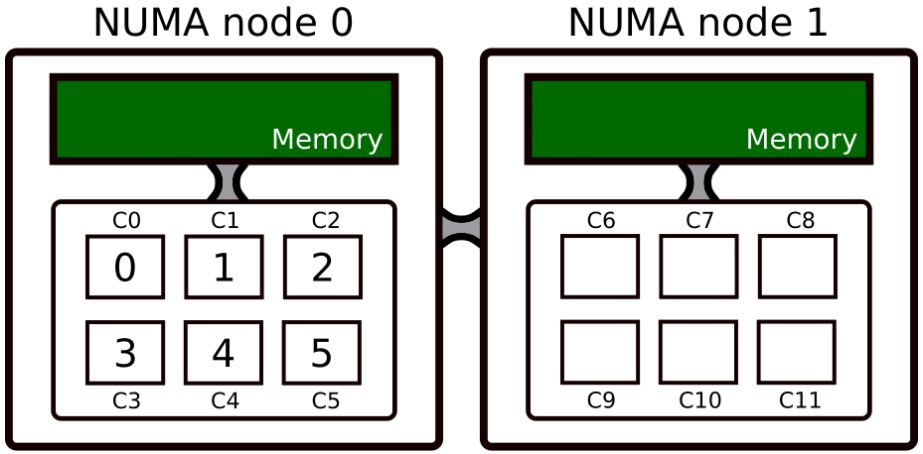
- NUMA node - set of cores and memory with the "same distance" to each other
  - Memory access to a different ("farther") node is slower!
- Karolina has 8 NUMA nodes (each has 16 cores and ~31 GiB RAM)
- Barbora has 2 NUMA nodes (each has 18 cores and ~94 GiB RAM)
- Check NUMA topology: `$ ml hwloc && lstopo --no-io --output-format txt`



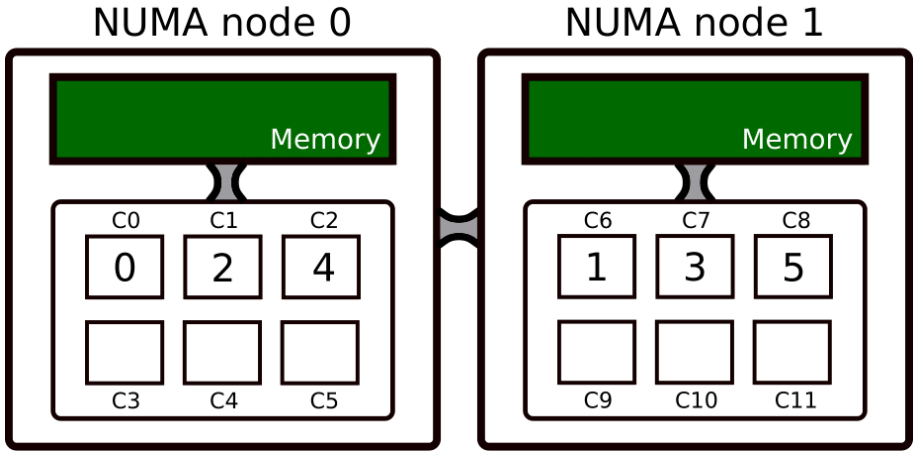
NUMA PLACEMENT

- You can control on which cores will your threads run
- Use numactl or OpenMP binding env. variables

