Workshop Agenda – Feb 25th 2015

Time	Presenter	Title
09:30	T. König	Talk – bwHPC Concept & bwHPC-C5 - Federated User Support Activities
09:45	R. Walter	Talk – bwHPC architecture (bwUniCluster, bwForCluster JUSTUS, ForHLR Phase I)
10:00	A. Fuchs	Talk – Cluster: Access, Data Transfer and Storage, GUI
10:30		*Break*
10:45	R. Barthel	Talk – File System, Software System (modulefiles), Batch System
11:10	A. Fuchs	Tutorial – bwUniCluster: Access, Data Transfer, Compiling, Modulefiles, Batch Job Scripting
11:50		*Lunch Break*
13:00	R. Barthel	Talk – Advanced Bash Scripting
13:30	R. Barthel	Tutorial – Advanced (Batch) Job Scripting
14:15		*Break*
14:30	A. Fuchs	Tutorial – Compiling, Makefile, Parallelising
15:15		User Forum – Solving User Cases
16:00		*End*

bw|HPC – C5

bwHPC course – Tutorial: Compiling, Makefile, Parallelising

Simon Raffeiner, Annika Fuchs, Robert Barthel

Funding: Baden-Württemberg MINISTERIUM FÜR WISSENSCHAFT, FORSCHUNG UND KUNST

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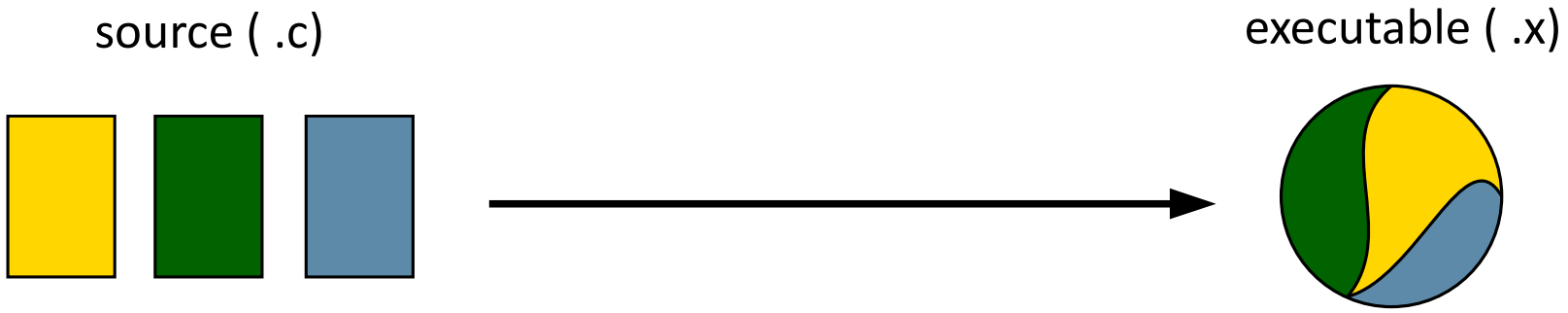
Outline

- Compiler + Numerical Libraries
  - commands
  - linking
- Makefile
  - Intro, Syntax (Explicit + Implicit Rules ...)
  -
- Parallelising
  - OpenMP
  - MPI

