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Ohio Supercomputer Center Using Glenn, the IBM Opteron 1350 Compilers

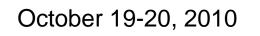


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Compilers available on Glenn/BALE Introduction to compiling using GNU MPI compiler wrappers Libraries Debuggers Material in this class can also be found at <u>http://www.osc.edu/supercomputing/software/apps/pgi.shtml</u> <u>http://www.osc.edu/supercomputing/software/apps/intel_compile.shtml</u>



Retrieve Workshop Problems

Retrieve examples/exercises:

>> svn checkout http://svn.osc.edu/repos/softdevtools/trunk/Compiling

More on SVN tomorrow. You may follow along with the Examples during the lecture. Time will be provided to complete the exercises later.

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Compilers at OSC Myriad of compilers in use **On OSC HPC machines** □gcc, g++ - the Gnu C compiler ifort, icc - Intel compilers mpicc, mpif90 - compiling MPI programs Use gcc to illustrate compiling concepts Compilers do the same thing Some arguments differ in syntax ---O3 (gcc) □-fast (ifort) Good compiling practices enhance software development Main interests Programs that run And run fast Forego the usual software engineering arguments Good and bad practices



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GNU Compilers

Compiler suite from the Free Software Foundation Freely available open source compiler system C (gcc) C++ (g++) Fortran 77/90 (g77/gfortran) Installed in /usr/bin and are on all users' \$PATH Quite good compilers in terms of standards conformance Primarily used in Makefiles for open source software builds Do not generate as fast code as other compilers – not recommended for high performance scientific code



Available on Glenn and BALE clusters

Better performance for AMD Opteron processors

Complete development environments C(pgcc) C++ (pgCC) Fortran 77 (pgf77) Fortran 90 (pgf90) High Performance Fortran (pghpf)

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Includes a debugger (pgdbg) and a profiler (pgprof)

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Complete manuals can be found at http://www.pgroup.com/resources/docs.htm



Load the PGI compilers into your environment using the module command: module load pgi

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The **pgi** module is loaded into each user's environment by default

Current default versions: 9.0-4 (glenn), 7.1-5 (BALE) Other versions available: through 10.5 (glenn), 9.0-1 (BALE) module switch pgi pgi-10.5





Compiler binaries (executables)

```
pgf77 (Fortran 77)
pgf90 (Fortran 90)
pgcc (C)
pgCC (C++)
```





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Always use man pages when uncertain!

General options

□-c (compile only, do not link; produces object file with .o suffix)

DMACRO[=value] (defines preprocessor macro MACRO with optional value; default value is 1)

g (generate symbols for debugging; disables optimization)

--I/dir/name (add /dir/name to the list of directories to be searched for #included files)

□-lname (add library libname.{a|so} to the list of libraries to be linked)
□-L/dir/name (add /dir/name to the list of directories to be searched for
library files)

□-o outfile (name executable file outfile; default is a.out)
□-UMACRO (removes definition of MACRO from preprocessor)



Optimization options -fast ("best" optimization) – on Glenn, equivalent to: -O2 -Munroll=c:1 -Mnoframe -Mlre -Mvect=sse -Mscalarsse -Mcache_align -Mflushz -00 (no optimization) -01 (light optimization; default) -02 (heavy optimization, same as -0) -O3 (aggressive optimization) -Munroll (enables loop unrolling) -Minline (controls function inlining) -Mvect=cachesize:numbytes (sets assumed L2 cache size to

- *numbytes* bytes)
- -Mconcur (enables automatic parallelization of loops)
- -mp (enables support for OpenMP and SGI-style PCF pragmas for parallelization)



- C Options
- -xa (enforces strict ANSI C compliance)
- -xc (enforces loose ANSI C compliance)
- -xs (enforces strict K&Rv1 C compliance)
- -xt (enforces loose K&Rv1 C compliance)

Recommended flags:

-Xa -fast



C++ Options -A (enforces strict ANSI C++ compliance) -exceptions (enables ANSI C++ exceptions) --prelink_objects (enables support for template libraries within template libraries) Recommended flags

