

Compiling environment

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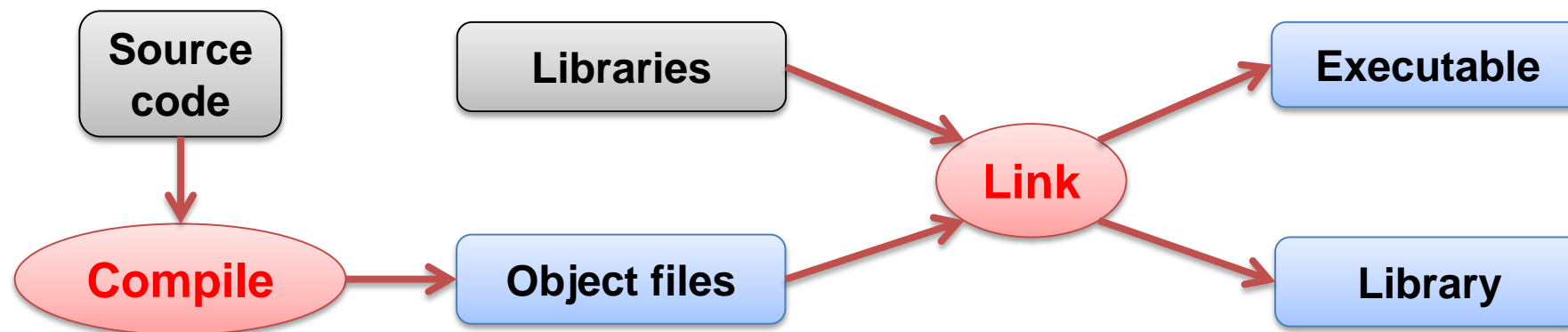
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Outline

- Introduction
- Fortran Compiler
- Linking
- Libraries
- Make
- Debugging
- Profiling
- Practical session

Introduction

- Compiling
 - Objects
- Linking
 - Libraries
 - static libraries
 - shared libraries



Introduction

- Why compiling at ECMWF?
 - decoding of (MARS) data
 - model runs
- Alternatives to compilation?
 - Grib_api tools, grib_api python interface
 - Netcdf format generated from MARS
 - Wgrib, cdo, ...
- Which platforms are available?
 - Linux server (ecgate)
 - Supercomputers (Cray: cca)

Introduction

- Which compilers?
 - Fortran (77/90/95/2003)
 - C/C++
- Which platform to use?
 - High Performance Computing Facility (cca) for computing intensive work, including parallel work.
 - Linux server (ecgate) for decoding or I/O bound work.

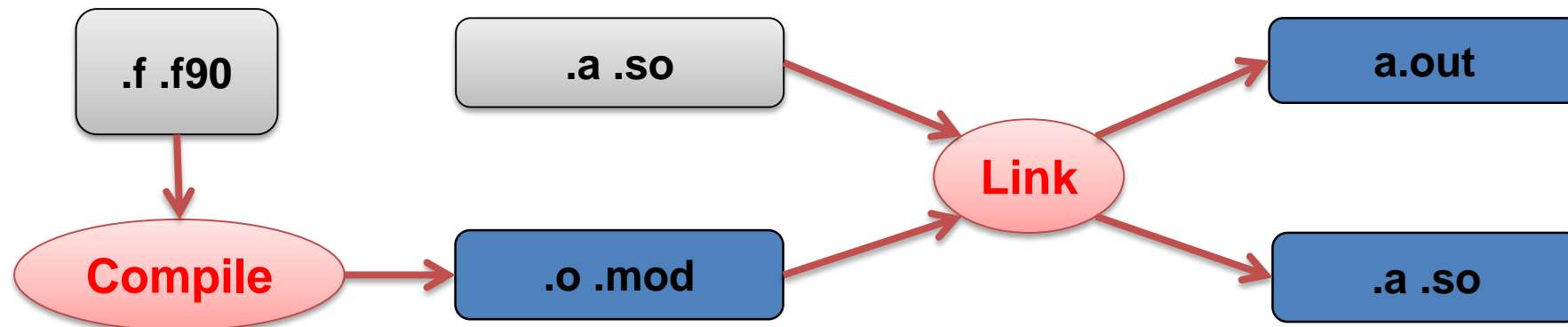
Compilers

- GNU compilers:
 - gfortran
 - gcc
 - g++
- Which version do I use?

```
$ gcc --version
gcc (GCC) 4.4.7 20120313 (Red Hat 4.4.7-3)
...
$ gfortran --version
GNU Fortran (GCC) 4.4.7 20120313 (Red Hat 4.4.7-3)
...
```

Compilers

- Common file suffixes and files
 - .f, .F, .f90, .F90 : source code
 - .o : object file
 - .a : archive file (library)
 - .so: share object (library)
 - .mod: fortran 90 module files
 - a.out: default name of executable



Fortran Compiler common options

- Fortran 77 / f90
 - -c compilation only, no linking
 - -fdefault-real-8 64bit real variables
 - -O[1-3] optimisation
 - -g debugging
 - -v verbose
 - --help display usage
- Many more options. See man page.