1. Compilation

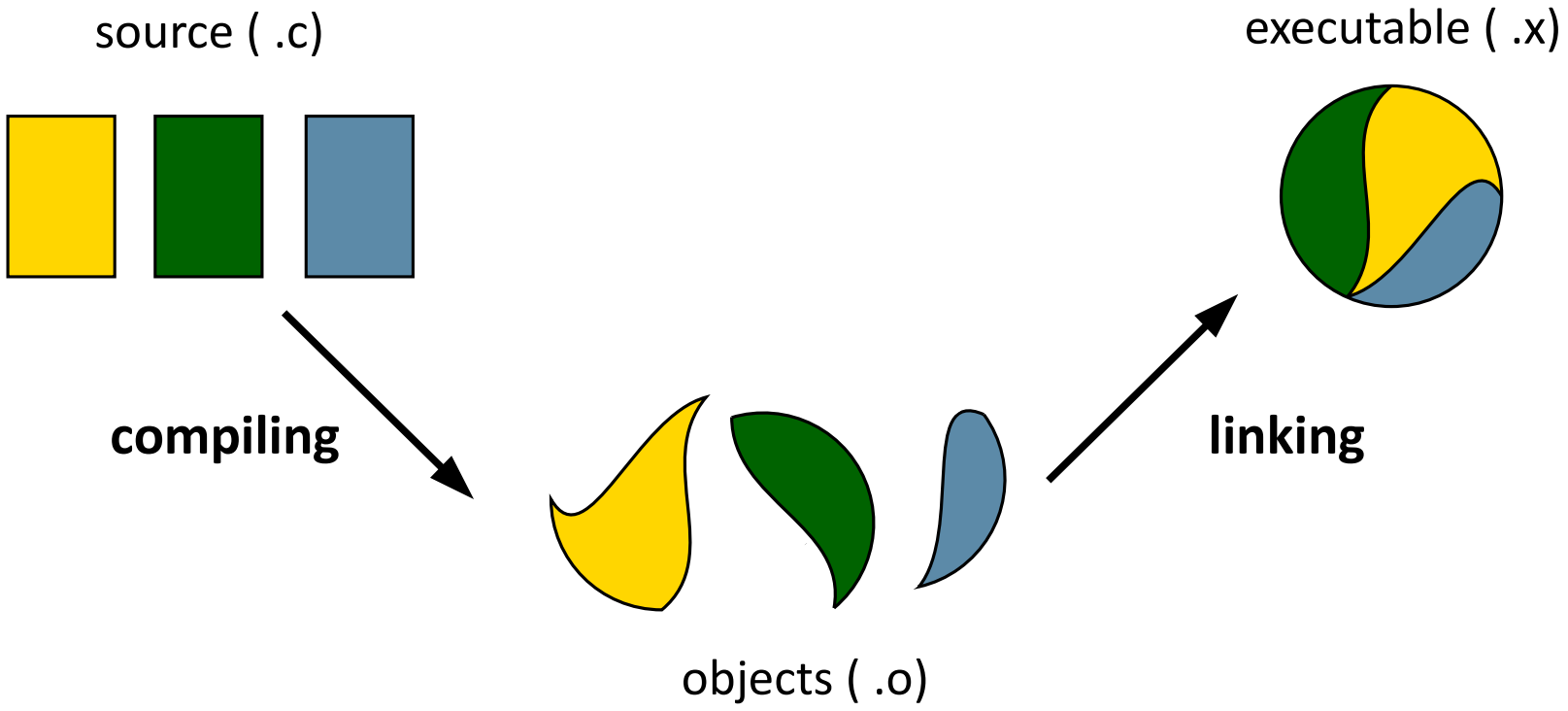
Object files



- Example:

```
$ gcc -o exec.x src1.c src2.c src3.c
$ ./exec.x
```

Object files




```
$ gcc -c src1.c; gcc -c src2.c; gcc -c src3.c
$ gcc -o exec.x src1.o src2.o src3.o
```

- Changes in a single file do not afford the compilation of all source code.

Include files

- Header files (.h)
  - Declaration of variables
  - Definition of static variables
  - Declaration of functions/subroutines
  - ..

- Example: include header file /home/myincs/header.h
  - Preprocessor directive in source code:

```
#include "header.h"
…
```
src1.c

'#' does **not** initiate command lines but preprocessor directives in C/C++ code!

  - Add header directory `-I<include_directory>`

```
$ gcc -I/home/myincs -c src1.c; gcc -c src2.c
$ gcc -o exec.x src1.o src2.o
$ ./exec.x
```

Example: Hello

Main Program

```
#include "hello.h"

int main(void){

  print_hello();

  return 0;
}
```

hello.c

Header (Declarations)

```
#ifndef _HELLO_H_
#define _HELLO_H_

int print_hello(void);

#endif
```

hello.h

Functions (Definitons)

```
#include <stdio.h>

int print_hello(void){

  printf(„hello!\n“);

  return 0;
}
```

