Tools and more for High-Performance Computing

Overview

- ❑ Environment & account setup
- ❑ Compilers
- ❑ IDEs, Libraries
- ❑ Make & Makefiles
- ❑ Version control
- ❑ Data analysis tools: awk & perl (self study)
- ❑ Visualization tools (self study)
- ❑ Resource Managers

The DTU computer system

The central DTU UNIX system

- Application servers:
  - 8 Huawei XH620 V3 (2x Intel Xeon E5-2660v3 2.6 GHz)
  - 7 Dell PowerEdge FC430 (2x Intel Xeon E5-2670v3 2.3 GHz)
  - Alma Linux 9.7
- Virtual GL servers:
  - 2 Lenovo ThinkSystem SR650 (2x Intel Xeon Gold 6226R 2.9 GHz + 2x NVIDIA Quadro RTX 5000)
- Desktop servers (ThinLinc):
  - 4 servers (AMD EPYC 7513, 2.6 GHz)
- 10000+ users (students + employees)

The DTU Unix systems

- HPC servers (for 'everybody'), e.g.
  - 48 Huawei XH620 V3 (2x Xeon E5-2660v3 2.6 GHz, 128 GB memory)
  - 40 Huawei XH620 V3 (2x Xeon E5-2650v4 2.2 GHz, 256 GB memory)
  - 24 Lenovo ThinkSystem SD530 (2x Xeon Gold 6126 2.6 GHz, 192-384 GB memory)
  - 4 Lenovo ThinkSystem SD530 (2x Xeon Gold 6142 2.6 GHz, 384 GB memory)
  - 28 Lenovo ThinkSystem SD530 (2x Xeon Gold 6226R 2.9 GHz, 384-768 GB memory)
  - 4 Lenovo ThinkSystem SD630 (2x Xeon Gold 6342 2.8 GHz, 512 GB memory)
- + “private” clusters (DTU departments)

Access to the system

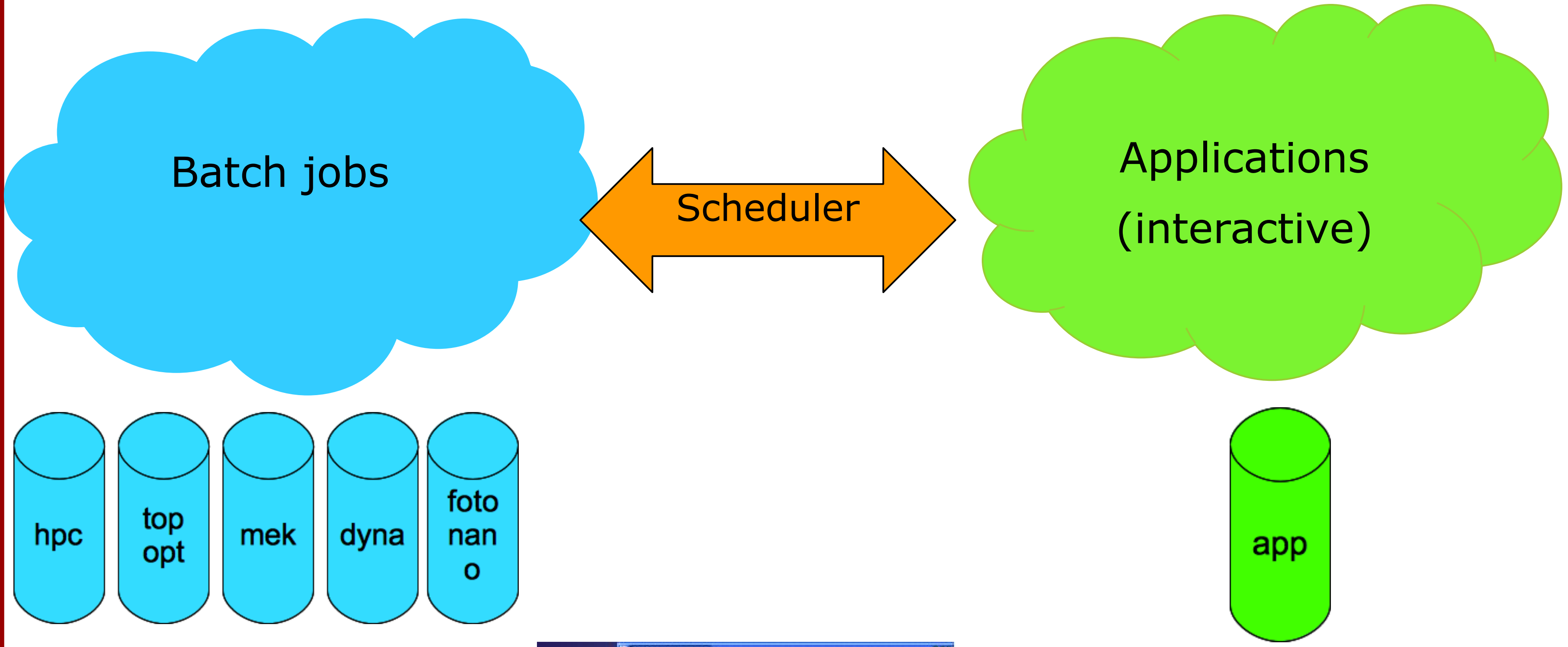
- Remote access, only:
  - ThinLinc remote desktop session:
    - download ThinLinc client from www.thinlinc.com
    - connect to thinlinc.gbar.dtu.dk
    - browser based: https://thinlinc.gbar.dtu.dk/
    - preferred way, if you work a lot with GUIs
  - Secure SHell (ssh) connection
    - login.hpc.dtu.dk or login2.hpc.dtu.dk
    - login.gbar.dtu.dk or login2.gbar.dtu.dk
  - Note: those machines are login nodes!
    - no computations here, please!
    - open a ‘xterm’ (ThinLinc) or do a ‘linuxsh’ (SSH)

