HPC Software – Modules, Libraries & Software

JSC Training Course

November 21, 2023 | R. Schöbel | JSC

Member of the Helmholtz Association

JÜLICH Forschungszentrum

Outline

Modular Programming

Software Implementation & Libraries

A **library** is a collection of resources.
In computer science: configuration data, documentation, help data, message templates, pre-written code and subroutines, classes, values or type specifications

- **Don't reinvent the wheel**: Recoding is time-consuming and error-prone
- **Best practice for own code**: Design interfaces and do different implementation separately (ideally separate files)

Modular Programming

Compiling & Linking

Example:

- Code decomposition into an executable and an outsourced subprogram *(C++: Link object files for different modules)*

  ```
  g++ -g -c -o main.o main.cpp
  g++ -g -c -o alibrary.o alibrary.cpp
  g++ -g main.o alibrary.o -o main
  ```

  (In real life: Use **make** or **cmake**)
- Copy *.o* and *.h* to separate directories (e.g. */base/lib/alibrary.o*) and add
  - The **-L** option for the path to the library's object, the object code using **-l**

    ```
    g++ -g -L/base/lib -o main main.o -lalibrary
    ```
  - The **-I** flag for include directories

Modular Programming

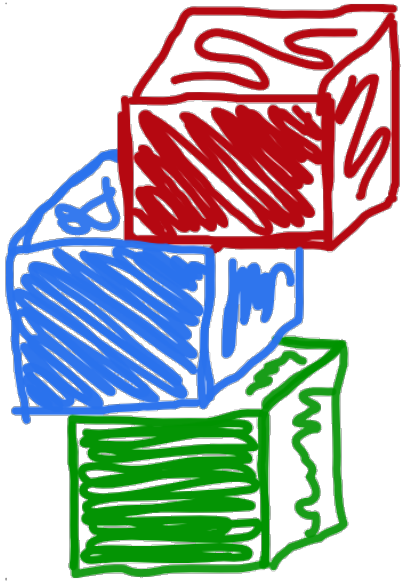
Compiling & Linking

- For libraries that are not in standard directories, you need to set **-I**/base/include and **-L**/base/lib for compiling/linking
- Or define linux **environment variables**:
  - You either enter the *export*-commands on the linux prompt before compiling, or, copy them into to the .bashrc file in your home folder
- Usually you do not need **-I** or **-L** for libraries accessed using the *module load* command on our supercomputers

Modular Programming

Installing Libraries from Source

- Library is not in the software module stack
- Common installation procedure:
  - make
    ./configure –prefix=base
    make; make install
  - cmake
    cmake -DCMAKE_INSTALL_PREFIX=base
    make; make install
  - Choose *base* as a directory you have write permissions



easybuild

Preinstalled HPC Software Packages

EasyBuild

Preinstalled HPC Software Packages

Navigating Modules

- Tools are available through **"modules"**
  - Allows to easily manage different versions of programs
  - Works by dynamic modification of a user's environment
- Module setup based on **EasyBuild** and **lmod**
  - **"Staged"**, hierarchical setup
  - Automatically manages dependencies via **"toolchains"**
- Consistent setup on JURECA, JUSUF and JUWELS (Cluster & Booster)

Preinstalled HPC Software Packages

Toolchains: Underlying Compiler and MPI Libraries

- **Base:** GCCcore
- **Compiler:**
  - Intel compiler
  - GNU compiler
  - NVIDIA (CUDA) compiler
- **MPI libraries:**
  - ParastationMPI
  - Intel MPI
  - OpenMPI
- **Math libraries:** e.g. FlexiBLAS

Preinstalled HPC Software Packages

Toolchains: Underlying Compiler and MPI Libraries

Current software stage is 2024

- **Base:** GCCcore *(12.3.0)*
- **Compiler:**
  - Intel compiler *(Intel 2023.2.1)*
  - GNU compiler *(GCC 12.3.0)*
  - NVIDIA (CUDA) compiler *(NVHPC 23.7)*
- **MPI libraries:**
  - ParastationMPI *(ParaStationMPI 5.9.2-1)*
  - Intel MPI *(Intel MPI 2021.10.0)*
  - OpenMPI *(OpenMPI 4.1.5)*
- **Math libraries:** e.g. FlexiBLAS *(MKL 2023.2.0, BLIS 0.9.0, OpenBLAS 0.3.23)*

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Modules Environment

Available Compiler/MPI Combinations in Stages/2024

Compiler	MPI	Cuda available
GCC	ParaStationMPI	yes
GCC	OpenMPI	yes
NVHPC	ParaStationMPI	yes
NVHPC	OpenMPI	yes
Intel	ParaStationMPI	yes
Intel	IntelMPI	no
Intel	OpenMPI	yes

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Toolchains: Underlying Compiler and MPI Libraries

