HPC tools for programming

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Justification

High Performance Computing requires, beyond simple use of a programming language, a number programming tools. These tutorials will introduce you to some of the more important ones.

Intro to file types

File types

Text files	
Source	Program text that you write
Header	also written by you, but not really program text.
Binary files	
Object file	The compiled result of a single source file
Library	Multiple object files bundled together
Executable	Binary file that can be invoked as a command
Data files	Written and read by a program

Text files

- Source files and headers
- You write them: *make sure you master an editor*
- The computer has no idea what these mean.
- They get compiled into programs.

(Also 'just text' files: READMEs and such)

Binary files

- Programs. (Also: object and library files.)
- Produced by a compiler.
- Unreadable by you; executable by the computer.

Also binary data files; usually specific to a program.
(Why don't programs write out their data in readable form?)

Compilation

Compilers

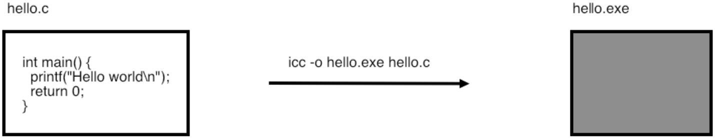
Compilers: a major CS success story.

- The first Fortran compiler (Backus, IBM, 1954): multiple man-years.
- These days: semester project for graduate students. Many tools available (`lex`, `yacc`, `clang-tidy`) Standard textbooks ('Dragon book')
- Compilers are very clever! You can be a little more clever in assembly – maybe but compiled languages are 10$\times$ more productive.

Compilation vs interpreted

- Interpreted languages: lines of code are compiled 'just-in-time'. Very flexible, sometimes very slow.
- Compiled languages: code is compiled to machine language: less flexible, very fast execution.
- Virtual machine: languages get compiled to an intermediate language
  (Pascal, Python, Java)
  pro: portable; con: does not play nice with other languages.
- Scientific computing languages:
  - Fortran: pretty elegant, great at array manipulation
    Note: Fortran20003 is modern; F77 and F90 are not so great.
  - C: low level, allows great control, tricky to use
  - C++: allows much control, more protection, more tools
    (kinda sucks at arrays)

Simple compilation



- From source straight to program.
- Use this only for short programs.

```
%% gcc hello.c
%% ./a.out
hello world
```

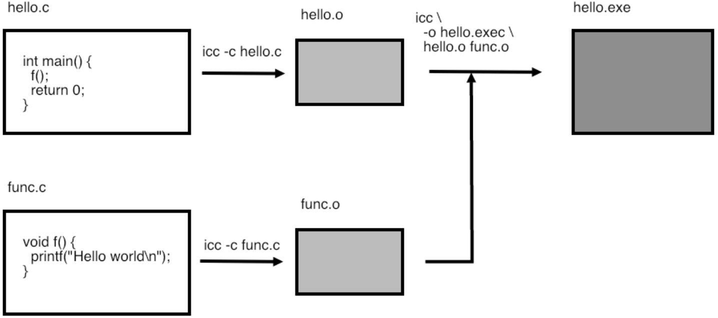
```
%% gcc -o helloprog hello.c
%% ./helloprog
hello world
```

Exercise 1

```
/****************************************************************
 ****
 **** This program source is part of
 **** Introduction to High-performance Scientific Computing
 **** by Victor Eijkhout
 **** copyright Victor Eijkhout 2011-2020
 ****
 **** hello.c : simple hello world program
 ****
 ****************************************************************
#include <stdlib.h>
#include <stdio.h>

int main() {
  printf("hello world\n");
  return 0;
}
```

Separate compilation



- Large programs best broken into small files,
- … and compiled separately (can you guess why?)
- Then 'linked' into a program; linker is usually the same as the compiler.

Exercise 2

Main program: fooprog.c

```
/*
   ****************************************************************
 ****
 **** This program source is
   part of
 **** Introduction to High-
   performance Scientific
   Computing
 **** by Victor Eijkhout
 **** copyright Victor
   Eijkhout 2011-2020
 ****
 **** fooprog.c : simple main
   program using external
   function
 ****

   ****************************************************************
   */
#include <stdlib.h>
```

Subprogram: foosub.c

```
/*
   ********************************
 ****
 **** This program source is
   part of
 **** Introduction to High-
   performance Scientific
   Computing
 **** by Victor Eijkhout
 **** copyright Victor
   Eijkhout 2011-2020
 ****
 **** foosub.c : declaration
   of function for fooprog.c
 ****

   ********************************
   */
#include <stdlib.h>
```