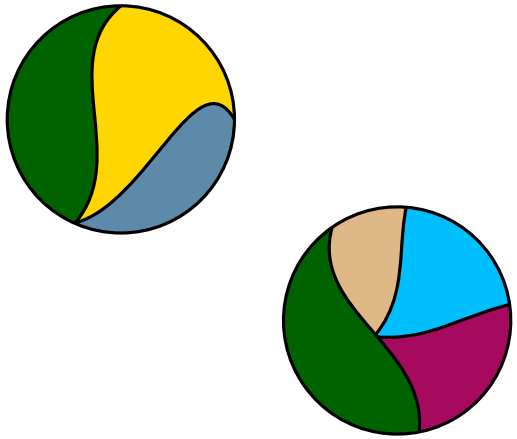
hello_fct.c

- Exercise: *hello*
  - Build objects hello.o hello_fct.o
  - Build executable by linking objects
  - `$ ./hello`

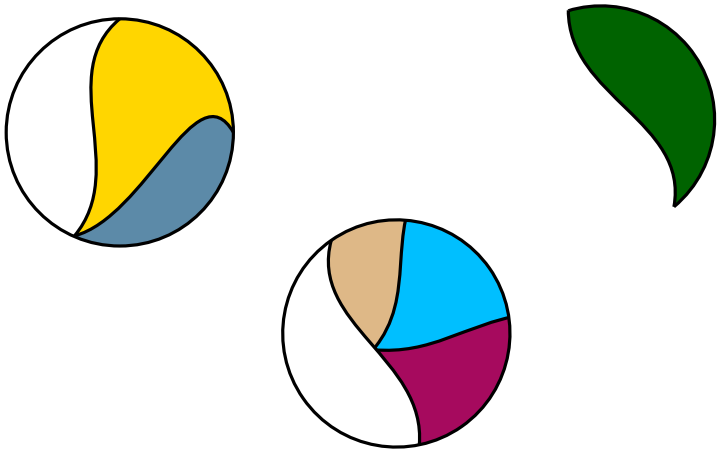
Shared object files and Libraries

- Objects can be used by different executables.
- A **library** contains program parts (subroutines, classes, type definitions, …) that can be used by different executables.

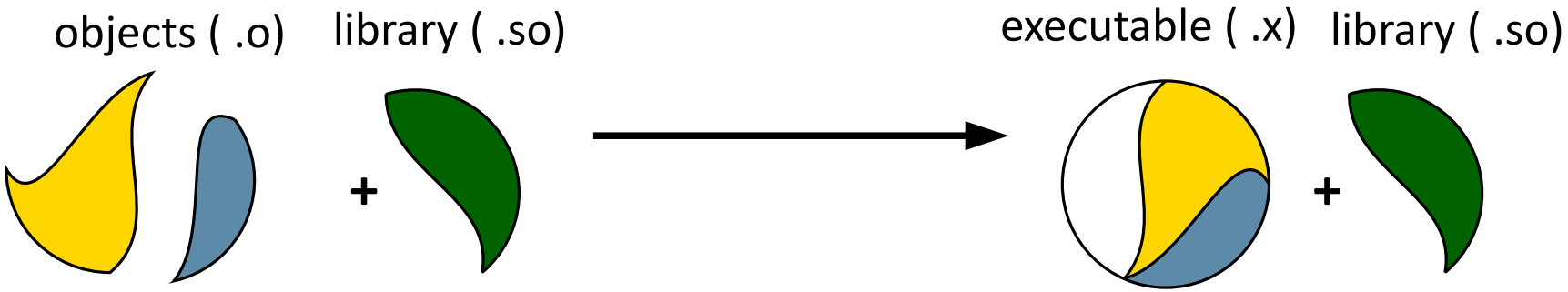
- Static library
  - Linked during building executable



- Shared library
  - Loaded during runtime



Shared Object files and Libraries



- Example: link library */home/mylibs/libexample.so*
  - Build executable:
    - Add library directory `-L<library_directory>`
    - load library `-l<library_name>` **after** refering source/object files

```
$ gcc -o exec.x src1.o src2.o -L/home/mylibs -lexample
```

  - Run executable:
    - Add `<library_directory>` to list of library directories `${LD_LIBRARY_PATH}`

```
$ export LD_LIBRARY_PATH=${LD_LIBRARY_PATH}:/home/mylibs
$ ./exec.x
```

Module files

- Module files set/prepare following environment variables amongst others:
  - `*_LIB_DIR = <library_directory>`
  - `*_INC_DIR = <include_directory>`
  - `${LD_LIBRARY_PATH}`