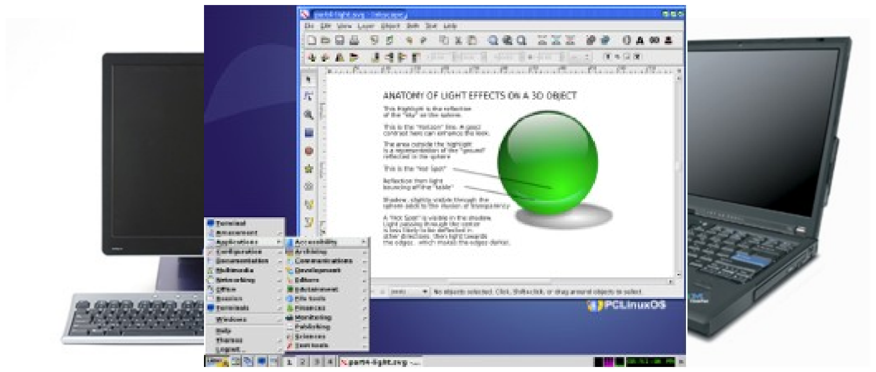
Access to the system

Please note – increased IT security:

- access with username & password only from a DTU network, e.g. WiFi on Campus (DTUsecure or eduroam), or via DTU VPN from outside.
- if you don't want to (or cannot) use the DTU VPN: SSH and ThinLinc (client) requires in addition a SSH keypair, when connecting from outside DTU.
  - for the setup see this page: https://www.hpc.dtu.dk/?page_id=4317
- the ThinLinc webclient (browser) does not work from outside the DTU networks (only via VPN)!

Our Setup


Batch jobs
Scheduler
Applications
(interactive)
hpc
top
opt
mek
dyna
foto
nan
o
app



The DTU computer system

Be aware of, that ...

- this is a multi-user system(!)
- (almost) all applications on the system are started by a load-balancing queueing system
- there are different
  - CPU types,
  - clock frequencies,
  - amounts of RAM,
  - etc
- Thus, the performance will vary!!!

The DTU computer system

Comparing performance numbers:

- make sure to be on the same machine type
  - `lscpu` command
  - `echo $CPUTYPEV`
- always report CPU type(s)
- check the load (interactive sessions)
  - `uptime` command
- check the # of CPU cores
  - `cpucount` command

Compilers

- GNU Compilers (C/C++)
  - gcc 11.5.0 (OS standard)
  - other versions: check with 'module avail gcc'
  - we provide version from 8.5 to latest GCC version
- other compilers:
  - clang (LLVM): check with ‘module avail clang’
  - Intel: check with ‘module avail intel’
- Note: 'cc' depends on the module loaded!!!
  - always use the specific names, i.e. gcc, clang, ...
  - in doubt: use the ‘--version’ option to check

Using modules

- modules help to organize certain Unix environment settings, e.g. PATH, MANPATH, LD_LIBRARY_PATH, etc. for different versions of the same application
- list available modules: `module avail gcc`
- load a module: `module load gcc`
  - loads the default version (13.3.0)
- swap a version: `module swap gcc/14.2.0`
- swap to default: `module swap gcc`
- info: http://gbar.dtu.dk/index.php/faq/83-modules

IDEs

- VSCode (`code`) – version 1.95.2
  - available under ThinLinc
    - start from menu
    - or command line: `code`
  - alternative: remote access with VSCode (guide will be on DTU Learn)
- Graphical debuggers:
  - Totalview (`totalview`)
  - Data Display Debugger (`ddd`)
    - GUI front-end to gdb

Alternative approach

- Develop the code on your computer
  - ... with the tools you know and like
- Transfer the code to the HPC system
  - ... with WinSCP, FileZilla, scp, rsync
  - or sync with repository (GitLab, GitHub, ...)
- Test and run on the HPC system
  - ... tests on the interactive nodes
  - ... timings/benchmarks via the batch system

Libraries

- Available Scientific Libraries:
  - ATLAS
    - BLAS, CBLAS, LAPACK, ...
    - optimized for generic x64 platform
  - OpenBLAS
    - module load openblas/<version>
    - optimized for different CPU types

Make & Makefiles

A tool for building and
maintaing software projects

Make – The ideas behind

- maintain, update and regenerate groups of programs
- useful tool in multi-source file software projects
- can be used for other tasks as well, e.g. typesetting projects, flat-file databases, etc
- in general: every task that involves updating files (i.e. result) from other files (i.e. sources) is a good candidate for make

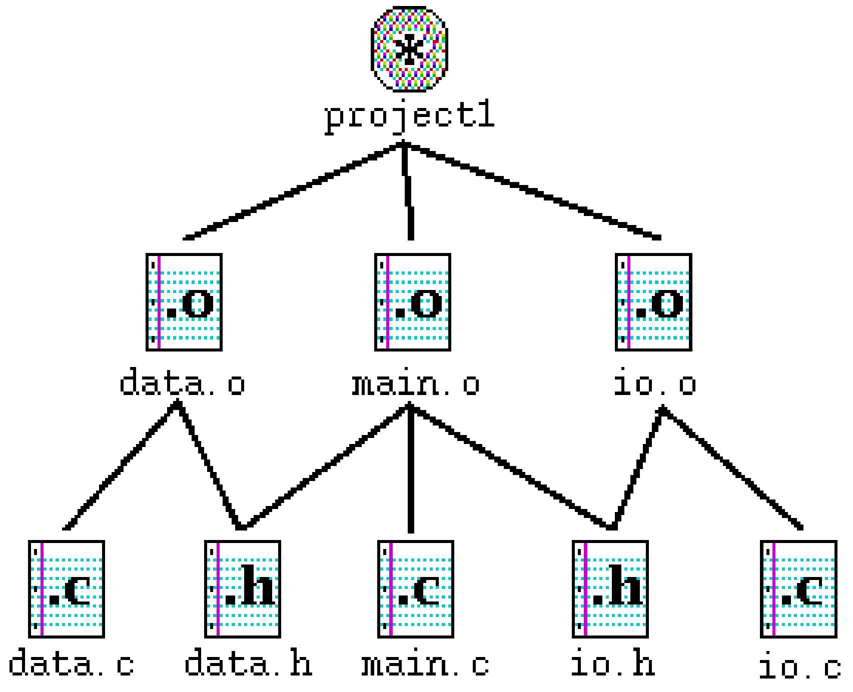
Make – The ideas behind

Dependency graph:

result (executable)