Compilation – return codes

- Return code
 - Successful compilation: 0
 - Failure: ($\neq 0$) 1, ...
 - gfortran messages:

```
grdemo.f90:2.12:  
use grib_api  
          1  
Fatal Error: Can't open module file 'grib_api.mod'  
for reading at (1): No such file or directory
```

Error severity

position

Error message

Word lengths – precision

- 32bit real and integer variables by default.
- The option `-fdefault-real-8` promotes real variables to 64bit entities.
- When using a library, check its precision, e.g. for EMOSLIB, MAGIC5. The GRIB_API is independent of the precision for floating points.

Fortran I/O

- GRIB and BUFR formats are pure binary formats, accessible with PBIO routines from EMOSLIB or with the GRIB API for GRIB (Edition 1 and 2).
- IEEE format - big-endian on IBM systems (old supercomputer) , little endian on Linux systems (ecgate and Cray supercomputer)
 - real*4: 6 significant digits
 - real*8: 15 significant digits
 - Use '-fconvert=big-endian' to read/write big-endian files.

Linking

- Use gfortran to link, e.g.

```
$ gfortran -o prog prog.f $EMOSLIB  
# equivalent to:  
$ gfortran -o prog prog.f -L/usr/local/apps/libemos/000437/lib -lemos.R32.D64.I32
```

- Use "ar" to build static libraries, eg.

```
$ gfortran -c *.f  
$ ar -vr libmy.a *.o
```

- Use gfortran -shared to build shared libraries, eg.

```
$ gfortran -c -fPIC *.f  
$ gfortran -shared -fPIC -o libmy.so *.o
```

Libraries

- ECMWF libraries
 - Graphics software library – MAGICS: `$MAGPLUSLIB_SHARED`(Magics++)
 - Meteorological Software - EMOS library - `$EMOSLIB`
 - Grib_api, for GRIB1 and GRIB2 format - `$GRIB_API_LIB`, `$GRIB_API_INCLUDE`
 - Locally produced software library - EC Library - `$ECLIB`
- Manufacturer/Public Domain Libraries
 - `BLAS/LAPACK` – public domain software
 - `HDF/NetCDF` available.

Libraries (cont)

- Many of our locally produced libraries have both 32-bit and 64-bit floating point versions (REAL numbers) - different libraries.
- Do NOT make the confusion between the precision (32/64 bit **REALS**) and the **ADDRESSING** mode (32/64 bit) of a library:
 - You will get **WRONG** results when mixing libraries of different precision.
 - You will not be able to link your program if you mix libraries of different addressing mode.

Make

- Easy to use utility to build a program or library.
- Suitable for different languages.
- **Makefile**: file containing rules on how to compile code and build library or executable.
- The 'make' command will read the Makefile and will figure out which code files (or libraries or executables) need to be rebuilt.
- make allows for compilations in parallel (make -j).

Makefiles

- Contain rules that will be applied in cascade:
- The command(s) to run for each rule must be preceded by a tab

No spaces!!!

- Syntax:

```
target1: source1
    command_to_run target1 source1
```

- Example:

```
hello: hello.f
    $(FC) -o $@ -ffixed-form $(FFLAGS) $<
```


Debugging

- checking:
 - array bounds checking: `-fbounds-check`

```
$ gfortran -fbound-check prog.f -o prog  
$ ./prog
```

- undefined reference checking

```
$ gfortran -finit-real=inf prog.f -o prog
```

checkings done at runtime!

- generating debug output:
 - Backtrace: `-fbacktrace`
 - Core file: `-fdump-core`

Debugging – floating point exceptions

- Nothing generated on floating point exception.
- Floating point trapping

```
$ gfortran -ffpe-trap=overflow,invalid,zero [-g] [-O0] prog.f -o prog  
$ ./prog
```

- interactive window based debugger: - totalview

```
$ module load totalview  
$ totalview ./prog
```

- Core files – how to get a backtrace

```
$ gdb -c core ./prog  
> where
```

Profiling - tuning

- time - command timer

```
$ time a.out
```

- -O and other options at compilation for faster execution. Try to use -O3
- other applications, like gprof

```
$ gfortran -O0 -g -pg -o prog prog.f  
$ ./prog  
$ gprof prog gmon.out
```

References

- **GNU manuals (fortran, C, ...):**
<http://gcc.gnu.org/onlinedocs/>
- **User Documentation:**
<https://software.ecmwf.int/wiki/display/UDOC/User+Documentation>
- **Job examples:**
<https://software.ecmwf.int/wiki/display/UDOC/Slurm+job+script+examples>