-A -fast --prelink-objects



F77/F90 Options

-byteswapio (uses byte-swapping with unformatted I/O; compatible with Sun and SGI systems)

- -i4 (assumes 4-byte INTEGERS; default)
- -i8 (assumes 8-byte INTEGERS)
- -r4 (interpret DOUBLE PRECISION variables as REAL)
- -r8 (Interpret REAL variables as DOUBLE PRECISION)

Recommended flags:

-fast



Better performance than GNU (excellent performance) Includes support for: C (icc) C++ (icpc) Fortran 77 and 90 (ifort) Includes a debugger and a profiler Debug with idb Profile with gprof Vendor documentation can be found here:

http://www.osc.edu/supercomputing/manuals/



Latest version: glenn: 11.1.056 BALE: 10.0.023

module load intel-compilers-11.1
intel-compilers-11.1 points to the 11.1.056 software
Compiler binaries (executables)
ifort (Fortran 77)
ifort (Fortran 90)
icc (C)
icpc (C++)



General Options

- -c (compile only; do not link)
- -DMACRO[=value] (defines preprocessor macro MACRO with optional value; default value is 1)
- -g (generate symbols for debugging; disables optimization)
- -I/dir/name (add /dir/name to the list of directories to be searched for #included files)
- -lname (add library libname.{a|so} to the list of libraries to be linked)
- -L/dir/name (add /dir/name to the list of directories to be searched for library files)
- -o outfile (name resulting output file outfile; default is a.out)
- -UMACRO (removes definition of MACRO from preprocessor)

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Optimization Options

-fast ("good" optimization, can cause numerical problems) – on Glenn, equivalent to:

-03 -ipo -static

- -00 (no optimization)
- -01 (light optimization; default)
- -02 (heavy optimization)
- -O3 (aggressive optimization, may change numerical results)
- -ipo (enable interprocedural optimizations between files)
- -funroll-loops (enables loop unrolling)
- -parallel (enables auto-parallelizer to generate multi-threaded code for safe loops)
- -openmp (enables parallelization using OpenMP directives)



C/C++ Options

-strict_ansi (enforces strict ANSI C/C++

compliance)

-ansi (enforces loose ANSI C/C++ compliance)

-wall (enable all warnings)

Recommended flags: -02 -ansi



Fortran 77, Fortran 90 Options

-convert bigendian (uses unformatted I/O compatible with Sun and SGI systems)

-convert cray (uses unformatted I/O compatible with Cray systems)

-i8 (makes 8-byte INTEGERs the default)

-module /dir/name (adds /dir/name to the list of directories searched for F90 modules)

-r8 (makes 8-byte **REAL**s the default)

-warn (enables all warning messages)

-warn nousage (suppresses warnings about questionable programming practices)

Recommended flags: -02



Transitioning From GNU to Intel/PGI

Makefiles that use GNU compilers can be modified to use Intel or PGI compilers: Generally the PGI compilers are more likely to work with an existing GNU Makefile

Be careful with optimization flags

Start with little or no optimization

Verify numerical correctness (some optimization techniques can affect

numerical stability)

Increase optimization



Compiling – Examples using GNU

Simple Compile Small C program hello.c: #include <stdio.h> int main (void) { printf ("Hello, world!\n"); return 0; }

Minimal single file compile
gcc hello.c
Produces executable a.out
Execute program with command ./a.out
If \$PATH includes ./, may type a.out
Executable file should have `x' set in permissions
 `./a.out: Permission denied."