- Show module file setup with `$ module show <module_file>`

- Example: link NETCDF library
  - Build executable:

```
$ module load compiler/intel
$ module load lib/netcdf
$ icc -I${NETCDF_INC_DIR} -c src1.c; gcc -c src2.c
$ icc -o exec.x src1.o src2.o -L${NETCDF_LIB_DIR} -lnetcdf
```

  - Run executable:

```
$ module load lib/netcdf
$ ./exec.x
```

2. Makefile

Motivation

- Interactively
  - `$ gcc -o hello -I. hello.c hello_fct.c`
  - Works as long as command history is active
- Shell script
  - `$ ./compile.sh`
  - Does always recompile the whole code
- Makefile
  - `$ make`
  - better organisation of code compilation
  - recompiles only updated files,

```
make: `hello' is up to date.
```

Makefile

- `$ make [<target>]`
  - executes script named *Makefile* or *makefile*
  - without argument first rule in *Makefile* is executed

- Rule definition (format):

```
target: prerequisites
<TAB>command
```

Rule has to be applied, if any of these files is changed

To apply the rule, command has to be executed.

Only works with beginning tab stop!

```
hello: hello.h hello.c hello_fct.c
	gcc -o hello -I. hello.c hello_fct.c
```

Makefile.1

- Exercise: *Makefile.1*
  - define a second rule named `clean` to remove the executable

Rules - Content

- Explicit rules
  - `hello.o:` rule to build target *hello.o*
- Wildcards
  - `hello: *.c` *hello* depends on all files with suffix *.c* in this directory
- Pattern rules
  - `%.o:` rule for all files with suffix *.o*
  - `%.o: %.c` `%` in prerequisites substitutes the same as `%` in the target
- Phony Targets
  - `.PHONY: clean` target *`clean`* is nothing to build

```
clean:
```

Variables

- Variable assignment
  - `=` recursively expanded (referenced by reference)
  - `:=` simply expanded (referenced by value)
  - `?=` only if variable is not defined yet (no overwrite)
  - `+=` add item to variable array

```
CC      ?= gcc
CFLAGS  = -I.
INC     := hello.h
OBJ     := hello.o
OBJ     += hello_fct.o
EXE     := hello

${EXE}: ${INC} ${OBJ}
        ${CC} -o ${EXE} ${CFLAGS} ${OBJ}

.PHONY: clean
clean:
        rm -f ${OBJ} ${EXE}
```

Makefile.2

- Exercise: *Makefile.2*
  - „*hello.o* depends on *hello.h*“
  - write an appropriate rule

Automatic Variables

- Automatic variables change from rule to rule

  `$@` = target

  `$<` = first item of prerequisites

  `$^` = all items of prerequisites separated by ' '

- Exercise: *Makefile.3*
  - Use automatic variables in rule to build *hello*

```
CC      ?= gcc
CFLAGS  = -I.
INC     := hello.h
OBJ     := hello.o
OBJ     += hello_fct.o
EXE     := hello

%.o: %.c ${INC}
        ${CC} -o $@ ${CFLAGS} -c $<

hello: hello.o hello_fct.o
        ${CC} -o ${EXE} ${CFLAGS} ${OBJ}

.PHONY: clean
clean:
        rm -f ${OBJ} ${EXE}
```

Makefile.3

Directives

- Conditions can be expressed by directives
  - if VAR is (not) defined

```
ifdef/ifndef VAR
  ..
else
  ..
endif
```

  - if A and B are (not) equal

```
ifeq/ifneq (A,B)
  ..
else
  ..
endif
```

- Example:
  - Conditional assignment `CC ?= gcc` is equivalent to

```
ifndef CC
  CC = gcc
endif
```

Include

- Parts of *Makefile* can be outsourced
  - e.g. platform specific statements
- External makefile code, e.g. file *make.inc*, can be loaded in *Makefile* via

```
include make.inc
```

- Exercise: *hello_omp*
  - *make.inc.gnu* and *make.inc.intel* contain compiler specific makefile statements
  - Adjust *Makefile.4*: include *make.inc* depending on `${CC}`
  - **`$ module load compiler/gnu`**
    `$ make`
  - **`$ module load compiler/intel`**
    `$ make`

```
CC      = gcc
CFLAGS = -I. -fopenmp
```

make.inc.gnu

```
CC      = icc
CFLAGS = -I. -openmp
```

make.inc.intel

```
include make.inc

hello_omp:hello_omp.o
        ${CC} -o $@ ${CFLAGS} $<
```