intermediate level

source file level



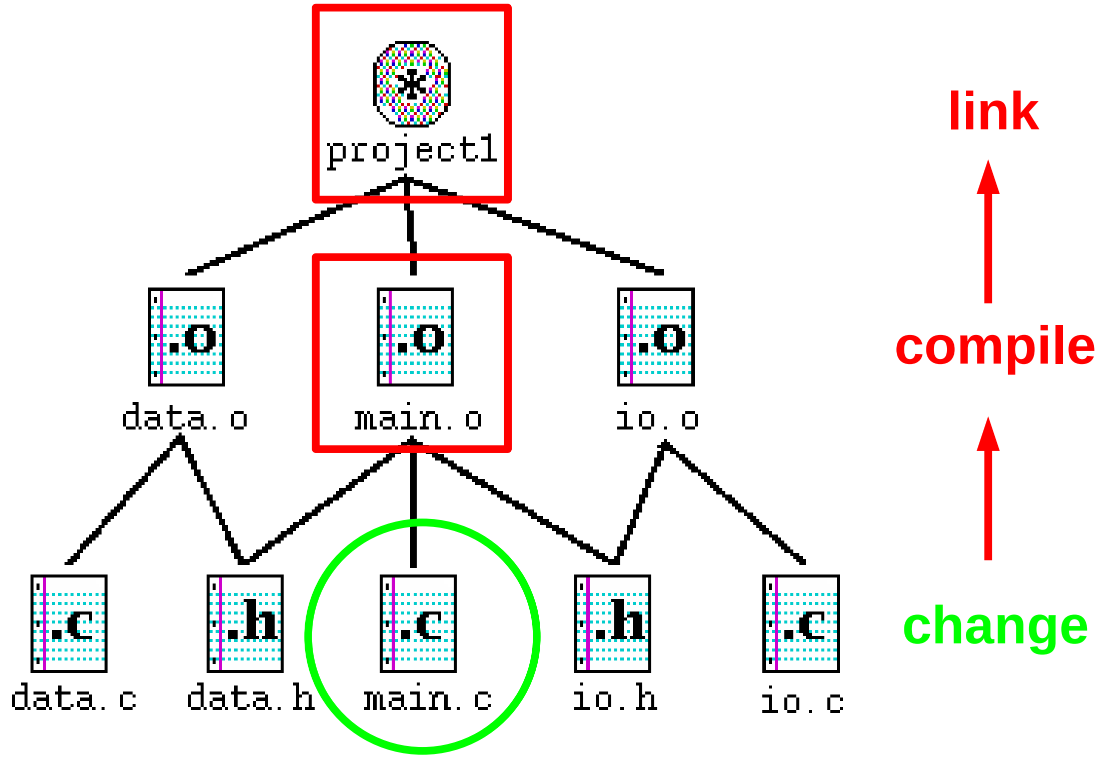
Make – The ideas behind

Dependency graph:

result (executable)

intermediate level

source file level



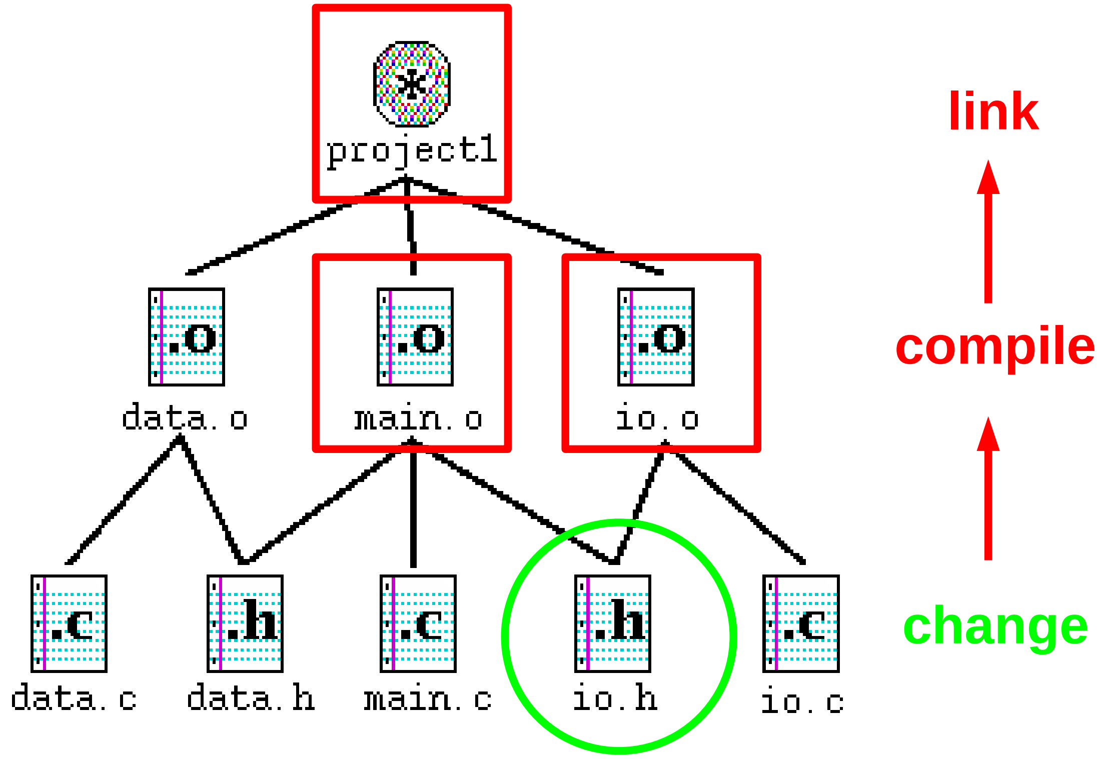
Make – The ideas behind

Dependency graph:

result (executable)

intermediate level

source file level



Make – The ideas behind

- Compiling by hand:
  - error prone
  - easy to forget a file
  - typos on the command line
- There is a tool that can help you:

make

Make – The ideas behind

Things 'make' has to know:

- file status (timestamp)
- file location (source/target directories)
- file dependencies
- file generation rules (compiling/linking)
  - general rules (.c → .o)
  - special rules (io.c → io.o)
- tools (compilers, etc.)