8 -rwxr-xr-x 1 pete G-0541 chmod a+x a.out 5144 Feb 24 05:18 a.out





Simple Compile Direct executable name to alternate file name gcc hello.c -o hello Execute with command ./hello Most compilers recognize the `-o' option Second simple program

```
duh.c:
#include <stdio.h>
int main (void) {
    printf ("Two plus two is %f\n", 4);
    return 0;
}
```

Try to compile and execute?

```
>> gcc duh.c -o duh
>> ./duh
Two plus two is -0.139606
>> [Truly, DOH!??]
```

We will revisit this later The need for feedback during the compile



Compiling Multiple Source Files

Having all the source in a single file is limiting As the file grows compilation time tends to grow for each little change, the whole program has to be re-compiled Impossible that several people will work on the same project together in this manner Managing your code becomes harder Split the source code into multiple files each containing a set of closely-related functions

Use a single command line to compile all the files

gcc -g -o imgdither make_pal.c convert.c io_image.c img_dither.c

All the source files will be recompiled Even those files not edited



Compiling Multiple Source Files

Alternate method Divide the compile into two phases Compiling

Compile object files for each source

gcc -c make_pal.c gcc -c convert.c gcc -c io_image.c gcc -c img_dither.c

□-c flag indicates just compile the object file More flexible

Unedited files need not be recompiled

Linking

Link all object files into one executable

gcc make_pal.o convert.o io_image.o img_dither.o -o imgdither

This will be more efficient when discussing 'make' and Makefiles



Compiling production line Objective is to create an executable file Specific to the architecture of the machine Compiling is multi-stage process Refer to gcc Front ends: gcc or g++Assembler: as Linker: Id Don't need to use each individually The compilation step with qcc uses all The simple *hello.c* example goes through all the steps -Uses headers Uses external libraries Use the -v flag during compilation < the output is on the next slide > The stages are: Preprocessing (macro expansion) Compilation (creating assembler language code) Assembling (create machine code) Linking (create final binary executable)



Compiling production line

pete@gromit: ~/ >> gcc -v hello.c Using built-in specs. Target: i386-redhat-linux Configured with: ../configure --prefix=/usr --mandir=/usr/share/man --infodir=/usr/share/info --enable-shared --enable-threads=posix --enable-checking=release --with-system-zlib --enable- cxa atexit --disable-libunwind-exceptions --enable-libgcj-multifile --enable-languages=c,c++,objc,obj-c++,java,fortran,ada --enable-java-awt=gtk --disable-dssi --enable-plugin --with-java-home=/usr/lib/jvm/java-1.4.2-gcj-1.4.2.0/jre --with-cpu=generic --host=i386-redhat-linux Thread model: posix gcc version 4.1.1 20070105 (Red Hat 4.1.1-51) /usr/libexec/gcc/i386-redhat-linux/4.1.1/ccl -quiet -v hello.c -quiet -dumpbase hello.c -mtune=generic -auxbase hello -version -o /tmp/ccbDwhXh.s ignoring nonexistent directory "/usr/lib/gcc/i386-redhat-linux/4.1.1/../../../i386-redhat-linux/include" #include "..." search starts here: #include <...> search starts here: /usr/local/include /usr/lib/gcc/i386-redhat-linux/4.1.1/include /usr/include End of search list. GNU C version 4.1.1 20070105 (Red Hat 4.1.1-51) (i386-redhat-linux) compiled by GNU C version 4.1.1 20070105 (Red Hat 4.1.1-51). GGC heuristics: --param ggc-min-expand=98 --param ggc-min-heapsize=129117 Compiler executable checksum: 98782966c6e2b1983484cce1a314172a as -V -Qy -o /tmp/ccr9lLjm.o /tmp/ccbDwhXh.s GNU assembler version 2.17.50.0.6-2.fc6 (i386-redhat-linux) using BFD version 2.17.50.0.6-2.fc6 20061020 /usr/libexec/gcc/i386-redhat-linux/4.1.1/collect2 --eh-frame-hdr -m elf i386 --hash-style=gnu -dynamic-linker /lib/ld-linux.so.2 /usr/lib/gcc/i386-redhat-linux/4.1.1/../../crt1.o /usr/lib/gcc/i386-redhat-linux/4.1.1/../../crt1.o /usr/lib/gcc/i386-redhat-linux/4.1.1/crtbegin.o -L/usr/lib/gcc/i386-redhat-linux/4.1.1 -L/usr/lib/gcc/i386-redhat-linux/4.1.1 -L/usr/lib/gcc/i386-redhat-linux/4.1.1/../.. /tmp/ccr91Ljm.o -lgcc --as-needed -lgcc_s --no-as-needed -lc -lgcc --as-needed -lqcc s --no-as-needed /usr/lib/qcc/i386-redhat-linux/4.1.1/crtend.o /usr/lib/qcc/i386-redhat-linux/4.1.1/../crtn.o pete@gromit: ~/ >>

