cesnet
metacentrum

LOKÁLNÍ INSTALACE SOFTWAROVÝCH BALÍČKŮ

SÉRIE WEBINÁŘŮ METACENTRA #4



DATUM
21. 10. 2026, 13:00



PŘEDNÁŠEJÍCÍ
Jiří Vorel



DÉLKA
90 min + diskuze

SLIDY A DOPROVODNÉ MATERIÁLY
events.cesnet.cz/e/meta4

OTÁZKY POKLÁDEJTE
v chatu nebo po skončení prezentace

V rámci této série webinářů jsme již představili:
23. 6. Úvod do možností využití výpočetní infrastruktury MetaCentrum
20. 7. AI nástroje (nejen) pro výzkum
2. 9. Efektivní práce s daty v infrastruktuře MetaCentrum
Materiály z těchto školení naleznete na https://github.com/CESNET/metacentrum-webinars.

Registrací na tuto akci potvrzujete, že:

1. berete na vědomí, že na této akci budou pořizovány audiovizuální záznamy, které budou dále využívány pro účely propagace této akce, a to v hmotné či elektronické podobě, včetně webových a sociálních stránek sdružení CESNET,
2. Vám byly poskytnuty veškeré potřebné informace o zpracování osobních údajů.

Začátek 21. 10. 2026 13:00
Konec 21. 10. 2026 14:30
Europe/Prague

Online

https://cesnet.zoom.us/j/96035402029?pwd=EqDQCnyakAFUhW0ZRWLbQakvvsBzPf.1

Doplňkové materiály (GitHub)

Registrace
Registrace jsou již otevřeny.