The most important module command

- module load <*name*> or ml <*name*>

- **GCCcore** is preloaded, which enables a lot of base software
- For HPC software you have to load a **compiler**, to expand the module tree
  e.g. `ml GCC` *(Default is 12.3.0)*
- Then you load an **MPI** version
  e.g. `ml ParaStationMPI` *(Default is 5.9.2-1)*
- Then you can load any other **math or application package**
  e.g. `ml PETSc/3.20.0`

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Preinstalled HPC Software Packages

Modules Environment

- After loading compiler and MPI `ml avail` shows the software available with that combination
- `ml avail` *name* and `ml help` *name* will show you details about the *name* package
- Many libraries are available for more than one combination/toolchain

- Write e-mail to `sc@fz-juelich.de` if you want special versions or new software
  - No guarantee the software will be installed
  - alternative: Install packages in User space

Preinstalled HPC Software Packages

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Preinstalled HPC Software Packages

Modules Environment

- `ml spider` *name* shows whether a library is available in the current stage and in which versions

  e.g. module spider petsc

  ⇒ PETSc/3.18.5,
  PETSc/3.20.0, ...

- `ml spider` *name/version* shows which environment you have to load before you can load that version

  e.g. module spider PETSc/3.20.0

  ⇒ Stages/2024 + GCC/12.3.0 + ParaStationMPI/5.9.2-1, ...

- Some packages are hidden. To see them use

  `ml -show-hidden spider` *name*

Preinstalled HPC Software Packages

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  `ml -show-hidden spider` *name*

Preinstalled HPC Software Packages

Modules Environment

- For R, Python and Perl we use bundles
  - You might be looking for a software package that is part of a bigger module
- Use `ml key software`
  `ml key numpy` will suggest `SciPy-Stack`
- You can use then `ml spider` to find out how to load the module

Preinstalled HPC Software Packages

Modules Environment

Stages

- The whole software stack of JURECA, JUSUF, JUWELS Cluster and Booster will be updated regularly
- Current stage is 2024
- Old stages are still accessible on JUWELS Cluster, but no guarantee
- To check availability in other stages first type

```
ml use $OTHERSTAGES
```

Preinstalled HPC Software Packages

Mathematical Libraries: FlexiBlas

FlexiBlas: wrapper library, includes MKL, BLIS, OpenBLAS

- Linear Algebra Packages (LAPACK, ScaLAPACK, ...)
- Iterative Sparse Solvers, Trust Region Solver
- Vector Math Library
- Vector Statistical Library
- Fourier Transform Functions
- Trigonometric Transform Functions
- GMP routines, Poisson Library, ...

Preinstalled HPC software packages

Mathematical Libraries: Sequential Packages

Public domain Libraries

- LAPACK (Linear Algebra PACKage)
- ARPACK (ARnoldi PACKage)
- GSL (Gnu Scientific Library)
- GMP (Gnu Multiple Precision Arithmetic Library)
- METIS (Serial Graph Partitioning and Fill-reducing Matrix Ordering)

Preinstalled HPC Software Packages

Mathematical Libraries: Parallel Packages

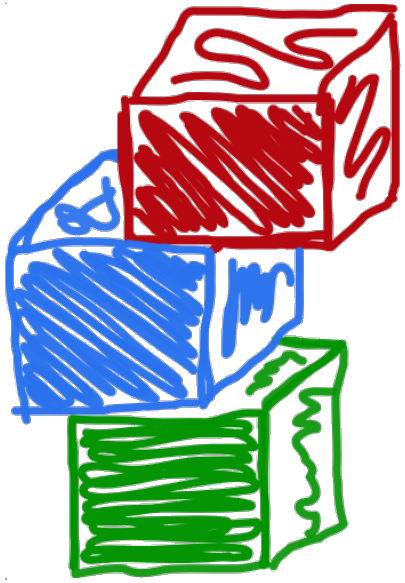
- ScaLAPACK (Scalable Linear Algebra PACKage)
- ELPA (Eigenvalue SoLvers for Petaflop-Applications)
- FFTW (Fastest Fourier Transform of the West)
- MUMPS (MUltifrontal Massively Parallel sparse direct Solver)
- ParMETIS (Parallel Graph Partitioning)
- SCOTCH (Parallel Graph Partitioning)
- Hypre (high performance preconditioners)
- ARPACK (Parallel ARPACK)
- SPRNG (Scalable Parallel Random Number Generator)
- SUNDIALS (SUite of Nonlinear and DIfferential/ALgebraic equation Solvers)

GPU Library

- MAGMA, Matrix Algebra on GPU and Multicore Architectures

Parallel Systems

- PETSc, toolkit for partial differential equations
  - PETSc for Python (petsc4py)
- SLEPc Scalable Library for Eigenvalue Problem Computations Extension to PETSc for the computation of eigenvalues and eigenvectors



easybuild

User Installations at JSC

EasyBuild

EasyBuild

How it is used at JSC

- Used by the software team to create software stacks since 2014
  - **Install in Production stage:**
    ml Stages/2024
    ml Developers
    eb packages-1.2.3.eb
- Allow users to install software on-top of the available modules
  - **Install in User space:**
    ml Stages/2024
    export USERINSTALLATIONS=/p/project/yourproject/user
    ml UserInstallations
    eb packages-1.2.3.eb