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Compiling production line

Preprocessing Source code Expand macros Included headers Usually files not saved unless the -save-temps option used . *i* for C code . *ii* for C++ code Compiling Compilation of preprocessed source code to assembly language For a specific processor

>> gcc -Wall -S hello.i

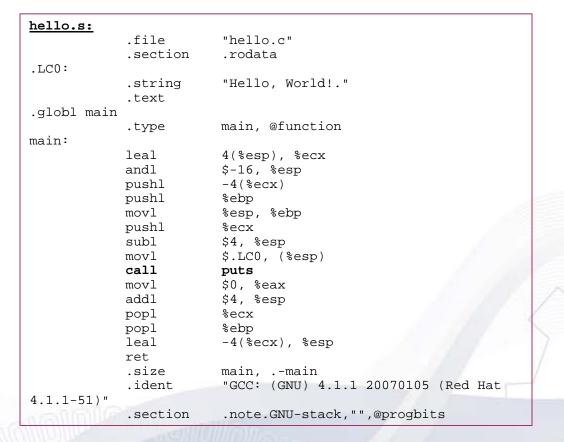
Use the command-line option -S

□Convert the preprocessed C source code to assembly language : □Assembly language is stored in the file hello.s:



Compiling production line

Compiling Assembler file for an Intel 386 processor on Fedora Core 6



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Compiling production line

Assembler

Assembler converts assembly language into machine code

Generates object file

Calls to external functions

addresses of the external functions are left undefined

Filled in later by the linker.

 \Box Assembler invoked with the $-\circ$ flag in the command line

>> as hello.s -o hello.o

Linking

Final stage of compilation

Linking of object files to create an executable Executable requires many external functions

From system and C run-time (crt) libraries

Internal link command, *1n*, is complicated

Id --eh-frame-hdr -m elf_i386 --hash-style=gnu -dynamic-linker /lib/ld-linux.so.2 /usr/lib/gcc/i386-redhat-linux/4.1.1/../../crt1.o /usr/lib/gcc/i386-redhat-linux/4.1.1/../../crti.o /usr/lib/gcc/i386-redhat-linux/4.1.1/crtbegin.o -L/usr/lib/gcc/i386-redhat-linux/4.1.1 -L/usr/lib/gcc/i386-redhat-linux/4.1.1 -L/usr/lib/gcc/i386-redhat-linux/4.1.1/../../tmp/ccr9ILjm.o -lgcc --as-needed -lgcc_s --no-as-needed -lc -lgcc --as-needed -lgcc_s --no-as-needed /usr/lib/gcc/i386-redhat-linux/4.1.1/crtend.o /usr/lib/gcc/i386-redhat-linux/4.1.1/../../crtn.o





Compiling production line Linker

Transparent to the process, fortunately

Links the object file

□To the C standard library

□To any other libraries as directed

 $\operatorname{\tilde{Using}} - \operatorname{L}$ in command line

~Environment variable : \$LD_LIBRARY_PATH

Produces the executable file a.out



Using Options For Compiling Control compiling features

Search paths used for locating libraries and include files Use of additional warnings and diagnostics **Preprocessor macros** C language dialects. Some desirable options are not default For specific options use the man For our purposes 'man gcc' Information overload But very specific to the architecture Eventually programmers must refer to the options Commonly-used GCC compiler options **Debugging with** -q Builds symbol table of the code Names of variables [~]Line numbers of commands and variables File size differ appreciably gcc -q main.c 6356 Feb 24 05:44 a.out ⊔8 -rwxr-xr-x 1 pete G-0541 gcc main.c G = 0.5415144 Feb 24 05:45 a.out 1 pete ⊓8 -rwxr-xr-x Look at this in greater detail in the *debugging* section -c and -o We have seen these in action Empower. Partner. Lead. Ohio Supercomputer Center 32