Registrovat se ihned

cesnet

metacentrum

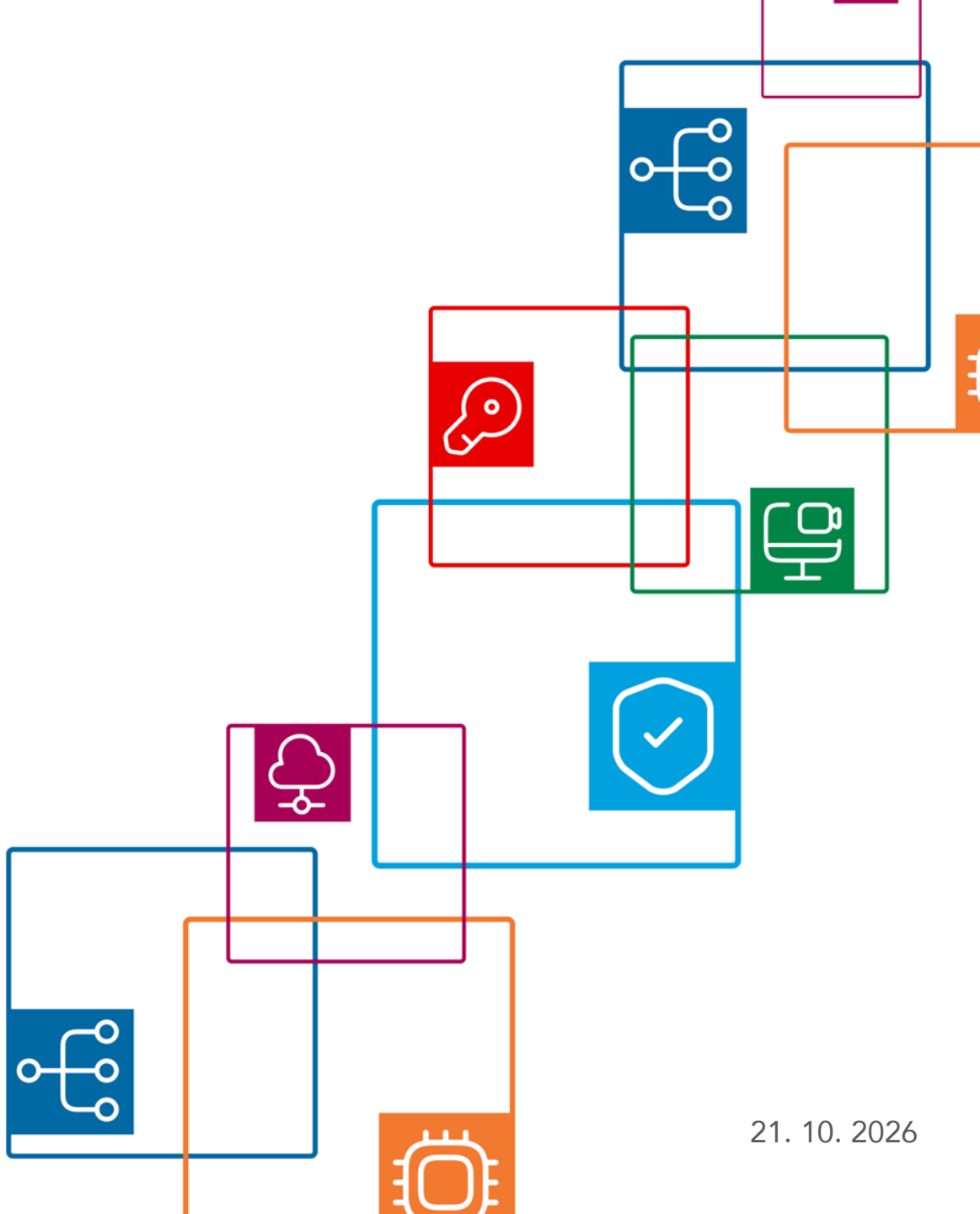
MetaCentrum NGI

The MetaCentrum webinar series

4. Local installation of software packages

Jiří Vorel

vorel@cesnet.cz meta@cesnet.cz



21. 10. 2026

Outline

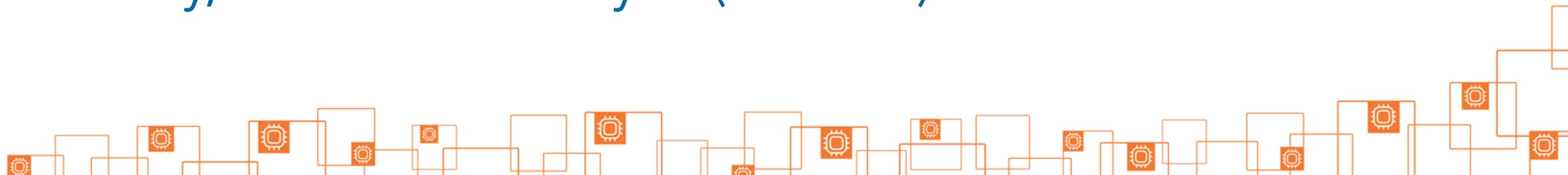
- Local installation in a nutshell
- Software modules
- Precompiled binaries
- Personal module file
- Debian libraries
- Python packages
- R packages
- Mamba package manager
- Singularity/Apptainer images
- Building and compiling source code
- Answering questions



https://docs.metacentrum.cz/en/docs/software/install-software

Local installation in a nutshell

- As a user, you can do it in your home directory
- Basically, anything can be installed...
  - Just make sure you do not violate the licence terms
  - Personal commercial software is OK (restricted access for the owner)
  - Apps for Windows are problematic in the grid, as we do not have a license
  - You can start a personal Windows licence in the cloud service
- Do not hesitate to ask for help (email us or contact any ambassador)
- Alternatively, we can do it for you (email us)



https://docs.metacentrum.cz/en/docs/software/install-software

Local installation in a nutshell

- Some installations take some time
  - It is better to start an interactive job

    `qsub -I ...` (capital letter i)
- A lot of temporary files can be produced
  - Tools with many dependencies installed by package managers (pip, Mamba, R)
  - Start an interactive job with a scratch storage
  - Redirect the temporary directory to the scratch directory

    `export TMPDIR=$SCRATCHDIR`



https://docs.metacentrum.cz/en/docs/software/install-software

Local installation in a nutshell

- We support and maintain many installation methods
  - Precompiled binaries (download, extract and use)
  - Debian libraries (apt-get)
  - Install packages for popular programming languages (Python, R, Rust, Julia, Perl, Ruby)
  - Package managers (Mamba, pip, Spack)
  - Singularity/Apptainer
  - Compiling source code
- Read the developer's instructions on how to install a given tool



https://docs.metacentrum.cz/en/docs/software/modules

Software modules

- Open source project Environment Modules

https://modules.readthedocs.io/en/latest/



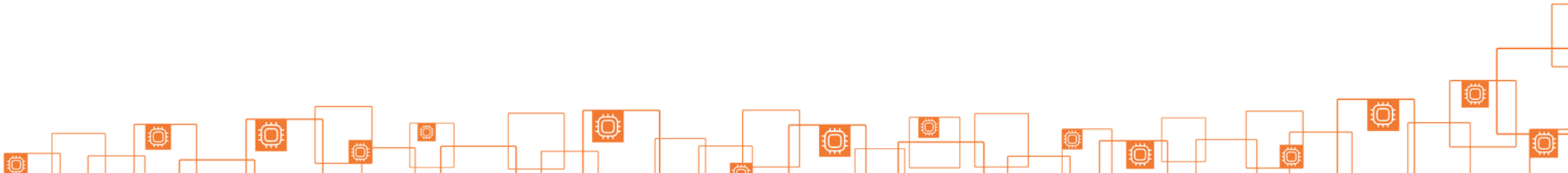
  - A tool for modifying user's environment

```
module --help
```