OMP_NUM_THREADS=6
OMP_PROC_BIND=close
OMP_PLACES=cores



OMP_NUM_THREADS=6
OMP_PROC_BIND=spread
OMP_PLACES=cores



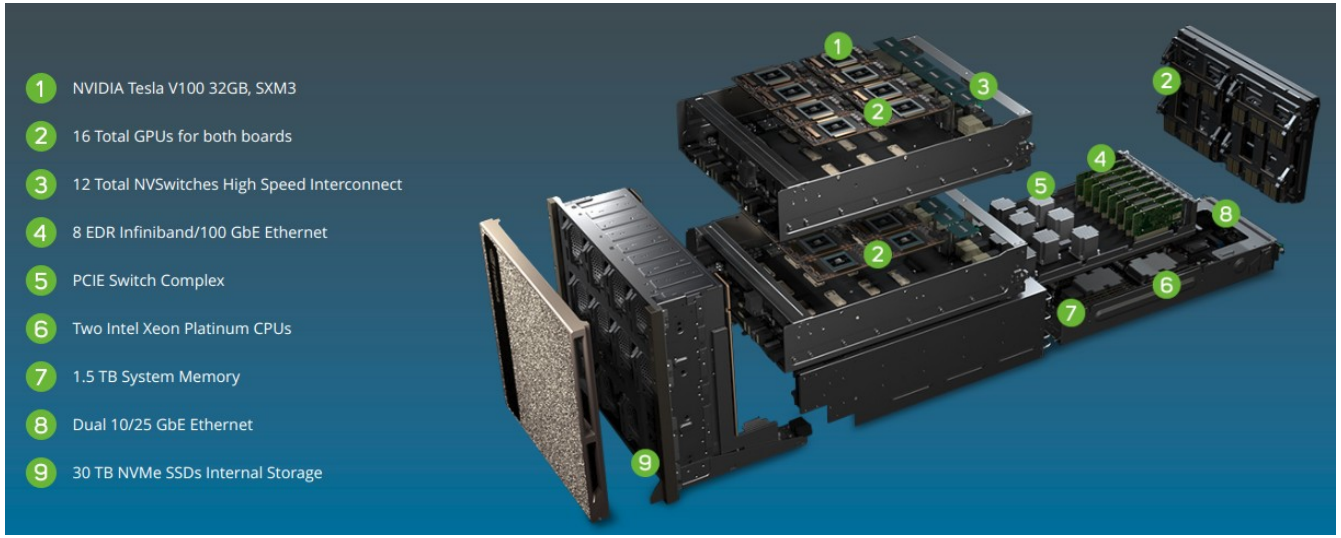
USING GPUS

- Available clusters with GPUs:
  - Karolina: 72 nodes, 8 A100 (40 GiB) GPUs per node
  - Barbora: 8 nodes, 4 V100 (16 GiB) GPUs per node
  - DGX: 16 V100 (32 GiB) GPUs
- Access to GPU resources must be requested for a project!
- Using only a single GPU might be wasteful
  - Check if your tool has support for Multi-GPU setups
  - Example: Keras
- Use prepared modules:
  - $ ml CUDA/11.3.1
  - When loading multiple GPU modules, match their versions!

```
$ ml CUDA/11.3.1 \
        cuDNN/8.2.1.32-CUDA-11.3.1 \
        NCCL/2.10.3-GCCcore-10.3.0-CUDA-11.3.1
```

DGX-2

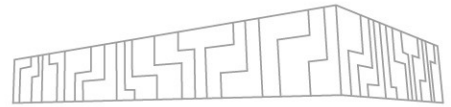
- Has a dedicated PBS queue
  - Accessible from Barbora
  - `$ ml DGX-2`
- Check if your tool has direct support for it
  - Dask-DGX



FAT NODES

- Nodes with a large amount of RAM
- Useful for programs that are hard to distribute
- Use the `qfat` queue
- Karolina
  - HPE Superdome Flex – 768 cores, 24 TiB RAM
- Barbora
  - BullSequana X808 – 128 cores, 6144 GiB RAM