Excerpt from PETSc easyconfig

https://github.com/easybuilders/JSC/blob/2024/Golden_Repo/p/PETSc/PETSc-3.20.0-gpsfbf-2023a.eb

```
04 name = "PETSc"
05 version = "3.20.0" # PETSc/3.20.0

#see Golden_Repo: g=GCC, ps=ParaStationMPI, fbf=FlexiBlas
18 toolchain = 'name': 'gpsfbf', 'version': '2023a'

# where the installation files are downloaded
23 source_urls = ['https://web.cels.anl.gov/...
24 sources = ['petsc-%s.tar.gz' % version]

#deps that are already present at stage 2023a
35 dependencies = [('METIS', '5.1.0'), ...

53 configopts = '–with-large-file-io'
```

Create new PETSc installation

PETSc-3.20.0-gpsfbf-2023a-myVersion.eb

```
04 name = "PETSc"
05 version = "3.20.0"
06 versionsuffix = '-myVersion' # PETSc/3.20.0-myVersion
18 toolchain = 'name': 'gpsfbf', 'version': '2023a'

# where the installation files are downloaded
23 source_urls = ['https://web.cels.anl.gov/...
24 sources = ['petsc-%s.tar.gz' % version]

#deps that are already present at stage 2023a
35 dependencies = [('METIS', '5.1.0'), ...

53 configopts = '–with-large-file-io'
54 configopts += '–something_fancy '
```

Create and run new PETSc installation

PETSc-3.20.0-gpsfbf-2023a-myVersion.eb

- **Install in User space:**
  ml Stages/2024
  export USERINSTALLATIONS=/p/project/yourproject/user
  ml UserInstallations
  eb PETSc-3.20.0-gpsfbf-2023a-myVersion.eb
- **Load and Use of new Software:**
  export USERINSTALLATIONS=/p/project/yourproject/user
  ml Stages/2024 && ml GCC && ml ParaStationMPI
  ml PETSc/3.20.0-myVersion

EasyBuild: Further Links

Documentation:

- EasyBuild Documentation
  `https://docs.easybuild.io`
- EasyBuild Tutorial
  `https://easybuild.io/tutorial`

Where do I find easyconfigs?

- JSC repository
  `https://gitlab.jsc.fz-juelich.de/software-team/easybuild`
- JSC public mirror
  `https://github.com/easybuilders/JSC`
- Upstream
  `https://github.com/easybuilders/easybuild-easyconfigs`

Containers

Apptainer

Containers

What they provide

- Containers package up pieces of software in a way that is **portable and reproducible**, they ...
  - manage different versions of programs
  - are more lightweight than virtual machines
  - provide the ability to build, ship, and run applications
- Some examples are Docker, Shifter, and **Apptainer/Singularity**
- They typically use so-called **"images"**
  - contain a file system including a minimal operating-system, the application, and some metadata

Apptainer Containers

First steps

- We provide an up-to-date version of **Apptainer**
  - Formerly, we provided Singularity on the Systems
  - We have replaced Singularity by Apptainer, a fork maintained by the linux foundation
- To be granted access to the container runtime, you have to go to our user portal **JuDoor**
  - *Software*
  - *Request access to restricted software*
  - *Access to other restricted software*
  - *Container*
  - *Get Access*
  - *Accept the Service Level Description*

Apptainer Containers

First steps

Environment variables:

- It might be helpful to overwrite some Apptainer environment variables

```
export APPTAINER_CACHEDIR =$(mktemp -d -p <DIR>)
```

```
export APPTAINER_TMPDIR= $(mktemp -d -p <DIR>)
```

Download an image:

- Use the pull command to download pre-built images from an external resource like Docker Hub

```
apptainer pull centos.sif docker://centos:7
```

Apptainer Containers

First steps

Call an executable:

- The shell command allows you to spawn a new shell within your container and interact with it

```
srun -N1 -p <part> –gres gpu:1 –pty apptainer shell –nv centos.sif
```

- To Slurm, Singularity is just another executable and can be called as such

Container Build System:

- JSC provides a build system that can build images on behalf of the user, based on a Docker- or Singularity-file
- For further information see `https://apps.fz-juelich.de/jsc/hps/jureca/container-runtime.html`

Further information and JSC-people

http://www.fz-juelich.de/ias/jsc/jureca
http://www.fz-juelich.de/ias/jsc/juwels
http://www.fz-juelich.de/ias/jsc/jusuf

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Supercomputer support:
sc@fz-juelich.de