  - Commonly known commands like

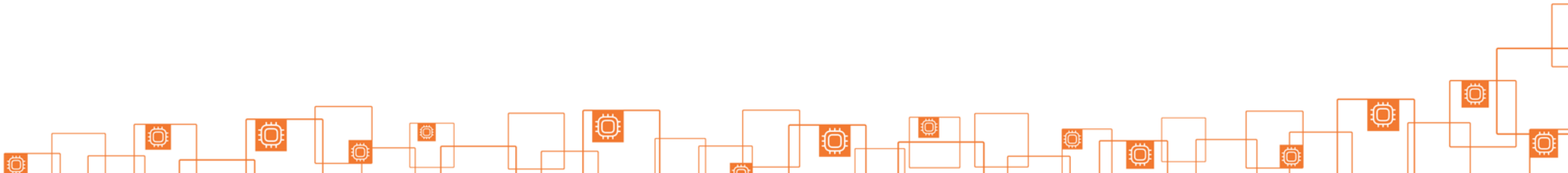
```
module ava/avail xyz/
module ava/avail xyz*/
module add/load xyz
module rm/unload xyz
module purge
```

  - Users can create their own module files for local installations



Precompiled binaries

- In most cases, this is the most straightforward way
- Download it - extract it, and use it
- However, this does not address the problem of dependencies
- It is also not highly optimised for a specific CPU architecture



Personal module file

- Should contain all the necessary settings
- Defined via the variable `MODULEPATH`
- Is written in the Tcl language

```
#%Module1.0
#!
#! Title: salmon
#! Version: 2.8.0
#! Description: Salmon is a fast program to produce a highly-accurate, transcript-level quantification estimates from RNA-seq data.
#!
#! Author: Jiri Vorel

proc ModulesHelp {} {
global ModulesCurrentModulefile
puts stdout "modulehelp $ModulesCurrentModulefile"
}

prepend-path PATH /storage/brno2/home/vorel/WEB_INSTALL/salmon/
```

Personal module file

- Should contain all the necessary settings
- Defined via
- Is written in

```
module add cuda/cuda-11.1.0-intel-19.0.4-j4dpull

prepend-path PATH /software/NAMD/3.0.2-gpu
prepend-path LD_LIBRARY_PATH /software/NAMD/3.0.2-gpu/lib
```

```
#%Module1.0
#!
#! Title: salmon
#! Version: 2.8.0
#! Description: Salmon is a
#!
#! Author: Jiri Vorel

proc ModulesHelp {} {
global ModulesCurrentModulef
puts stdout "modulehelp $Mod
}

prepe
```

```
(TRIXIE)vorel@nympha:~/UMItools-1.1.5/lib$ pwd
/storage/plzen1/home/vorel/UMItools-1.1.5/lib
(TRIXIE)vorel@nympha:~/UMItools-1.1.5/lib$ ls
cmake                   libcurl.so              libhistory.so.8
itcl4.2.3               libcurl.so.4            libhistory.so.8.2
krb5                    libcurl.so.4.8.0        libitm.so
```

```
export LD_LIBRARY_PATH=/storage/plzen1/home/vorel/UMItools-1.1.5/lib/:$LD_LIBRARY_PATH
```

https://docs.metacentrum.cz/en/docs/software/install-software#debian-packages

Debian libraries

- Debian users can download the missing system libraries using the `apt-get` command
  - Installation requires sudo (as tutorials say) = problem for users

```
error while loading shared libraries: libgsl.so.28: cannot open shared object file: No such file or directory
```

```
(TRIXIE)vorel@nympha:~/TEST_LIB$ apt-get install libgsl28
E: Could not open lock file /var/lib/dpkg/lock-frontend - open (13: Permission denied)
E: Unable to acquire the dpkg frontend lock (/var/lib/dpkg/lock-frontend), are you root?
(TRIXIE)vorel@nympha:~/TEST_LIB$ sudo apt-get install libgsl28
[sudo] password for vorel:
```

