The Cray Compilation Environment (CCE)

Additional Information

CCE Overview

- **Cray technology focused on scientific applications**
  - Takes advantage of automatic vectorization
  - Takes advantage of automatic shared memory parallelization
- **Standard conforming languages and programming models**
  - ANSI/ISO Fortran 2008 standards compliant
  - ANSI/ISO C99 and C++2003 compliant
  - OpenMP 3.1 compliant, working on OpenMP 4.0
  - OpenACC 2.0
- **OpenMP and automatic multithreading fully integrated**
  - Share the same runtime and resource pool
  - Aggressive loop restructuring and scalar optimization done in the presence of OpenMP
  - Consistent interface for managing OpenMP and automatic multithreading
- **PGAS languages (UPC & Fortran coarrays) fully optimized and integrated into the compiler**

General Cray Compiler Flags

- **Optimisation Options**

-O2	safe flags [enabled by default]
-O3	aggressive optimization
-O ipaN (ftn) or **-hipaN (cc/CC)**	inlining, N=0-5 [default N=3]

- **Create listing files with optimization info**

-hlist=a	creates a listing file with all optimization info
-hlist=m	produces a source listing with loopmark information

- **Parallelization Options**

-h omp	Recognize OpenMP directives [default]
-h threadN	control the compilation and optimization of OpenMP directives, N=0-3 [default N=2]

➔ **More info: man crayftn, man craycc, man crayCC**

Inlining with CCE

- **Inlining is enabled by default**
  - Command line option **-OipaN (ftn)** or **-hipaN (cc/CC)** where N=0…5, provides a set of choices for inlining behavior
    - 0 - All inlining and cloning are disabled. All inlining and cloning compiler directives are ignored.
    - 1 - Directive inlining. Inlining is attempted for call sites and routines that are under the control of an inlining compiler directive. Cloning disabled and cloning directives are ignored.
    - 2 - Inlining. Inline a call site to an arbitrary depth as long as the expansion does not exceed some compiler-determined threshold. Cloning disabled and cloning directives are ignored.
    - 3 (default) - Constant actual argument inlining and tiny routine inlining. This includes levels 1 and 2, plus any call site that contains a constant actual argument. Cloning disabled and cloning directives are ignored.
    - 4 - Aggressive inlining. This includes levels 1, 2, and 3, plus a call site does not have to reside in a loop body to inline. Cloning disabled and cloning directives are ignored.
    - 5 - Cloning. This includes levels 1, 2, 3, and 4, plus routine cloning is attempted if inlining fails at a given call site. Cloning directives are enabled.

Inlining with CCE (cont)

- **By default, all inlining candidates come from the current source file**
- **The -Oipafrom= (ftn) or -hipafrom= (cc/CC) option instructs the compiler to look for inlining candidates from other source files, or a directory of source files**
  - "ftn -Oipafrom=b.f a.f" tells the compiler to look for inlining candidates within b.f when compiling a.f
  - "cc -hipafrom=./dir src.c" tells the compiler to look for inlining candidates in all the valid source files that exist in the directory ./dir when compiling src.c
- **Cross language inlining is not supported**

Whole-Program Compilation

- **The Program Library (PL) feature allows the user to specify a repository of compiler information for an application build**
  - This repository provides the framework for future productivity features such as
    - Whole program static error detection
    - Incremental recompilation
    - Provide support for the future Cray interactive whole program performance analysis and tuning assistant Reveal
- **Two command line options control the Program Library functionality**
  - **-h pl = <PL_path>** specifies the repository
    - -hpl=./PL.1 tells the compiler to either update the Program Library "./PL.1" if it exists, or create it if it does not exist.
    - <PL_path> should specify a single location to be used for entire application build. If a makefile changes directories during a build, an absolute path might be necessary.
  - **-h wp** enables whole-program mode
- **Needed by Reveal (to be covered in the tool talk on Thursday)**

Whole-Program Compilation (cont)

- **Whole-program mode (-hwp) requires a program library (-hpl=) and both options must be specified on all compilation command lines as well as on the link line.**
  - The compiler frontend is invoked for the compilation (-c) command lines
  - The compiler backend (inliner, optimizer, code generator) is invoked for all source files when the link line is specified.
  - While **-hwp** might have a negative affect on overall compile time due to increased inlining, it is most usually a compile time shift, where -c compilations become quite fast and the time spent on the link step increases.
  - Setting the environment variable “NPROC” to a number greater than 1 instructs the compiler to invoke NPROC backend processes concurrently. The backend invocations are independent of each other and setting NPROC to a level that is appropriate for the host build machine can improve compile time.
- **Whole-program mode (-hwp) allows the inliner to see all inline candidates in the application.**
  - This option makes cross file inlining automatic
    - Removes the need for **-O/-h ipafrom=**
    - Inlining heuristics are still controlled by **-O/-h ipaN**