Using Options For Compiling – Warnings

-W(exp): Commonly-used GCC compiler options

Warnings with -Wall

■Essential potpourri of individual warning flags ■Should always be included in the compile ■Can catch many errors during compilation ■Full list of options included in man gcc ■Revisit our previous duh.c problem

>> gcc duh.c
>> ./a.out
Two plus two is -0.703465.
>>

Problem printing correct value

-Wall includes the warning -Wformat

[~]Checks for incorrect use of format strings

In functions such as printf and scanf

format specifier does not agree with the variable type

```
>> gcc -Wall duh.c
duh.c: In function 'main':
duh.c:4: warning: format '%f' expects type 'double', but argument 2 has type 'int'
>> ./a.out
Two plus two is 4.
>>
```

All listed in *man gcc* □Will say something like (Included in -Wall)



<u>Using Options For Compiling - Warnings</u> Other warning options not included in -Wall Source code may be technically valid But may cause problems Not included in -Wall

-Flag only possible problems

-W

```
int testInt (unsigned int x) {
    if (x < 0) return 0;
    else return 1;
}
>> gcc -W -c testInt.c
testInt.c: In function 'testInt':
testInt.c:2: warning: comparison of unsigned expression < 0 is always false
>>
```



Using Options For Compiling - Optimizing

Optimizing the code

Want the program to run faster or take less space

Replace the '-g' flag with the '-O' argument

Compilation takes longer

Compiler applies various optimization algorithms

Optimization is designed to be conservative

Ensures code will function the same as without optimization

Can ramp up the optimization

□Add number arguments to '-Ox': '-O2', '-O3', '-O4'

The higher the number the greater the optimization and slower the compiler Optimization can alter code

Chances are higher that an improper optimization will actually alter our code Some of them tend to be non-conservative, complex, and contain bugs





Using Options For Compiling - Optimizing

Common in-source optimization References programming practices Eliminate subexpressions

Reduce the number of operators

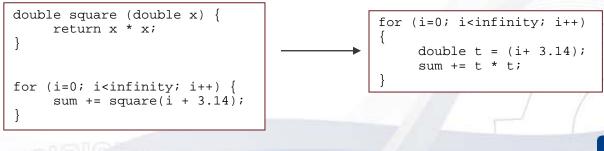
X = (1 - t 2) + 3*(1 - t 2) 3 - 2*(1 - t 2) 5;

Pre-calculate a common expression

m = 1 - t 2;X = (m) + 3 * (m) 3 - 2 * (m) 5;

 $\hfill \ensuremath{\mathsf{Reduces}}$ the size of the code and increases the speed Function inlining

Overhead calling functions







Using Options For Compiling - Optimizing

Control compilation-time and compiler memory usage Tradeoffs between speed and space for the resulting executable GCC provides a range of general optimization levels

Numbered from 0—3

Individual options for specific types

An optimization level is given in the command line options

 \square -OLEVEL, LEVEL is 0-3

-00 or no -0 option (default)

Does not perform any optimization

Compiles the source code in the most straightforward way possible Each command converted directly to the corresponding instructions

Best option to use when debugging

-01 **or** -0

Most common form of optimization

□Executables should be smaller and faster than with -00

Expensive optimizations are not used at this level.

[~]Instruction scheduling

□Takes less time than compiling with -00

[~]Reduced amounts of data not processed after simple optimizations.



Using Options For Compiling - Optimizing

-02

Turns on further optimizations

□Additional to those used by -01

Includes instruction scheduling

No optimizations that require any speed-space tradeoffs are used

□executable should not increase in size

Takes longer to compile and requires more memory than with -01 Best choice

Provides maximum optimization without increasing the executable size Default optimization level for GNU

-03

More expensive optimizations

□Function inlining

As well as all the optimizations of the levels -02 and -01

May increase the speed executable

Could also increase its size

May make a program slower and create spurious results Not recommended



Using Options For Compiling - Optimizing

-funroll-loops
Turns on loop-unrolling
Independent of other optimization options
Will increase the size of an executable
Results unclear, must be considered case-by-case
-Os
Reduces the size of an executable
Produces the smallest possible executable
For systems constrained by memory or disk space
Possible that smaller executable runs faster
Better cache usage.
Cost of optimization
Greater complexity in debugging