- filesystem
- Makefile
- environment

Makefile – rulesets...and more

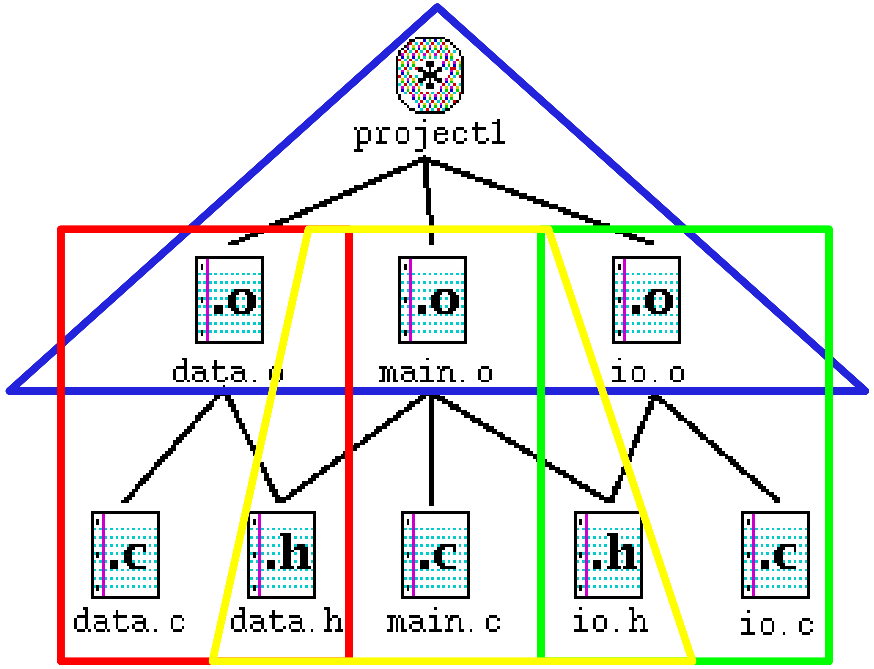
- make needs a set of rules to do its job
- rules are defined in a text file – the *Makefile*
- standard names: Makefile or makefile
- non-standard names can be used with the '-f' option of make: `make -f mymf` ...
- preview/dryrun option: `make -n` ...

Makefile – rulesets...and more

There are two major object types in a Makefile

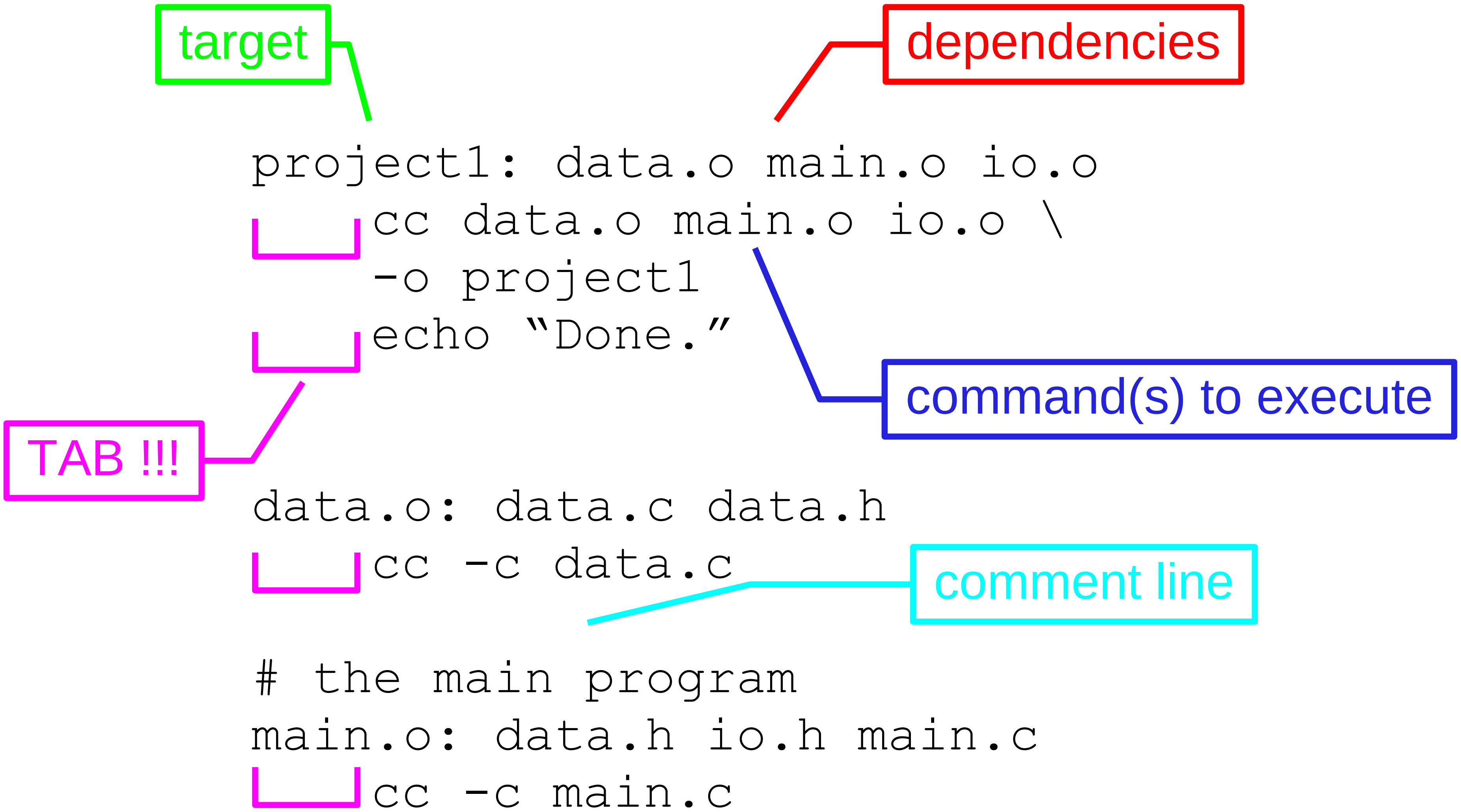
- targets
  - definition by a “:”
  - followed by the dependencies (same line)
  - followed by lines with the commands to execute
- macros
  - definition by “=”
  - single line (use “\” to extend lines)
- ... and comments: (lines) starting with #