Compiler options 101

- You have just seen two compiler options.
- Commandlines look like

  ```
  command [ options ] [ argument ]
  ```

  where square brackets mean: 'optional'
- Some options have an argument

  ```
  icc -o myprogram mysource.c
  ```

- Some options do not.

  ```
  icc -g -o myprogram mysource.c
  ```

- Question: does `-c` have an argument? How can you find out?

  ```
  icc -g -c mysource.c
  ```

Object files

- Object files are unreable. (Try it. How do you normally view files? Which tool sort of works?)
- But you can get some information about them.

```
#include <stdlib.h>
#include <stdio.h>
void bar(char *s) {
  printf("%s",s);
}
```

```
[c:264] nm foosub.o
0000000000000000 T _bar
U _printf
```

Where `T`: stuff defined in this file
`U`: stuff used in this file

Compiler options 102

- Optimization level: `-O0`, `-O1`, `-O2`, `-O3`
  ('I compiled my program with oh-two')
  Higher levels usually give faster code. Level 3 can be unsafe. (Why?)
-
- `-g` is needed to run your code in a debugger. Always include this.
- The ultimate source is the 'man page' for your compiler.

Example of optimization

Givens program

```
// rotate.c
void rotate(double *x,double *y,double alpha) {
  double x0 = *x, y0 = *y;
  *x = cos(alpha) * x0 - sin(alpha) * y0;
  *y = sin(alpha) * x0 + cos(alpha) * y0;
  return;
}
```

Run with optimization level 0,1,2,3 we get:

```
Done after 8.649492e-02
Done after 2.650118e-02
Done after 5.869865e-04
Done after 6.787777e-04
```

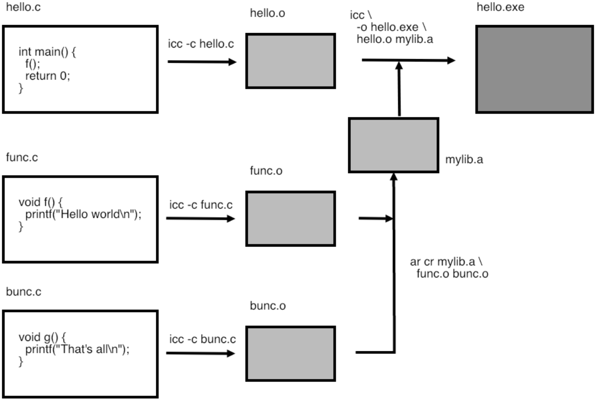
Exercise 3

The file `rotate.c` can be speeded up by compiler transformations.
Compile this file with optimization levels `0,1,2,3`
(try both the Intel and gcc compilers)
observe run time and conjecture what transformations can explain this.

Write a report of your investigations.

Libraries

Libraries



- Sometimes you have many object files: convenient to bundle them
- Easier to link to
- Easy to distribute as a product.
- Software library: collection of object files that can be linked to a main program.

Static / non-shared libraries

- Static libraries are created with `ar`
- Inspect them with `nm`
- Link as object file:

  ```
  icc -o myprogram main.o ../lib/libfoo.a
  ```
- Or:

  ```
  icc -o myprogram main.o -L../lib -lfoo.a
  ```

```
mkdir ../lib
ar cr ../lib/libfoo.a foosub.o
```

```
%% nm ../lib/libfoo.a

../lib/libfoo.a(foosub.o):
00000000 T _bar
         U _printf
```

Static library example

Use `ar` to add object files to `.a` file.

```
icc -g -O2 -std=c99 -c foosub.c
for o in foosub.o ; do \
  ar cr libs/libfoo.a ${o} ; \
done
icc  -o staticprogram fooprog.o -Llibs -lfoo
-rwx------ 1 eijkhout G-25072 38192 Sep 23 18:15 staticprogram
./staticprogram
hello world
```

Dynamic/shared libraries

Created with the compiler,
`-shared` flag.

```
icc -O2 -std=c99 -fPIC -c foosub.c
icc -o libs/libfoo.so -shared foosub.o
icc -o dynamicprogram fooprog.o -Llibs -lfoo
```

Executable size

Static libraries are baked into the executable
shared libraries are linked at runtime.

```
# Making static library
icc  -o staticprogram fooprog.o -Llibs -lfoo
-rwx------ 1 eijkhout G-25072 28232 Sep 23 14:25 staticprogram
# Using dynamic library
icc -o dynamicprogram fooprog.o -Llibs -lfoo
-rwx------ 1 eijkhout G-25072 28160 Sep 23 14:25 dynamicprogram
```