Increased time and memory requirements during compilation

Best rule of thumb

□Use -00 for debugging □Use -02 for production

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Using Options For Compiling - Optimizing

Optimization and compiler warnings Some compiler warnings do not appear without optimization Data flow analysis

□Compiler examines the use of all variables and initial values □Basis of optimization strategies

Compiler can detect the use of un-initialized variables

Create a file with the following code:

-Wuninitialized (included in -Wall)

DWarns about un-initialized variables

Only works with optimization turned on

Try the two compile commands

gcc -Wall -c checkex.c

gcc -Wall -O2 -c checkex.c

<u>checkex.c:</u>
<pre>float check (float x) {</pre>
float s;
if (x == 0.0)
s = 0.0;
else if (x != 0.0)
s = 1/x;
return s;
}





Using Options For Compiling – Libraries

Precompiled object files which can be linked into programs Most commonly used in the C library *sqrt, fabs* functions in the C *math* library

Two flavors

static libraries

Have the extension *.a*May be referenced directly in the compile command

gcc -Wall calc.c /usr/lib/libm.a -o calc

shared libraries

Have the extension .so More compatible with code reuse Linked in at runtime Library locations Specify specific libraries in compile command $\Box = 1(name) - [lower case el](name)$ Example: libm. a would be -lmTake off the 'ib' and the '.a' $\Box gcc -g -Wall - o$ myfunc myfunc.c -L/home/user/libs - lmylibs $\Box Gompiler will look for a library libmylibs.a or libmylibs.so$ $<math>\Box In the directory /home/user/libs$

Using Options For Compiling – Libraries

Library locations

```
As with header files, libraries may reside outside the system install
      Compilers look in /usr/lib and /usr/local/lib by default
      -Ldir in the compile command
            <sup>~</sup>May be repeated
                         qcc -L. -L/home/me/libs ...
      □$LD LIBRARY PATH
            The command module user interface to Modules package
            <sup>•</sup> Provides for dynamic modification of user environment
              [opt-login01] ~ :: module list
              Currently Loaded Modulefiles:
                1) pqi
                                                     4) torque
                           7) modules
                2) intel-compilers-10.0
                                                     5) mpi
                3) moab
                                                     6) mpirun-compat
              [opt-login01] ~ :: module show intel-compilers-10.0
              /usr/local/share/modulefiles/intel-compilers-10.0:
              module-whatis
                                loads the Intel C/C++/F95 compilers
                                LM LICENSE FILE 28519@license2.osc.edu
              prepend-path
              prepend-path
                                MANPATH /usr/local/intel-10.0.023/man
              prepend-path
                                PATH /usr/local/intel-10.0.023/bin
              append-path
                                LD LIBRARY PATH /usr/local/intel-10.0.023/lib
              set-alias
                                efc ifort
              set-alias
                                ecc icc
              [opt-login01] ~ ::
```

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Using Options For Compiling – Include Files

Include files contain information for a program Variable declaration and initialization Function declaration and prototyping <stdio.h>

Directed to look in standard system default locations u/usr/include, /usr/local/include

beme (me / in glude / muser b"

"/home/me/include/myown.h"

Look in a specified directory

Include locations for header files

Header files in your source code

-Most system header files in /usr/include and /usr/local/include
--Idir - that's [cap i]dir
-Also repeatable
-Need to access other directories

gcc -g -Wall -I/home/me/includes

Direct the compiler to look into /home/me/includes for referenced headers Use the <> in the source file





<u>Using Options For Compiling – Include Files</u>

Include locations for header files Environment variables

□C_INCLUDE_PATH □CPLUS_INCLUDE_PATH

Using Options For Compiling – Search Paths

Order of search

- 1. Command-line options -I and -L, left to right
- 2. Environment variables
- 3. Default system directories





<u>Using Options For Compiling – Preprocessing</u>

Alter execution of program Using #ifdef

```
#include <stdio.h>
int main(void) {
#ifdef DEBUG
    printf ("This might be interesting.\n");
#endif
    printf ("This is running mode.\n");
    return 0;
}
```

Preprocessor includes code
 □#endif terminates block
 -Dname defines a macro
 □Part of the command line

gcc -DDEBUG ...