CONTAINERIZATION USING SINGULARITY



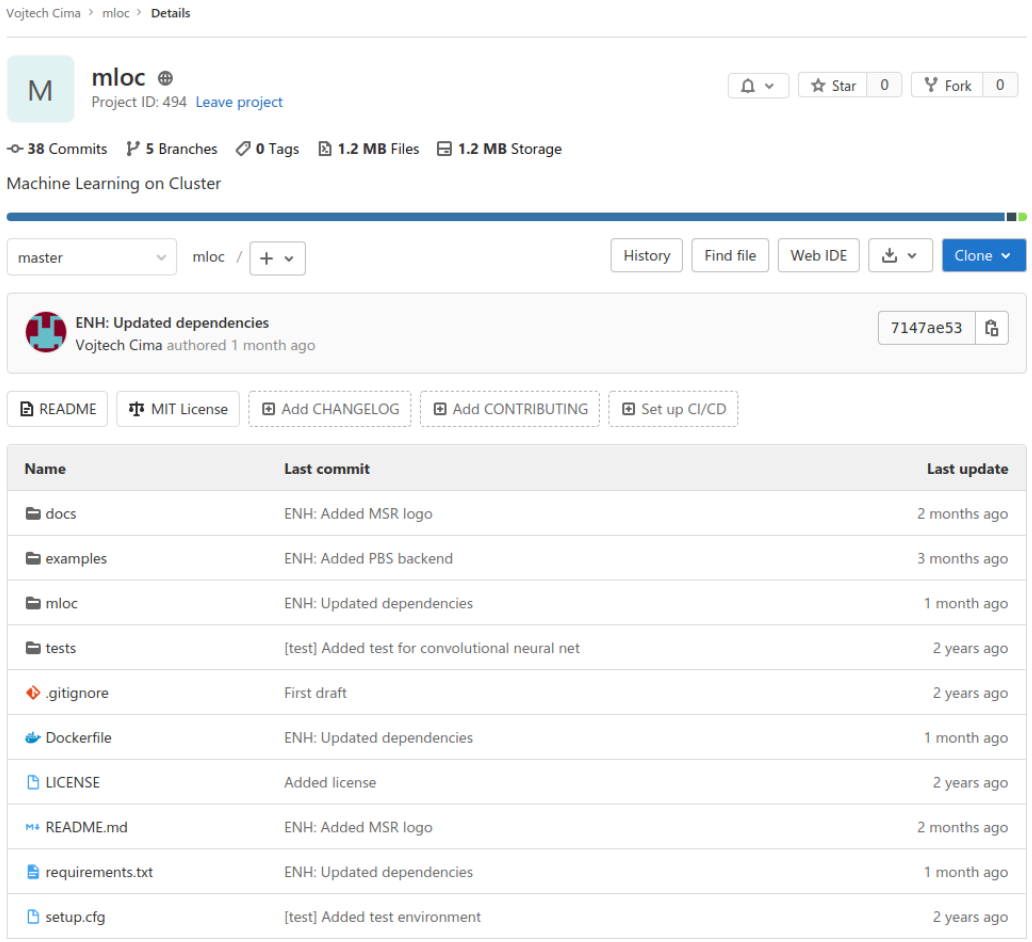
- Containers allow you to
  - Prepare your code and all dependencies
  - Distribute them easily in the form of an archive (image)
  - Execute them in a sandboxed environment
- Popular container solution is Docker
  - It cannot be used on IT4I clusters directly because of security issues
- You can use Singularity instead
  - Preferred deployment method on DGX-2
  - Nvidia containers available at NGC

```
# Load Singularity module
$ ml Singularity

# Run Docker image directly
$ singularity shell docker://centos:latest

# Build Singularity image from Docker image
$ singularity build ubuntu.img docker://ubuntu:latest

# Run interactive shell with image + mount /scratch
$ singularity shell -B /scratch ubuntu.img
```

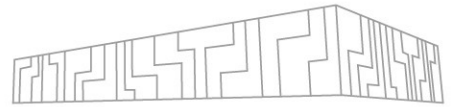
IT4I helper Singularity wrappers (https://docs.it4i.cz/software/tools/singularity-it4i/)

GITLAB

- IT4I hosts a GitLab instance at https://code.it4i.cz
- Code storage, sharing and review (repositories, pull requests)
- Project management (issue tracker, wiki)
- Container repository
- Continuous integration



GITLAB CI (CONTINUOUS INTEGRATION)



- Pipelines = scripts executed after a push to a repository
  - IT4I has 5 shared runners that can run pipelines
- Check that your code was not broken by a commit
  - Correctness (unit tests)
  - Performance (benchmarks)
  - Code style, lints, …
- Deploy built artifacts
- Configured with `.gitlab-ci.yml`