Unrolling

- **By default, the compiler attempts to unroll all loops, unless the `NOUNROLL` directive is specified for a loop**
  - Generally, unrolling loops increases single processor performance at the cost of increased compile time and code size
- **-hunrollN (cc/CC) where N=0,1,2, globally control loop unrolling and changes the assertiveness of the UNROLL directive**
  - **0**: No unrolling (ignore all `UNROLL` directives and do not attempt to unroll other loops)
  - **1**: Attempt to unroll loops if there is proof that the loop will benefit
  - **2**: (Default) Attempt to unroll all loops (includes array syntax implied loops), except those marked with the `NOUNROLL` directive.

Vectorization

- **-hvectorN (cc/CC) where N=0…3, specify the level of automatic vectorizing to be performed. Vectorization results in significant performance improvements with a small increase in object code size. Vectorization directives are unaffected by this option**
  - **0**: No automatic vectorization
  - **1**: Specifies conservative vectorization. Loop nests are restructured. No vectorizations that might create false exceptions are performed. Results may differ slightly from results obtained when N=0 is specified because of vector reductions
  - **2**: (Default) Specifies moderate vectorization. Characteristics include moderate compile time and size. Loop nests are restructured
  - **3**: Specifies aggressive vectorization. Loop nests are restructured. Vectorizations that might create false exceptions in rare cases may be performed.

Floating-Point Optimizations

- **The -hfpN option, where N=0…4, controls the level of floating-point optimizations: N=0 gives the compiler minimum freedom to optimize floating-point operations, while N=4 gives it maximum freedom. The higher the level, the less the floating-point operations conform to the IEEE standard.**
  - **N=0 and N=1**: Use this option only when your code pushes the limits of IEEE accuracy or requires strong IEEE standard conformance. Executable code is slower than higher floating-point optimization levels
  - **N=2**: default value. It performs various generally safe, non-conforming IEEE optimizations
  - **N=3**: This option should be used when performance is more critical than the level of IEEE standard conformance provided by N=2. This is the suggested level of optimization for many applications.
  - **N=4**:You should only use this option if your application uses algorithms which are tolerant of reduced precision.

Floating-Point Optimization Flags Comparison

The **-hfpN** option, where N=0…4, controls the level of floating-point optimizations

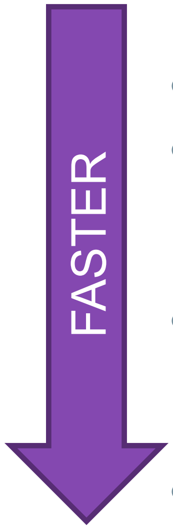
Optimization	fp0	fp1	fp2 (default)	fp3	fp4
Safety	Maximum	High	High	Moderate	Low
Complex divisions	Accurate and slower	Accurate and slower	Fast	Fast	Fast
Exponentiation rewrite	None	None	When benefit is very high	Always	Always
Strength reduction	None	None	Fast	Fast	Fast
Rewrite division as reciprocal equivalent	None	None	Yes	Aggressive	Aggressive
Floating point reductions	Slow	Fast	Fast	Fast	Fast
Expression factoring	None	Yes	Yes	Yes	Yes
Inline 32-bit operations	No	No	No	Yes	Yes

Why are CCE's results sometimes different?

- **We do expect applications to be conformant to language requirements**
  - This include not over-indexing arrays, no overlap between Fortran subroutine arguments, and so on
  - Applications that violate these rules may lead to incorrect results or segmentation faults
  - Note that languages do not require left-to-right evaluation of arithmetic operations, unless fully parenthesized
    - This can often lead to numeric differences between different compilers
    - Use **-hadd_paren** to add automatically parenthesis to select associative operations (+,–,*). Default is **-hnoadd_paren**
- **We are also fairly aggressive at floating point optimizations that violate IEEE requirements**
  - Use **-hfp[0-4]** flag to control that

About reproducibility

- **Results can vary with the number of ranks or threads**
  - Use **-hflex_mp=option** to control the aggressiveness of optimizations which may affect floating point and complex repeatability when application requirements require identical results when varying the number of ranks or threads.
  - **option** in order from least aggressive to most is:
    - intolerant: has the highest probability of repeatable results, but also has the highest performance penalty
    - strict: uses some safe optimizations, with high probability of repeatable results.
    - conservative: uses more aggressive optimization and yields higher performance than intolerant, but results may not be sufficiently repeatable for some applications
    - default: uses more aggressive optimization and yields higher performance than conservative, but results may not be sufficiently repeatable for some applications
    - tolerant: uses most aggressive optimization and yields highest performance, but results may not be sufficiently repeatable for some applications