Making Static Libraries

Additional commands ar GNU program which creates, extracts and modifies from <u>archives</u> an archive is single file holding a collection of other files ranlib generates an index to the contents of an archive and stores it in the archive.



Making Static Libraries : Creating

Often code may be collected and used over and over again This involves compiling the reusable code into a static library First Create source files Containing functions that will be used Library can contain multiple object files Compile files into object files

Creating a library

ar rc speciallib.a objfile1.o objfile2.o objfile3.o

Create a static library Rename the "speciallib" portion of the name Create an index inside the library

ranlib libmylib.a

copying the library ⊔use the -p option with cp to preserve permissions





Making Static Library : Usage Prototype library function calls Do not want implicit declaration errors When linking to the libraries

gcc -o main -L. -lmylib main.o

Specify where the library can be found -L. tells gcc to look in the current directory for libmylib.a.



Making Shared Libraries : Creating

Creating shared or dynamic libraries is simple also. Using the previous example, to create a shared library:

```
>> gcc -fPIC -c objfile1.c
>> gcc -fPIC -c objfile2.c
>> gcc -fPIC -c objfile3.c
>> gcc -shared -o libmylib.so objfile1.o objfile2.o objfile3.o
```

-fpic option

tells compiler to create Position Independent Code

□create libraries using relative addresses

no absolute addresses because these libraries can be loaded multiple times

```
-shared option
```

specifies architecture-dependent shared library is being created not all platforms support this flag.

Compile the actual program

using the libraries:

>> gcc -o foo -L. -lmylib foo.o

□Same as creating a static library □none of the actual library code is inserted into the executable



Making Shared Libraries : Usage Programs using static libraries

Can run on its own

Shared libraries dynamically access libraries at run-time

program needs to know where the shared library is stored

The advantage of using Dynamic Libraries

The executable is much smaller

□No need to compile it into the executable at compile time

Programs working with dynamic libraries use LD_LIBRARY_PATH environment variable

Make sure to **append** the desired path to the variable

>> echo \$LD LIBRARY PATH /usr/lib:/local/lib:/local/peteFiles/vtk5.0/lib:/local/peteFiles/AVS7.0/express/lib/linux >> setenv LD_LIBRARY_PATH /home/pete/libs:\${LD_LIBRARY_PATH} >> echo \$LD_LIBRARY_PATH /home/pete/libs:/usr/lib:/local/lib:/local/peteFiles/vtk5.0/lib:/local/peteFiles/AVS7.0/express/lib/linux

Not overwrite it – erases all the system settings

Mistake: setenv LD_LIBRARY_PATH /home/pete/libs



MPI Compiler Wrappers

The MVAPICH implementation of MPI for Infiniband

Uses a set of compiler scripts

- Need not remember path names for libraries and include files
- □MPI compilation scripts support the following languages

~C (mpicc - wrapper for pgcc)

[~]C++ (mpiCC – wrapper for pgCC)

- [~]Fortran 77 (mpif77 wrapper for pgf77)
- [~]Fortran 90 (mpif90 wrapper for pgf90)

DAccept the same arguments as the compiler they wrap

- mpicc accepts the same arguments as pgcc
- mpif77 accepts the same arguments as pgf77
- [~]See manual pages for details on argument options



MPI Compiler Wrappers
 Default compiler suite is PGI
 To use Intel compilers:

module switch mpi mvapich-1.1-intel



MPI Compiler Wrappers Break

Occasionally, quoting of compiler arguments:

□will not work with the MPI compiler wrappers (which are, after all, only shell scripts)

in these cases, you can use the Portland Group compilers directly:

[~]Compile with

```
□$MPI_CFLAGS (C)
□$MPI_CXXFLAGS (C++)
□$MPI_FFLAGS (F77)
□$MPI_F90FLAGS (F90)
~Link with $MPI_LIBS
```