Makefile – rulesets...and more



```
project1: data.o main.o io.o
     cc data.o main.o io.o -o project1
data.o: data.c data.h
     cc -c data.c
main.o: data.h io.h main.c
     cc -c main.c
io.o: io.h io.c
     cc -c io.c
```

Makefile – rulesets...and more



```
project1: data.o main.o io.o
	cc data.o main.o io.o \
	-o project1
	echo "Done."

data.o: data.c data.h
	cc -c data.c

# the main program
main.o: data.h io.h main.c
	cc -c main.c
```

Makefile – rulesets...and more

```
# Sample Makefile
CC      = gcc
OPT     = -g -O3
WARN    = -Wall
CFLAGS = $(OPT) $(WARN)     # the C compiler flags
OBJECTS   = data.o main.o io.o

project1 : $(OBJECTS)
     $(CC) $(CFLAGS) -o project1 $(OBJECTS)

clean:
     @rm -f *.o core

realclean : clean
     @rm -f project1

# file dependecies
data.o : data.c data.h
main.o : data.h io.h main.c
io.o   : io.h io.c
```

Macro definitions

Macro reference

Where are my rules
for compiling the .o files?

Makefile – rulesets...and more

Running make:

```
myhost $ make
gcc -g -O3 -Wall   -c -o data.o data.c
gcc -g -O3 -Wall   -c -o main.o main.c
gcc -g -O3 -Wall   -c -o io.o io.c
gcc -g -O3 -Wall -o project1 data.o main.o io.o
```

How did **make** know how to build data.o, ... ?

Makefile – rulesets...and more

built-in data base of "*standard rules*" and "*standard macros*":

- known rules:
  - compile .o files from a .c/.cpp/.f/... source file
  - link executables from .o files
- pre-defined macros:
  - CC, CFLAGS, FC, FFLAGS, LD, LDFLAGS
- view with `make -p -f /dev/null` (long listing!)

Makefile – rulesets...and more

```
# GNU Make 3.80
# Variables
...
# default
OUTPUT_OPTION = -o $@
# makefile (from `Makefile', line 3)
CC = gcc
# environment
MACHTYPE = i686-suse-linux
# makefile (from `Makefile', line 6)
CFLAGS = $(OPT) $(WARN)
# makefile (from `Makefile', line 4)
OPT = -g -O3
# makefile (from `Makefile', line 5)
WARN = -Wall
# default
COMPILE.c = $(CC) $(CFLAGS) $(CPPFLAGS) -c
# makefile (from `Makefile', line 8)
OBJECTS = data.o main.o io.o
...
```

Makefile – rulesets...and more

```
...

# Implicit Rules
.c.o:
#  commands to execute (built-in):
	$(COMPILE.c) $(OUTPUT_OPTION) $<

...

data.o: data.c data.c data.h
#  Implicit rule search has been done.
#  Implicit/static pattern stem: `data'
#  Last modified 2004-08-27 10:08:56.008831584
#  File has been updated.
#  Successfully updated.
#  commands to execute (built-in):
	$(COMPILE.c) $(OUTPUT_OPTION) $<
```

Makefile – rulesets...and more

Practical hints:

- preview/dryrun option: `make -n ...`
- switch off built-in rules/macros:

  `make -r ...`
- check the known suffixes (.SUFFIXES) and implicit rules for your source files, e.g. does gmake still fail for .f90/.f95
- add suffixes needed:

```
.SUFFIXES: .f90
```

Makefile – rulesets...and more

Practical hints (cont'd):

- be aware of timestamps (Network-FS)
- override macros on the command line:

```
myhost $ make
gcc -g -O3 -Wall     -c -o data.o data.c
gcc -g -O3 -Wall     -c -o main.o main.c
gcc -g -O3 -Wall     -c -o io.o io.c
gcc -g -O3 -Wall-o project1 data.o main.o io.o

myhost $ make CFLAGS=-g
gcc -g   -c -o data.o data.c
gcc -g   -c -o main.o main.c
gcc -g   -c -o io.o io.c
gcc -g -o project1 data.o main.o io.o
```

Makefile – rulesets...and more

Special variables/targets:

- the first target in Makefile is the one used when you call make without arguments!
- automatic variables:
  - $< - The name of the first prerequisite.
  - $@ - The file name of the target of the rule.
- for more information:
  - man make
  - info make

Makefile – rulesets...and more

Makefile design – Best practice:

- start with the macros/variables
- call your first target “all:” and make it depend on all targets you want to build
- have a target “clean:” for cleaning up
- avoid explicit rules where possible, i.e. use redundancy

Makefile – rulesets...and more

Makefile design – Best practice (cont'd):

- check your dependencies:
  - by hand
  - most C/C++ compilers can generate Makefile dependencies (see compiler documentation)
    - GCC: `gcc -MM`
    - clang and Intel support this option, too
  - external tool: `makedepend -Y`
  - Note: the option above ignores system headers, like the ones from `/usr/include`

Makefile – rulesets...and more

Common mistakes:

- missing TAB in “command lines”
- wrong variable references:

  $VAR instead of $(VAR)
- missing/wrong dependencies
- remember: each command is carried out in a new sub-shell

Make and Makefiles: Labs

- There are five short lab exercises
- download from DTU Learn
- unzip the file
- the exercises are in the directories lab_N
- read the README files for instructions

Make and Makefiles: Labs

- Hints:
  - M_PI is a definition from <math.h>
  - sin() is a function from libm.so, so you have to link with that library (use -lm the right place)

Version control

- Larger – but also simple – software projects need to keep track of different versions
- This is very useful during development, e.g. to be able to go back to the last working version
- Versioning Tools:

RCS	– single user, standalone
CVS	– multi-user, network based
Subversion	– multi-user, network based
git	– multi-user, network based

Version control

- Some info about Git and GitLab:
  - http://gbar.dtu.dk/faq/41-git
  - http://www.gbar.dtu.dk/faq/94-gitlab