- The procedure involves
  - Downloading the package, extraction and linking



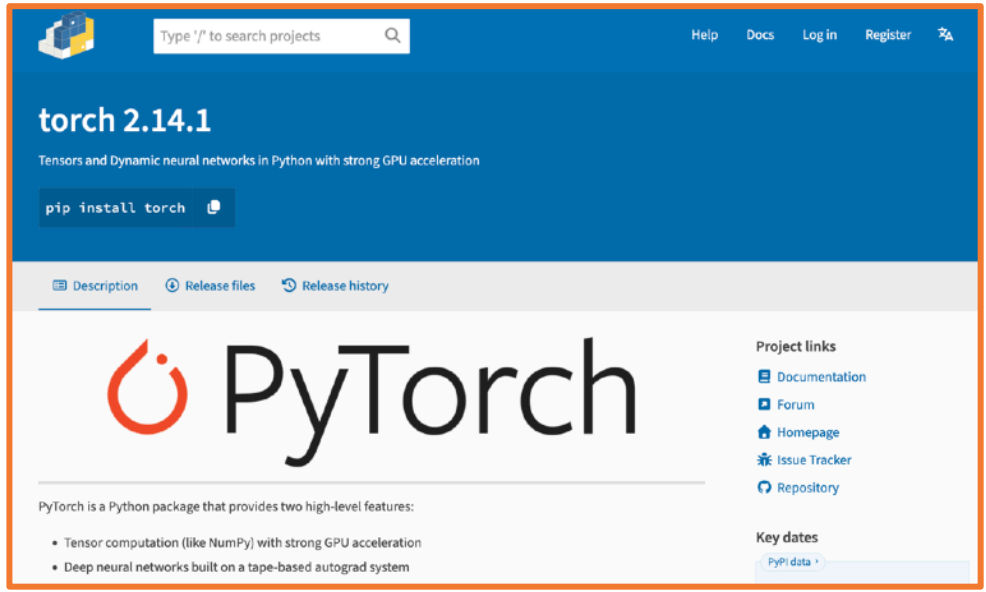
https://docs.metacentrum.cz/en/docs/software/install-software#python-packages

Python packages

- pip
  - Package manager and installer for Python
  - Repository at pypi.org
  - Installing of larger packages can exceed the root quota

```
ERROR: Could not install packages due to an OSError: [Errno 122] Disk quota exceeded
```

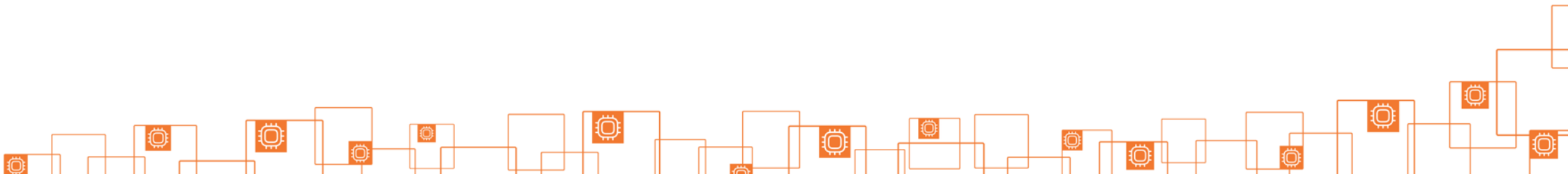
  - Let's try to install PyTorch
- venv
  - Isolated Python project environment
  - Let's try to install Pandas



https://docs.metacentrum.cz/en/docs/software/install-software#r-packages

R packages

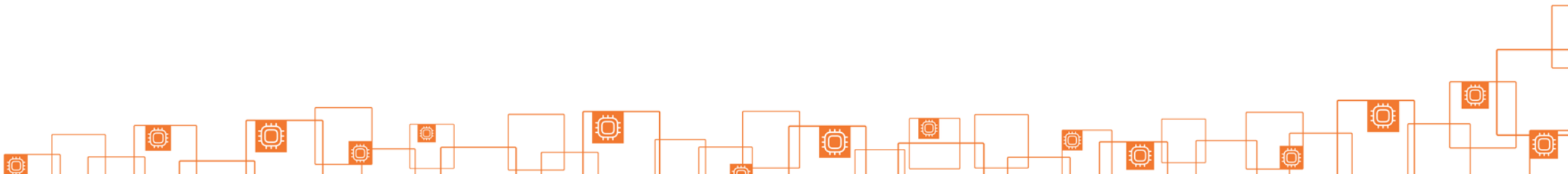
- Works in CLI and in GUI (Rstudio in OnDemand)
- Bioconductor - popular repository for bioinformatics packages
  - R package manager `BiocManager`
- Using `install.packages()` function
- Sometimes it can be complicated and dependent on build tools



https://docs.metacentrum.cz/en/docs/software/sw-list/conda-modules

Mamba package manager

- One of the most powerful package manager https://anaconda.org/
- An improved version of the Conda manager
- The syntax remains the same
- The most crucial channels are `bioconda` and `conda-forge`
- Mamba is a native part of the MetaCentrum system
  - There is no need to load the module



https://docs.metacentrum.cz/en/docs/software/containers

Singularity/Apptainer images

- Alternatives to Docker containers for HPC
  - No admin rights needed
  - Works smoothly with job schedulers and shared file systems
  - Supports Docker images
- Apptainer is a community-driven fork of Singularity
- We will probably switch to Apptainer by the end of the year
  - Users should not notice
  - The prompt will change from `Singularity>` to `Apptainer>`
- Create your images on the builder.metacentrum.cz



Building and compiling source code

- A very complex topic
- Literally anything can go wrong
  - From errors in the source code to bugs in the compiler
- This is a topic for a separate webinar :-/