Makefile.4

3. Parallelisation

Overview

- OpenMP is an **easy**, **portable** and **incremental** specification for node-level parallelisation
- Thread-based, shared memory, single-node (in contrast to MPI)

- How does it work?
  - Annotate the C/C++/FORTRAN source code with pragmas
  - The compiler transparently generates the necessary code
  - Non-parallel blocks are only executed by the main thread
  - Parallel blocks are handed to a team-of-threads and executed in parallel

- If the compiler has no support for OpenMP, or if you do not activate OpenMP, the pragmas will be ignored, the code will only run on a single core and still yield the correct result

Core syntax

- Most OpenMP pragmas apply to a „structured block“ or „parallel region“
  - A single instruction, or
  - A number of statements with a single entry point at the top and a single exit at the bottom

```
#pragma omp parallel
{
    // statements
}
```

```
!$omp parallel
    // statements
!$omp end parallel
```

- Only statements inside a block marked with the „parallel“ clause will be executed in parallel
- It is allowed to abort the execution of the whole application within a structured block

Library functions

- Many of these will only work correctly inside of a parallel region!

- Get the number of threads in the current team: `omp_get_num_threads()`
- Get the ID of the current thread: `omp_get_thread_num()`
- Get the number of processors available: `omp_get_num_procs()`

- Get the elapsed wall clock time: `omp_get_wtime()`

Compiling

- GCC

```
gcc -fopenmp -o openmp openmp.c
```

- Intel

```
icc -openmp -o openmp openmp.c


# Get information about which loops were parallelized and which not
icc -openmp -openmp-report 2 -o openmp openmp.c


# Get hints about weaknesses in the code regarding parallelisation
icc -openmp -diag-enable sc-parallel3 -o openmp openmp.c
```

Hello World example

```c
#include <stdio.h>
#include <stdlib.h>

#include <omp.h>


int main(int argc, char** argv)
{
    #pragma omp parallel
    {
        printf("Thread %i\n", omp_get_thread_num());
    }

    printf("All done!\n");

    return EXIT_SUCCESS;
}
```

Output:

```
Thread 0
Thread 3
Thread 2
Thread 1
All done!
```

Loops and reduction

```
#include <stdlib.h>
#include <stdio.h>
#include <omp.h>

static int VECTOR_LENGTH = 5;

int main (int argc, char * argv[])
{
    int i;
    double * v;
    double norm2 = 0.0, t1, tdiff;

    v = malloc (VECTOR_LENGTH * sizeof(double));

    t1 = omp_get_wtime();

    #pragma omp parallel for
    for (i=0; i < len; i++)
        v[i] = i;

    #pragma omp parallel for reduction(+:norm2)
    for(i=0; i < len; i++)
        norm2 += (v[i]*v[i]);

    tdiff = omp_get_wtime() - t1;

    printf ("norm2: %f Time:%f\n", norm2, tdiff);
    return 0;
}
```

Variable scopes

- A shared variable points to the same memory location for all threads
- A private variable points to an unique memory location for every thread

- Global variables are automatically shared
- Variables declared inside a parallel region are automatically private
- The control variable of a **do / for** construct is automatically private

- Variable handling can be controlled using the **private**, **shared**, **firstprivate** and **lastprivate** directives

Sections

```
#include <stdio.h>
#include <stdlib.h>

#include <omp.h>


int main(int argc, char** argv)
{
    #pragma omp sections
    {
        #pragma omp section
        {
            printf ("id = %d\n", omp_get_thread_num());
        }

        #pragma omp section
        {
            printf ("id = %d\n", omp_get_thread_num());
        }
    }

    return EXIT_SUCCESS;
}
```

Output 1:

```
id = 0
id = 0
```

Output 2:

```
id = 1
id = 0
```

Additional OpenMP clauses

- **critical:** Only one thread at a time executes the following region
- **atomic:** Only one thread at a time can update the following memory location
- **barrier:** The thread will wait until all other threads have reached the barrier
- **ordered:** Threads will execute the following region in serial order

- **single:** Only one of the threads executes the following region
- **master:** Only thread 0 executes the following region