Data analysis tools

- Scientific software usually produces lots of data/datafiles
- There are good tools to do (a quick) analysis:
  - awk – standard UNIX/Linux tool
  - perl – standard on many platforms
- Both tools can be used
  - from the command line
  - with scripts

Data analysis tools – awk

- awk operators:

```
Field reference:                   $
 $0: the whole line - $n: the n-th field
Increment or decrement:            ++ --
Exponentiate:                      ^
Multiply, divide, modulus:         * / %
Add, subtract:                     + -
Concatenation:                    (blank space)
Relational:                       < <= > >= != ==
Match regular expression:         ~ !~
Logical:                          && ||
C-style assignment:            = += -= *= /= %= ^=
```

Data analysis tools – awk

Examples:

- Print first two fields in opposite order:

```
awk '{ print $2, $1 }' file
```

- Print column 3 if column 1 > column 2:

```
awk '$1 > $2 {print $3}' file
```

- Print line (default action) if col. 3 > col. 2:

```
awk '$3 > $2' file
```

Data analysis tools – awk

Examples (cont'd):

- Add up first column, print sum and average:

```
awk '{s += $1}; END { print "sum
is", s," avg is", s/NR}' file
```

- Special keywords/variables:

```
BEGIN   do before the first record
END     do after the last record
NR      number of records
NF      number of fields
$NF     the value of the last field
```

Data analysis tools

- Other useful standard Unix tools for data analysis:
  - sort
  - uniq
  - head, tail
  - wc
  - sed
  - ...
- check the man pages for options, etc

Data analysis tools – perl

- Perl is a very powerful tool, that combines the features of awk, grep, sed, sort, and other Unix-tools into one language
- Good tool for more complex data analysis tasks
- Web-site: http://perl.org/
- Archive of perl programs:
  - Comprehensive Perl Archive Network – CPAN
  - http://www.cpan.org/

Data analysis tools – perl

Perl example script:

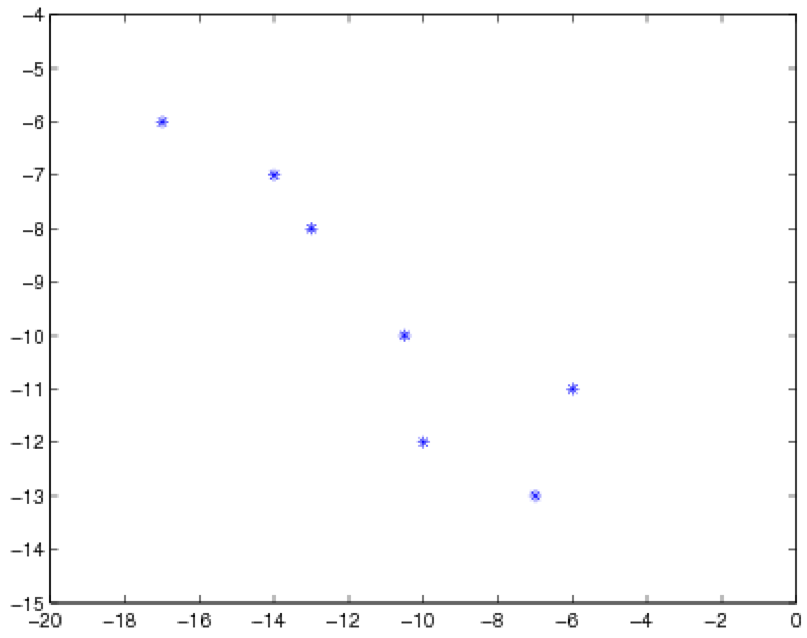
```
#!/usr/bin/perl

while (<>) {

    next if /^#/;          # skip comment lines
    @fields = split();  # split the line

    if ($#fields == 2 ) { # 3(!) elements
        print "$fields[0] $fields[2]\n";
    }
    else {
        print;
    }
}
```

Visualization

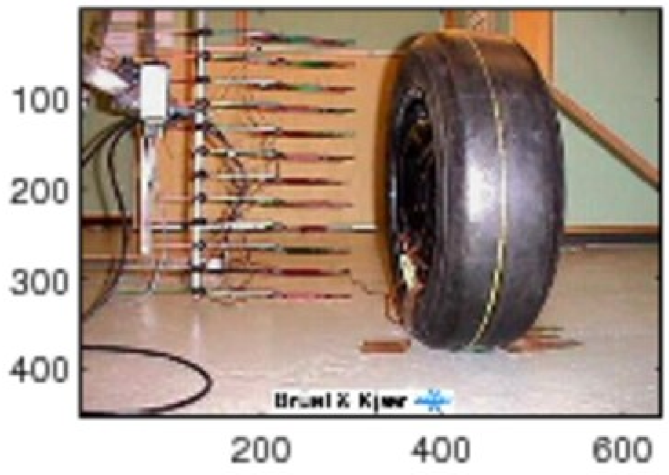
Visualization is an important part of Scientific Computing

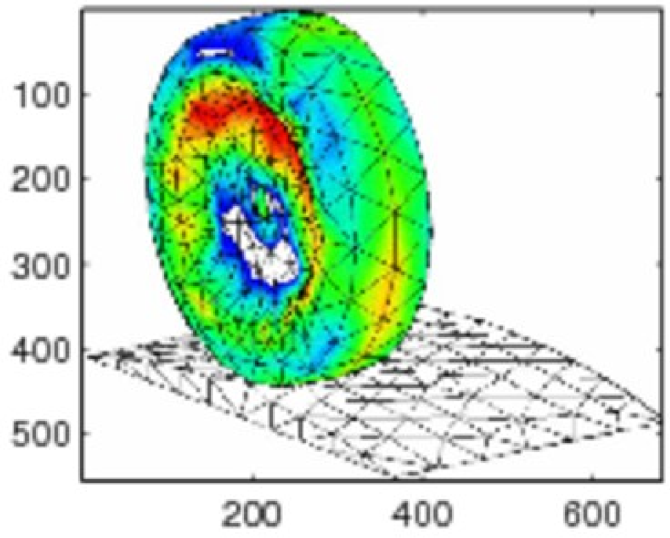
Motivation: What's that?

```
A (  -17,  -6)
B (  -14,  -7)
C (  -13,  -8)
D (-10.5, -10)
E (   -6, -11)
F (   -7, -13)
G (  -10, -12)
```



