Compilers Tools for Scientists and Engineers

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Outline of Today's Topics

- Introduction to PGI Compilers and Tools
- Documentation. Getting Help
- Basic Compiler Options
- Optimization Strategies
- Questions and Answers



PGI Compilers and Tools, features

- Optimization State-of-the-art vector, parallel, IPA, Feedback, ...
- Cross-platform AMD & Intel, 32/64-bit, Linux & Windows
- PGI Unified Binary for AMD and Intel processors
- Tools Integrated OpenMP/MPI debug & profile, IDE integration
- Parallel MPI, OpenMP 2.5, auto-parallel for Multi-core
- Comprehensive OS Support Red Hat 7.3 9.0, RHEL 3.0/4.0, Fedora Core 2/3/4/5, SuSE 7.1 – 10.1, SLES 8/9/10, Windows XP, Windows x64



PGI Tools Enable Developers to:

- View x64 as a unified CPU architecture
- Extract peak performance from x64 CPUs
- Ride innovation waves from both Intel and AMD
- Use a single source base and toolset across Linux and Windows
- Develop, debug, tune parallel applications for Multi-core, Multi-core SMP, Clustered Multi-core SMP



PGI Documentation and Support

- PGI provided documentation
- PGI User Forums, at <u>www.pgroup.com</u>
- PGI FAQs, Tips & Techniques pages
- Email support, via <u>trs@pgroup.com</u>
- Web support, a form-based system similar to email support
- Fax support



PGI Docs & Support, cont.

- Legacy phone support, direct access, etc.
- PGI download web page
- PGI prepared/personalized training
- PGI ISV program
- PGI Premier Service program

PGI Basic Compiler Options

- Basic Usage
- Language Dialects
- Target Architectures
- Debugging aids
- Optimization switches



PGI Basic Compiler Usage

- A compiler driver interprets options and invokes pre-processors, compilers, assembler, linker, etc.
- Options precedence: if options conflict, last option on command line takes precedence
- Use -Minfo to see a listing of optimizations and transformations performed by the compiler
- Use -help to list all options or see details on how to use a given option, e.g. pgf90 -Mvect -help
- Use man pages for more details on options, e.g. "man pgf90"
- Use –v to see under the hood



Flags to support language dialects

Fortran

- pgf77, pgf90, pgf95, pghpf tools
- Suffixes .f, .F, .for, .fpp, .f90, .F90, .f95, .F95, .hpf, .HPF
- Mextend, -Mfixed, -Mfreeform
- Type size –i2, -i4, -i8, -r4, -r8, etc.
- -Mcray, -Mbyteswapio, -Mupcase, -Mnomain, -Mrecursive, etc.

C/C++

- pgcc, pgCC, aka pgcpp
- Suffixes .c, .C, .cc, .cpp, .i
- -B, -c89, -c9x, -Xa, -Xc, -Xs, -Xt
- -Msignextend, -Mfcon, -Msingle, -Muchar, -Mgccbugs



Specifying the target architecture

- Not an issue on XT.
- Defaults to the type of processor/OS you are running on
- Use the "tp" switch.
 - -tp k8-64 or -tp p7-64 or -tp core2-64 for 64-bit code.
 - -tp amd64e for AMD opteron rev E or later
 - -tp x64 for unified binary
 - -tp k8-32, k7, p7, piv, piii, p6, p5, px for 32 bit code



Flags for debugging aids

- g generates symbolic debug information used by a debugger
- gopt generates debug information in the presence of optimization
- -Mbounds adds array bounds checking
- v gives verbose output, useful for debugging system or build problems
- -Mlist will generate a listing
- -Minfo provides feedback on optimizations made by the compiler
- -S or –Mkeepasm to see the exact assembly generated



Basic optimization switches

- Traditional optimization controlled through -O[<n>], n is 0 to 4.
- -fast switch combines common set into one simple switch, is equal to -O2 -Munroll=c:1 -Mnoframe -Mlre
 - For -Munroll, c specifies completely unroll loops with this loop count or less
 - -Munroll=n:<m> says unroll other loops m times
- -Mnoframe does not set up a stack frame
- -MIre is loop-carried redundancy elimination



Basic optimization switches, cont.