Status	Pipeline	Triggerer	Commit	Stages	
passed	#12563 latest		routing_lib 4ee1d985 ENH: PTDR base for wrapper		00:08:02 4 months ago
passed	#12544 latest		master 848f9c28 Update .gitlab-ci.yml		00:08:07 4 months ago
passed	#12492		settings_Di… 848f9c28 Update .gitlab-ci.yml		00:07:57 4 months ago
failed	#12491		settings_Di… 508be6f0 Update .gitlab-ci.yml		00:00:52 4 months ago

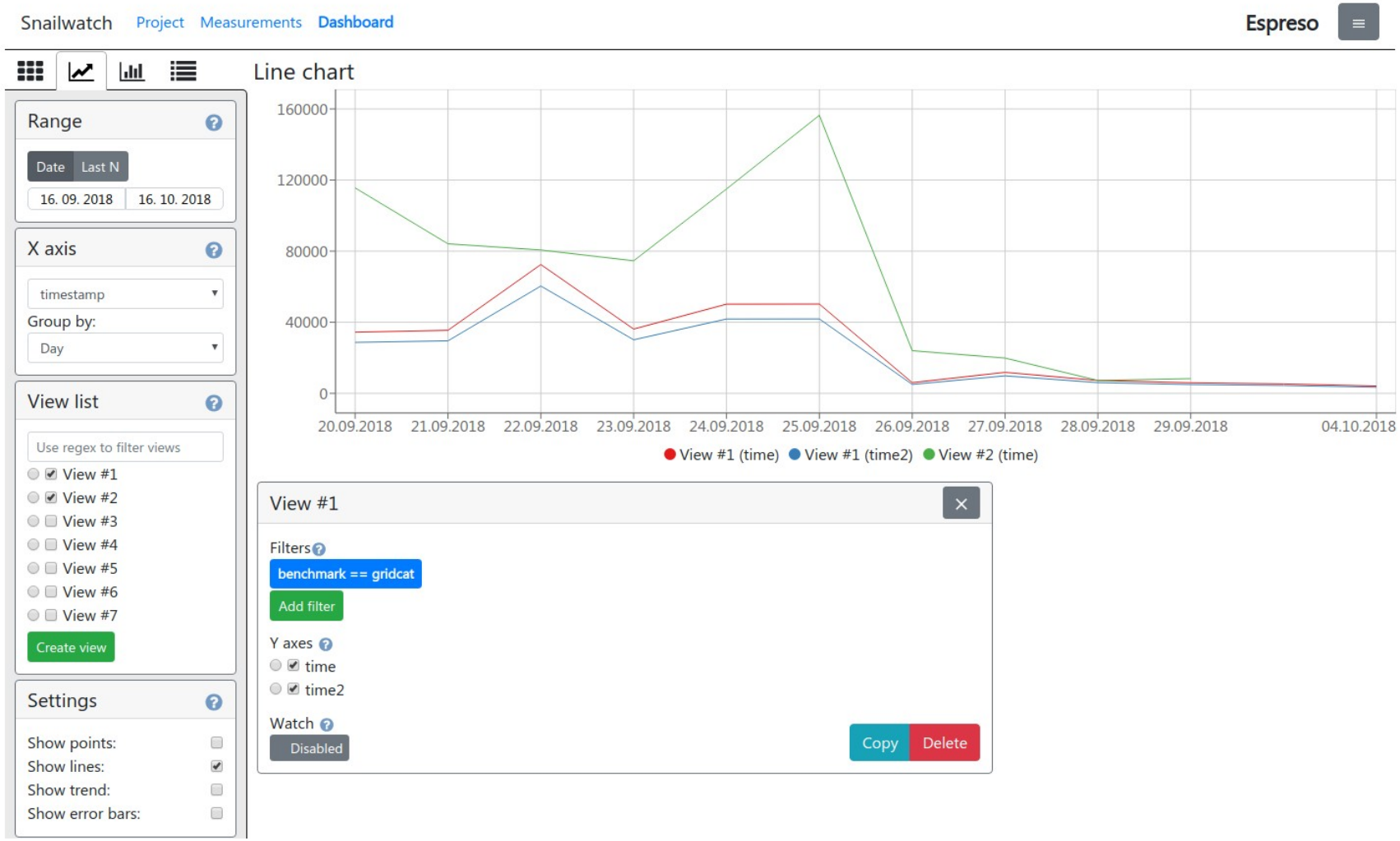
.gitlab-ci.yml 798 Bytes

```yaml
image: 'rust:latest'

stages:
  - build
  - test

variables:
  CARGO_HOME: $CI_PROJECT_DIR/cargo
  RUSTUP_TOOLCHAIN: stable

before_script:
  - apt-get update -yq
  - apt-get install --no-install-recommends -y libzmq3-dev

build:routing:
  stage: build
  artifacts:
    paths:
      - build/
    expire_in: 6h
  script:
    - mkdir build
    - cd build
    - cmake -DCMAKE_BUILD_TYPE=Release ..
    - make -j4
```