Visualization





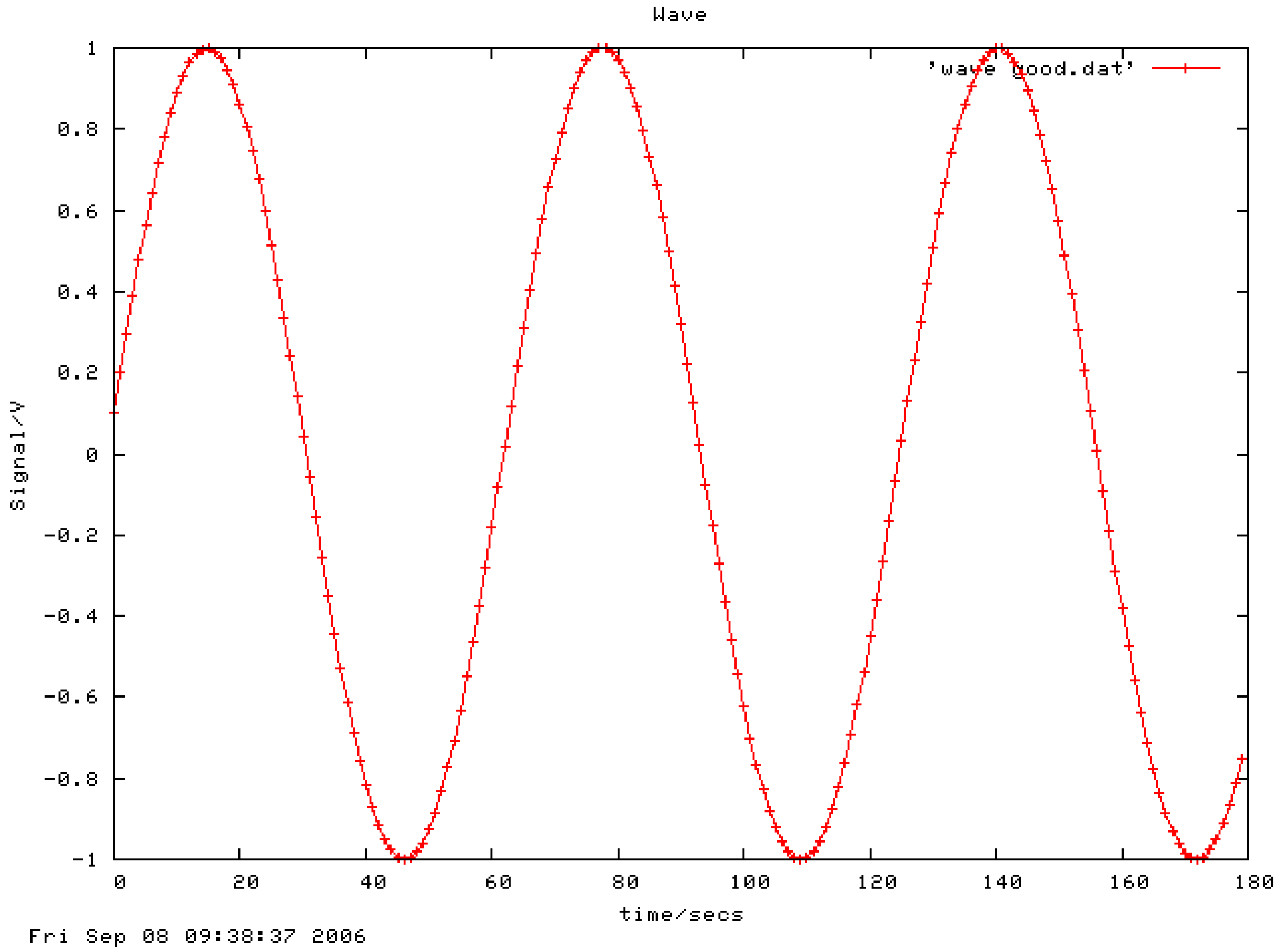
Visualization

- Simple tools to visualize data:
  - Gnuplot (`gnuplot`)
    - command based, flexible
    - good for scripting, batch analysis
    - limited graphics (not always suitable for publishing)
  - Grace (`xmgrace`)
    - GUI-based
    - difficult to do scripting, batch analysis
    - very good graphics (publication-ready)
  - ... or whatever tool you like/prefer

Visualization

Gnuplot example:

```
gnuplot>
gnuplot>
gnuplot>
gnuplot>
gnuplot>
```



Visualization

- Best practice:
  - label the axes
  - use legends (and titles)
  - use the right scaling
    - a plot of a circle should be a circle
  - don't overload figures with information – use more figures instead
  - colors are useful – but can also be confusing

And not to forget ...

... a very powerful tool/language for Scientific Computing:

- Python
  - built-in vector and matrix types (NumPy, SciPy)
  - data plot functionality (matplotlib)
  - interfaces to different languages
  - GPU support (PyOpenCL, PyCUDA)
  - and, and, and ....

Resource Managers

To handle the workload on an HPC installation, one needs a tool to manage and assign the resources: a Resource Manager – sometimes also called 'batch queue system'

- Most common systems:
  - Torque/PBS based (PBSpro, OpenPBS, ...)
  - LSF
  - Grid Engine
  - Slurm

Resource Managers

Before submitting a job, one has to specify the resources needed, e.g.

- # of CPUs/cores
- amount of memory
- expected run time (wall-clock time)
- other resources, like disk space, GPUs, etc

This is done in a special job script and is system (RM) dependent – but similar for all RMs.