Needs something more

Program can not immediately be run.
Use `ldd` to see what libraries it needs:

```
./dynamicprogram: error while loading shared libraries:
      libfoo.so: cannot open shared object file: No such file or director

ldd dynamicprogram | grep libfoo
        libfoo.so => not found
```

The ell-dee library path

Libraries are found by updating the `LD_LIBRARY_PATH`:

```
export LD_LIBRARY_PATH=${LD_LIBRARY_PATH}:./libs
ldd dynamicprogram | grep libfoo
        libfoo.so => ./libs/libfoo.so (0x00002ad6604c1000)
./libs dynamicprogram
hello world
```

The rpath

You can also bake the path into the program:

```
icc -O2 -std=c99 -fPIC -c foosub.c
icc -o libs/libfoo.so -shared foosub.o
icc -o rpathprogram fooprog.o \
    -Wl,-rpath=./libs -Llibs -lfoo
-rwx------ 1 eijkhout G-25072 28160 Sep 23 13:41 rpathprogram
./rpathprogram
hello world
```

(Notice the bizarre combination of minuses and commas)

Cross-language linking

-

Profiling and debugging; optimization and programming strategies.

Analysis basics

- Measurements: repeated and controlled
  beware of transients, do you know where your data is?
- Document everything
- Script everything

Compiler options

- Defaults are a starting point
- use reporting options: `-opt-report`, `-vec-report`
  useful to check if optimization happened / could not happen
- test numerical correctness before/after optimization change
  (there are options for numerical corretness)

Optimization basics

- Use libraries when possible: don't reinvent the wheel
- Premature optimization is the root of all evil (Knuth)

Code design for performance

- Keep inner loops simple: no conditionals, function calls, casts
- Avoid small functions: try macros or inlining
- Keep in mind all the cache,TLB, SIMD stuff from before
- SIMD: Fortran array syntax helps

Multicore / multithread

- Use `numactl`: prevent process migration
- 'first touch' policy: allocate data where it will be used
- Scaling behaviour mostly influenced by bandwidth

Multinode performance

- Influenced by load balancing
- Use HPCtoolkit, Scalasca, TAU for plotting
- Explore ‘eager’ limit (mvapich2: environment variables)

Classes of programming errors

Logic errors:
functions behave differently from how you thought,
or interact in ways you didn't envision

Hard to debug

Coding errors:
send without receive
forget to allocate buffer

Debuggers can help

Defensive programming

Defensive programming

- Keep It Simple (‘restrict expressivity’)
- Example: use collective instead of spelling it out
- easier to write / harder to get wrong
  the library and runtime are likely to be better at optimizing than you

Memory management

Beware of memory leaks:
keep allocation and free in same lexical scope

Modular design

Design for debuggability, also easier to optimize

Separation of concerns: try to keep code aspects separate

Premature optimization is the root of all evil (Knuth)

MPI performance design

Be aware of latencies: bundle messages
(this may go again separation of concerns)

Consider ‘eager limit’

Process placement, reduction in number of processes

Debugging

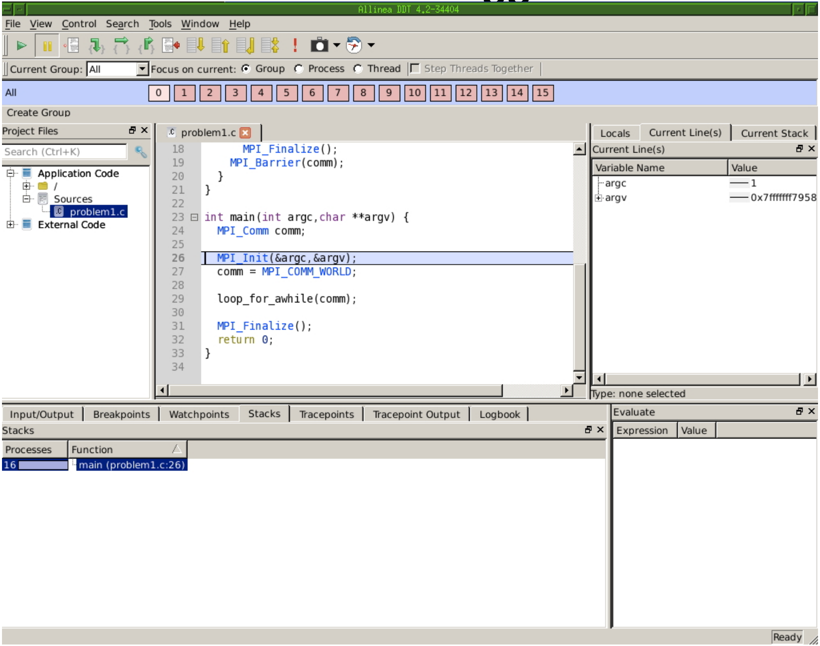
Debugging

I assume you know about gdb and valgrind…

- Interactive use of gdb, starting up multiple xterms
  feasible on small scale
- Use gdb to inspect dump:
  can be useful, often a program crashes hard and leaves no dump