.MPI Compiler Wrappers Break .Example

```
[opt-login1] pgcc -O2 \
$MPI_CFLAGS -DVERSION=' " v0.2 build 1/21/00" ' -c vbcast.c
```

.Example

[opt-login1] pgf90 -O2 \
\$MPI_FFLAGS -DSIZE=`128' cp3.F -o cp3-128 \$MPI_LIBS



Program Development Tools and Libraries

Libraries

Several Fortran numerical libraries installed

Can be used in conjunction with the compiler being used

AMD Core Math Library

Includes BLAS, LAPACK, FFT

Link with \$ACML

Requires loading the module specific to the compiler

```
[opt-login1] module avail acml
...
acml-gfortran acml-gnu acml-intel acml-pgi
...
[opt-login1] module load acml-pgi
```

Type the command 'module show acml-xxx' for specific settings





gdb command line symbolic debugger

Intel compilers include a debugger, idb

Portland Group compilers include a debugger, pgdbg

totalview parallel debugger

module load totalview





totalview within a batch job

Designed for parallel programs

MPI, OpenMP, or pthreads

MPI jobs run only through the PBS batch system

PBS allows for <u>interactive batch jobs</u> □Used to run interactive programs □Within the framework of a batch job □**qsub** -I





totalview example Specify on the command line

```
[opt-login1.osc.edu] > qsub -I -l nodes=2:ppn=4 \
  -l walltime=1:00:00 -j oe -N totalview -S /bin/ksh \
  -v DISPLAY
```

Obtain an interactive shell

□On one of the compute nodes □Has all the limits of your batch request □Run mpiexec with the -tv option

[opt0838] > cd \$PBS_O_WORKDIR
[opt0838] > module load totalview
[opt0838] > mpiexec -tv a.out



Debuggers

Totalview basic look

Process window Pull-down menus Control buttons 4 panes Interact with totalview via mouse Set breakpoints Examine variables "step" button

_ cdi	nz3d						•	
<u>File</u>	Edit <u>V</u> iew	<u>G</u> roup <u>P</u>	rocess <u>T</u> hread	Action Po	int Too <u>l</u> s	Window	Help	
Group - Control - Go Halt Next Step Out Run To Next Step P+ T- T+								
Process 0; cdnz3d (Exited or Never Created)								
No current thread								
Stack Trace Stack Frame								
No current thread								
		Function N	/AIN in [/usr/lo	cal/pgi=4.0).1/linux86/lii	b/libpac.sol		
	0 x 44 0 x 44	D16e336: D16e337: D16e338: D16e338: D16e33c: D16e33c: D16e332: D16e334: D16e341: D16e342: D16e344: D16e344: D16e344: D16e3445: D16e347: D16e345: D16e35: D16e35: D16e35: D16e35: D16e35: D16e35: D16e35: D16e35: D16e35: D16e35: D16e35: D16e35: D16e35: D16e35: D16e55: D16e35: D16e55; D16e55; D16e55; D16e55; D16e55; D16e55; D16e55;		0x00 0x00 0x00 0x8d 0xbf 0x00 0x00 0x00 0x00 0x55 0x85 0x85 0x85	addb addb pushl movl subl	<pre>%al, (%eax) %cl,191(%ebp) %dl,-119(%ebp) %ebp %esp,%ebp \$8,%esp 0x4016e347</pre>	1	
	0x40	016e348:		Oxff				
	0x40	016e349:		Oxff				
Threads (0) Action Points								
Proce		o thread:	s A				Z Z	

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DA good tutorial for totalview can be found at https://computing.llnl.gov/tutorials/totalview/



Reference

1. <u>http://www.network-theory.co.uk/docs/gccintro/index.html</u>, good online reference



Compiling Exercises

Retrieve the copies of the examples and exercises from Subversion repository

- 1. svn checkout http://svn.osc.edu/repos/softdevtools/trunk/Compiling
- 2. Each directory has a 'README' and/or 'HTML' file that will direct you through the exercise.