Resource Managers

The simplest job script:

```
#!/bin/bash
sleep 60
```

simple.sh

```
$ bsub < simple.sh
Job <702572> is submitted to default queue <hpc>.
$ bstat
JOBID  USER    QUEUE   JOB_NAME SLOTS STAT  START_TIME        ELAPSED
702572 gbarbd  hpc     NONAME       1 RUN   Dec 13 12:17      0:00:00
$ bjobs
JOBID  USER    QUEUE   JOB_NAME SLOTS STAT  START_TIME    TIME_LEFT
702572 gbarbd  hpc     NONAME       1 RUN   Dec 13 12:17 00:15:00 L
$ ls -g
total 4
-rw-r--r-- 1 gbar 1493 Dec 13 12:18 NONAME_702572.out
-rw-r--r-- 1 gbar   22 Dec 13 12:05 simple.sh
```

Resource Managers

The simplest job script – the full story:

```
#!/bin/bash
sleep 60
```

simple.sh

```
$ bsub < simple.sh
bsub info: Job has no name! Setting it to NONAME!
bsub info: Job has no wall-clock time! Setting it to 15 minutes!
bsub info: Job has no output file! Setting it to NONAME_%J.out!
bsub info: Job has no memory requirements! Setting it to 1024 MB!
bsub info:   You need to specify at least -R "rusage[mem=...]"!
Job <702608> is submitted to default queue <hpc>.
```

Resource Managers

A simple job script:

```
#!/bin/bash
#BSUB -J sleeper
#BSUB -o sleeper_%J.out
#BSUB -q hpcintro
#BSUB -W 2
#BSUB -R “rusage[mem=512MB]”

sleep 60
```

```
$ bsub < submit.sh
Job <702645> is submitted to queue <hpcintro>.
```

```
$ ls -g
total 3
-rw-r--r-- 1 gbar  121 Dec 13 12:32 submit.sh
-rw-r--r-- 1 gbar 1592 Dec 13 12:36 sleeper_702646.out
```

Resource Managers

- The output file:

```
Sender: LSF System <lsfadmin@n-62-21-20>
Subject: Job 702646: <sleeper> in cluster <dcc> Done

Job <sleeper> was submitted from host <hpclogin3> by user <gbarbd> in
cluster <dcc> at Wed Dec 13 12:34:59 2017.
Job was executed on host(s) <n-62-21-20>, in queue <hpc>, as user  <g-
barbd> in cluster <dcc> at Wed Dec 13 12:34:59 2017.
</zhome/../././...> was used as the home directory.
</zhome/../././.../02614/Batch/LSF> was used as the working directory.
Started at Wed Dec 13 12:34:59 2017.
Terminated at Wed Dec 13 12:36:00 2017.
Results reported at Wed Dec 13 12:36:00 2017.

Your job looked like:

------------------------------------------------------------

# LSBATCH: User input
#!/bin/bash
#BSUB -J sleeper
#BSUB -o sleeper_%J.out
```

Resource Managers

- The output file (cont'd):
  - job summary

```
Successfully completed.

Resource usage summary:

    CPU time :                                   0.28 sec.
    Max Memory :                                 4 MB
    Average Memory :                             4.00 MB
    Total Requested Memory :                     512.00 MB
    Delta Memory :                               508.00 MB
    Max Swap :                                   -
    Max Processes :                              4
    Max Threads :                                5
    Run time :                                   65 sec.
    Turnaround time :                            61 sec.

The output (if any) is above this job summary.
```

Resource Managers

Separating output and errors:

```
#!/bin/bash
#BSUB -J sleeper
#BSUB -o sleeper_%J.out
#BSUB -e sleeper_%J.err
#BSUB -q hpcintro
#BSUB -W 2 -R "rusage[mem=512MB]"

rm nonexistent.txt
echo "Just a minute ..."
sleep 60
```

```
$ bsub < submit2.sh
...
$ ls -g
total 3
-rw-r--r-- 1 gbar  184 Dec 13 13:56 submit2.sh
-rw-r--r-- 1 gbar   63 Dec 13 13:59 sleeper_702793.err
-rw-r--r-- 1 gbar 1744 Dec 13 14:00 sleeper_702793.out
```

Resource Managers

Separating output, errors – and mail summary:

```
#!/bin/bash
#BSUB -J sleeper
#BSUB -o sleeper_%J.out
#BSUB -e sleeper_%J.err
#BSUB -q hpcintro
#BSUB -W 2 -R "rusage[mem=512MB]"

rm nonexistent.txt
echo "Just a minute ..."
sleep 60
```

```
$ bsub -N < submit2.sh
...
$ ls -g
total 3
-rw-r--r-- 1 gbar  184 Dec 13 13:56 submit2.sh
-rw-r--r-- 1 gbar   63 Dec 13 14:04 sleeper_702814.err
-rw-r--r-- 1 gbar   18 Dec 13 14:04 sleeper_702814.out
```

send summary at end of job

Resource Managers

A simple parallel job script:

- for OpenMP (single node), using 4 cores

```
#!/bin/bash
#BSUB -J openmp_para
#BSUB -o openmp_para_%J.out
#BSUB -q hpcintro
#BSUB -W 2 -R "rusage[mem=512MB]"
#BSUB -n 4 -R "span[hosts=1]"

export OMP_NUM_THREADS=$LSB_DJOB_NUMPROC
...
```

Resource Managers

Another parallel job script:

- for MPI: two nodes, using 4 cores/node

```
#!/bin/bash
#BSUB -J mpi_para
#BSUB -o mpi_para_%J.out
#BSUB -q hpcintro
#BSUB -W 2 -R "rusage[mem=512MB]"
#BSUB -n 8 -R "span[ptile=4]"

module load mpi
mpirun ...
```

Resource Managers

more options and examples:

- see http://www.hpc.dtu.dk/ under
  - LSF User Guides
    - http://www.hpc.dtu.dk/?page_id=2534
- do the lab exercises
- use 'man bsub', 'man bjobs', etc

Resource Managers

DTU Computing Center specific commands:

- bstat – shows the status of your jobs; use ‘bstat -h’ for help for other options
- classstat – shows the status of the queues, e.g. free and used cores, pending jobs, etc
- nodestat – shows the current status of all nodes (use 'nodestat hpc' for the nodes of the 'hpc' queue)
- all commands above have a help (-h) option, but no man-page!

Resource Managers

- There are a few hands-on exercises on DTU Learn, to get you aquainted with the batch system
- more information can be found on www.hpc.dtu.dk under LSF User Guides
- we have a special queue for this course, '`hpcintro`', so please use '`-q hpcintro`' instead of '`-q hpc`' in your job scripts!