Note: compile options `-g -O0`

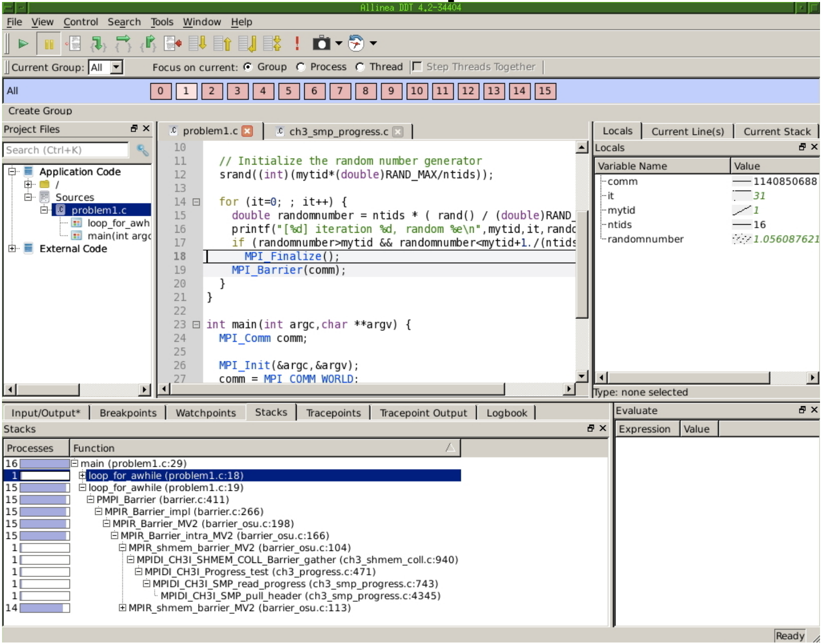
Parallel debuggers



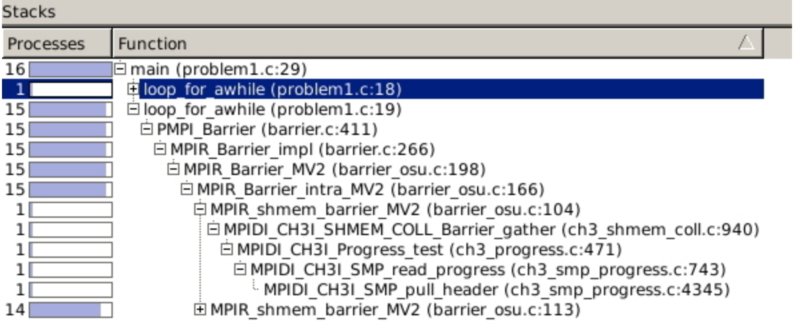
Buggy code

```
for (it=0; ; it++) {
  double randomnumber = ntids * ( rand() / (double)RAND_MAX
  printf("[%d] iteration %d, random %e\n",mytid,it,randomnum
  if (randomnumber>mytid && randomnumber<mytid+1./(ntids+1))
    MPI_Finalize();
  MPI_Barrier(comm);
}
```

Parallel inspection



Stack trace


Stacks
Processes
Function
16 main (problem1.c:29)
1 loop_for_awhile (problem1.c:18)
15 loop_for_awhile (problem1.c:19)
15 PMPI_Barrier (barrier.c:411)
15 MPIR_Barrier_impl (barrier.c:266)
15 MPIR_Barrier_MV2 (barrier_osu.c:198)
15 MPIR_Barrier_intra_MV2 (barrier_osu.c:166)
1 MPIR_shmem_barrier_MV2 (barrier_osu.c:104)
1 MPIDI_CH3I_SHMEM_COLL_Barrier_gather (ch3_shmem_coll.c:940)
1 MPIDI_CH3I_Progress_test (ch3_progress.c:471)
1 MPIDI_CH3I_SMP_read_progress (ch3_smp_progress.c:743)
1 MPIDI_CH3I_SMP_pull_header (ch3_smp_progress.c:4345)
14 MPIR_shmem_barrier_MV2 (barrier_osu.c:113)

Variable inspection