- fastsse switch is commonly used, extends –fast to SSE hardware, and vectorization
- -fastsse is equal to -O2 -Munroll=c:1 -Mnoframe -Mlre (-fast) plus -Mvect=sse, -Mscalarsse -Mcache_align, -Mflushz
- -Mcache_align aligns top level arrays and objects on cache-line boundaries
- -Mflushz flushes SSE denormal numbers to zero



Node level tuning

- Vectorization packed SSE instructions maximize performance
- Interprocedural Analysis (IPA) use it! motivating examples
- Function Inlining especially important for C and C++
- Parallelization for Cray XT CNL and multi-core processors
- □ Miscellaneous Optimizations hit or miss, but worth a try



Vectorizable F90 Array Syntax Data is REAL*4

350 !

351 ! Initialize vertex, similarity and coordinate arrays

352 !

- 353 Do Index = 1, NodeCount
- $354 \qquad IX = MOD (Index 1, NodesX) + 1$
- 355 IY = ((Index 1) / NodesX) + 1
- 356 CoordX (IX, IY) = Position (1) + (IX 1) * StepX
- 357 CoordY (IX, IY) = Position (2) + (IY 1) * StepY
- 358 JetSim (Index) = SUM (Graph (:, :, Index) * &
- 359 & GaborTrafo (:, :, CoordX(IX,IY), CoordY(IX,IY)))
- 360 VertexX (Index) = MOD (Params%Graph%RandomIndex (Index) 1, NodesX) + 1
- 361 VertexY (Index) = ((Params%Graph%RandomIndex(Index) 1) / NodesX) + 1
- 362 End Do

Inner "loop" at line 358 is vectorizable, can used packed SSE instructions



–fastsse to Enable SSE Vectorization
–Minfo to List Optimizations to stderr

% ftn -fastsse -Mipa=fast -Minfo -S graphRoutines.f90

localmove:

. . .

334, Loop unrolled 1 times (completely unrolled)
343, Loop unrolled 2 times (completely unrolled)
358, Generated an alternate loop for the inner loop Generated vector sse code for inner loop Generated 2 prefetch instructions for this loop Generated 2 prefetch instructions for this loop



Vectorizable C Code Fragment?

```
217 void func4(float *u1, float *u2, float *u3, ...
```

```
221 for (i = -NE+1, p1 = u2-ny, p2 = n2+ny; i < nx+NE-1; i++)
```

```
222 u3[i] += clz * (p1[i] + p2[i]);
```

```
223 for (i = -NI+1, i < nx+NE-1; i++) {
```

```
float vdt = v[i] * dt;
```

```
225 u3[i] = 2.*u2[i]-u1[i]+vdt*vdt*u3[i];
```

```
226 }
```

. . .

% pgcc –fastsse –Minfo functions.c func4:

221, Loop unrolled 4 times

221, Loop not vectorized due to data dependency

223, Loop not vectorized due to data dependency



Pointer Arguments Inhibit Vectorization

```
217 void func4(float *u1, float *u2, float *u3, ...
```

```
221 for (i = -NE+1, p1 = u2-ny, p2 = n2+ny; i < nx+NE-1; i++)
```

```
222 u3[i] += clz * (p1[i] + p2[i]);
```

```
223 for (i = -NI+1, i < nx+NE-1; i++) {
```

```
float vdt = v[i] * dt;
```

```
225 u3[i] = 2.*u2[i]-u1[i]+vdt*vdt*u3[i];
```

```
226 }
```

. . .

% pgcc –fastsse –Msafeptr –Minfo functions.c func4:

221, Generated vector SSE code for inner loopGenerated 3 prefetch instructions for this loop223, Unrolled inner loop 4 times



C Constant Inhibits Vectorization

```
217 void func4(float *u1, float *u2, float *u3, ...
```

```
221 for (i = -NE+1, p1 = u2-ny, p2 = n2+ny; i < nx+NE-1; i++)
```

```
222 u3[i] += clz * (p1[i] + p2[i]);
```

- 223 for (i = -NI+1, i < nx+NE-1; i++) {
- float vdt = v[i] * dt;
- 225 u3[i] = 2.*u2[i]-u1[i]+vdt*vdt*u3[i];

226 }

% pgcc –fastsse –Msafeptr –Mfcon –Minfo functions.c func4:

221, Generated vector SSE code for inner loop
Generated 3 prefetch instructions for this loop
223, Generated vector SSE code for inner loop
Generated 4 prefetch instructions for this loop



-Msafeptr Option and Pragma

-M[no]safeptr[=all | arg | auto | dummy | local | static | global]

- all All pointers are safe
- arg Argument pointers are safe
- local local pointers are safe
- static static local pointers are safe
- global global pointers are safe

#pragma [scope] [no]safeptr={arg | local | global | static | all},...