Fortran Source Preprocessing

For a source file to be preprocessed automatically, it must have an uppercase extension, either .F (for a file in fixed source form), or .F90, .F95, .F03, .F08, or .FTN (for a file in free source form). To specify preprocessing of source files with other extensions, including lowercase ones, use the -eP or -eZ options

- **-eP**: Performs source preprocessing on Fortran source files, **but does not compile**. Generates file.1, which contains the source code after the preprocessing has been performed and the effects have been applied to the source program.
- **-eZ**: similar to **-eP**, but it also performs compilation on Fortran source files

Other flags in brief

- **-h restrict=[a|f]**
  - C/C++ option which tells the compiler to treat certain classes of pointers as restricted pointers. You can use this option to enhance optimizations (this includes vectorization).

- **-h cacheN**
  - Specifies the levels of automatic cache management to perform. Values for N are between 0 (cache blocking turned off) and 3 (aggressive automatic cache management). Symbols are placed in the cache when the possibility of cache reuse exists. Default value is N=2.

Other flags in brief (cont)

- **-h Pic**
  - Generate position independent code (PIC), which allows a virtual address change from one process to another, as is necessary in the case of shared, dynamically linked objects. The virtual addresses of the instructions and data in PIC code are not known until dynamic link time.
- **-h[system|default]_alloc**
  - The **-hsystem_alloc** option causes the compiler to use the native malloc implementation provided by the OS. By default, the compiler uses a modified malloc implementation which offers better support for Cray memory needs. This is a link-time option.

Diagnostic Flags

- **-Rb (ftn) or -h bounds (cc/CC)**
  - Fortran: Enables checking of array bounds at runtime.
  - C/C++: Enables checking of pointer and array references at runtime. **-h nobounds** disables these checks.
- **-eo (ftn) or -hdisplay_opt (cc/CC)**
  - Display the compiler optimization settings currently in force.
- **-T (ftn)**
  - Disables the compiler but displays all options currently in effect.

Recommended CCE Compilation Options

- **Use default optimization levels**
  - It's the equivalent of most other compilers -O3 or -fast
  - It is also our most thoroughly tested configuration
- **Use -O3,fp3 (or -O3 -hfp3, or some variation) if the application runs cleanly with these options**
  - **-O3** only gives you slightly more than the default **-O2**
  - We also test this thoroughly
  - **-hfp3** gives you a lot more floating point optimization (default is **-hfp2**)
- **If an application is intolerant of floating point reordering, try a lower -hfp number**
  - Try **-hfp1** first, only **-hfp0** if absolutely necessary (**-hfp4** is the maximum)
  - Might be needed for tests that require strict IEEE conformance
  - Or applications that have 'validated' results from a different compiler
  - Higher numbers are not always correlated with better performance

OpenMP

- **OpenMP is ON by default**
  - This is the opposite default behavior that you get from GNU and Intel compilers
  - Optimizations controlled by **-OthreadN (ftn)** or **-hthreadN (cc/CC)**, N=0-3 [default N=2]
  - To shut off use **-O/-h thread0** or **-xomp (ftn)** or **-hnoomp**

- **Autothreading is off by default**
  - **-hautothread** to turn on
  - Interacts with OpenMP directives

- **If you do not want to use OpenMP and have OMP directives in the code, make sure to shut off OpenMP at compile time**

CCE Directives

- **The Cray compiler supports a full and growing set of directives and pragmas**
  - Fortran:
    - `!dir$ concurrent`
    - `!dir$ ivdep`
    - `!dir$ interchange`
    - `!dir$ unroll`
    - `!dir$ loop_info [max_trips] [cache_na]` ... Many more
    - `!dir$ blockable`
  - For C/C++ replace `!dir$` with `#pragma [_CRI]`
    - The `_CRI` specification is optional; it ensures that the compiler will issue a message concerning any directives that it does not recognize. Diagnostics are not generated for directives that do not contain the `_CRI` specification.