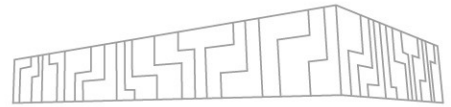
Gitlab CI documentation can be found here

CONTINUOUS BENCHMARKING

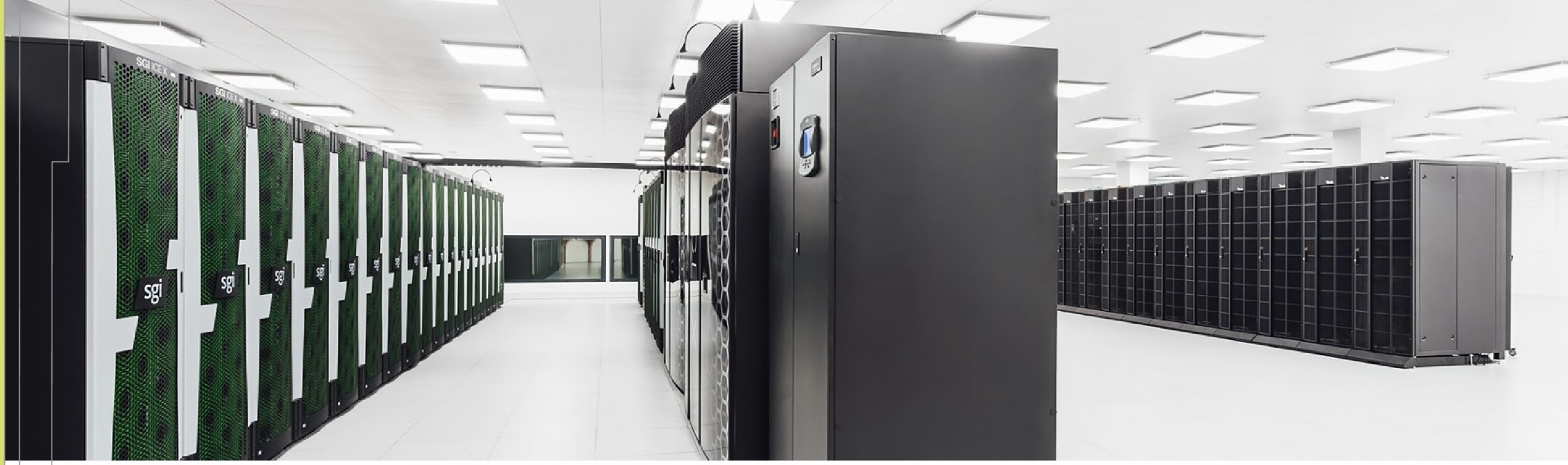
- Snailwatch
- Benchmark your code after each commit in CI, observe trends



FURTHER READING



- Productivity tools workshop
  - Git
  - EasyBuild
  - Gitlab CI
  - Singularity
  - Lmod
  - kvm



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