➔ More info: man directives
man loop_info

Macros

- **Cray compilers define the following macros:**
  - Fortran: `_CRAYFTN`
  - C/C++: `_CRAYC`

- **For example, the macros can be used to ensures that other compilers will not interpret the directives by encapsulating them inside `#if` … `#endif`**

```
    #if _CRAYC
          #pragma _CRI directive
    #endif
```

- **Some compilers diagnose any directives that they do not recognize. The Cray C/C++ compilers diagnose directives that are not recognized only if the _CRI specification is used.**

Compiler Message System

- The `explain` command displays an explanation of any message issued by the compiler. The command takes as an argument, the message number, including the number's prefix (`ftn-` for ftn or `CC-` for cc/CC)

  Example:

```
% cc bug.c
CC-24 cc: ERROR File = bug.c, Line = 1
An invalid octal constant is used.
int i = 018;
          ^
1 error detected in the compilation of "bug.c".
% explain CC-24
An invalid octal constant is used.
Each digit of an octal constant must be between 0 and
7, inclusive. One or more digits in the indicated
octal constant are outside of this range. Change each
digit in the octal constant to be within the valid
range.
```

➔ **More info: man explain (when PrgEnv-cray loaded)**

Compiler Message System (cont)

- **-h [no]msgs**
  - Enables or disables the writing of optimization messages to `stderr`. Default is **-h nomsgs**
- **-h [no]negmsgs**
  - Enables or disables the writing of messages to `stderr` that indicate why optimizations such as vectorization, inlining, or cloning did not occur in a given instance. Default is -h nonegmsgs
- **-m *n* (ftn) or -h msglevel_*n* (cc/CC)**
  - Specifies the lowest level of severity of messages to be issued. Messages at the specified level and above are issued. Values of ***n*** are:
    - 0: Comment
    - 1: Note
    - 2: Caution
    - 3: Warning (default)
    - 4: Error
- **-M msg*n*[,…] (ftn) or -h nomessage=*n*[:...] (cc/CC)**
  - Suppresses specific messages at the warning, caution, note, and comment levels, where ***n*** is the number of a message to be disabled (multiple numbers are possible)

Brief Overview on Intel and GNU Compilers

Additional Information

CCE – GNU – Intel compilers

- **More or less all optimizations and features provided by CCE are available in Intel and GNU compilers**
  - GNU compiler serves a wide range of users & needs
    - Default compiler with Linux, some people only test with GNU
    - Defaults are conservative (e.g. -O1)
      - -O3 includes vectorization and most inlining
    - Performance users set additional options
  - Intel compiler is typically more aggressive in the optimizations
    - Defaults are more aggressive (e.g -O2), to give better performance "out-of-the-box"
      - Includes vectorization; some loop transformations such as unrolling; inlining within source file
    - Options to scale back optimizations for better floating-point reproducibility, easier debugging, etc.
    - Additional options for optimizations less sure to benefit all applications
  - CCE is even more aggressive in the optimizations by default
    - Better inlining and vectorization
    - Aggressive floating-point optimizations
    - OpenMP enabled by default

Cray, Intel and GNU compiler flags

Feature	Cray	Intel	GNU
Listing	-hlist=a	-opt-report3	-fdump-tree-all
Free format (ftn)	-f free	-free	-ffree-form
Vectorization	By default at -O1 and above	By default at -O2 and above	By default at -O3 or using -ftree-vectorize
Inter-Procedural Optimization	-hwp	-ipo	-flto (note: link-time optimization)
Floating-point optimizations	-hfpN, N=0...4	-fp-model [fast|fast=2|precise|except|strict]	-f[no-]fast-math or -funsafe-math-optimizations
Suggested Optimization	(default)	-O2 -xAVX	-O2 -mavx -ftree-vectorize -ffast-math -funroll-loops
Aggressive Optimization	-O3 -hfp3	-fast	-Ofast -mavx -funroll-loops
OpenMP recognition	(default)	-fopenmp	-fopenmp
Variables size (ftn)	-s real64 -s integer64	-real-size 64 -integer-size 64	-freal-4-real-8 -finteger-4-integer-8

Linking with MKL and PrgEnv-cray

- **PrgEnv-cray compatible with sequential, not threaded, MKL**
  - MKL can be used as an alternative to Cray's libsci for CCE
- **Examples assume you have loaded the Intel module (to define the env var INTEL_PATH)**
  - Typical case: You want to use MKL BLAS and/or LAPACK

    ```
    -L ${INTEL_PATH}/mkl/lib/intel64/ \
    -Wl,--start-group \
    -lmkl_intel_lp64 -lmkl_sequential -lmkl_core \
    -Wl,--end-group
    ```
  - Another typical case: You want to use MKL serial FFTs/DFTs

    Same as above (need more for FFTW interface)
  - A less typical case: You want to use MKL distributed FFTs

    ```
    -L ${INTEL_PATH}/mkl/lib/intel64/ \
    -Wl,--start-group \
    -lmkl_cdft_core -lmkl_intel_lp64 -lmkl_sequential \
    -lmkl_core -lmkl_blacs_intelmpi_lp64 \
    -Wl,--end-group
    ```
- **The Intel MKL Link Line Advisor can tell you what to add to your link line**
  - http://software.intel.com/sites/products/mkl/