Where *scope* is *global*, *routine* or *loop*



Common Barriers to SSE Vectorization

- Potential Dependencies & C Pointers Give compiler more info with –Msafeptr, pragmas, or restrict type qualifer
- **Function Calls** Try inlining with –Minline or –Mipa=inline
- **Type conversions** manually convert constants or use flags
- Large Number of Statements Try Mvect=nosizelimit
- Too few iterations Usually better to unroll the loop
- □ **Real dependencies** Must restructure loop, if possible



Barriers to Efficient Execution of Vector SSE Loops

- Not enough work vectors are too short
- Vectors not aligned to a cache line boundary
- Non unity strides
- Code bloat if altcode is generated



- Vectorization packed SSE instructions maximize performance
- Interprocedural Analysis (IPA) use it! motivating example
- Function Inlining especially important for C and C++
- Parallelization for Cray XD1 and multi-core processors
- Miscellaneous Optimizations hit or miss, but worth a try



What can Interprocedural Analysis and Optimization with –Mipa do for You?

- Interprocedural constant propagation
- Pointer disambiguation
- Alignment detection, Alignment propagation
- Global variable mod/ref detection
- **F90 shape propagation**
- Function inlining
- IPA optimization of libraries, including inlining



Effect of IPA on the WUPWISE Benchmark

PGF95 Compiler Options	Execution Time in Seconds
-fastsse	156.49
-fastsse -Mipa=fast	121.65
–fastsse –Mipa=fast,inline	91.72

- Mipa=fast => constant propagation => compiler sees complex matrices are all 4x3 => completely unrolls loops
- —Mipa=fast,inline => small matrix multiplies are all inlined



Using Interprocedural Analysis

- Must be used at both compile time and link time
- Non-disruptive to development process edit/build/run
- Speed-ups of 5% 10% are common
- -Mipa=safe:<*name>* safe to optimize functions which call or are called from unknown function/library *name*
- –Mipa=libopt perform IPA optimizations on libraries
- –Mipa=libinline perform IPA inlining from libraries



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-Minline[=[lib:] <inlib> [name:]<func> except:<func> size:<n> levels:<n>]</n></n></func></func></inlib>	
[lib:] <inlib></inlib>	Inline extracted functions from inlib
[name:] <func></func>	Inline function func
except: <func></func>	Do not inline function func
size: <n></n>	Inline only functions smaller than n statements (approximate)
levels: <n></n>	Inline n levels of functions

For C++ Codes, PGI Recommends IPA-based inlining or –Minline=levels:10!



Other C++ recommendations

- Encapsulation, Data Hiding small functions, inline!
- Exception Handling use no_exceptions until 7.0
- Overloaded operators, overloaded functions okay
- Pointer Chasing -Msafeptr, restrict qualifer, 32 bits?
- **Templates, Generic Programming –** now okay
- Inheritance, polymorphism, virtual functions runtime lookup or check, no inlining, potential performance penalties



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SMP Parallelization

mp=nonuma to enable OpenMP 2.5 parallel programming model

- > See PGI User's Guide or OpenMP 2.5 standard
- > OpenMP programs compiled w/out –mp=nonuma "just work"
- Supported on Cray XT



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Miscellaneous Optimizations (1)

- Image: Market And American Straight And American Straight Ameri
- Mprefetch=d:,n:<q> control prefetching distance, max number of prefetch instructions per loop
- -tp k8-32 can result in big performance win on some C/C++ codes that don't require > 2GB addressing; pointer and long data become 32-bits



Miscellaneous Optimizations (2)

- -O3 more aggressive hoisting and scalar replacement; not part of –fastsse, always time your code to make sure it's faster
- For C++ codes: —no_exceptions –Minline=levels:10
- -M[no]movnt disable / force non-temporal moves
- -V[version] to switch between PGI releases at file level
- -Mvect=noaltcode disable multiple versions of loops

Pathscale programming environment

- Pathscale module available
 - module load pathscale
- Use standard compiler driver: ftn
 - ftn -O3 -OPT:Ofast ...



Pathscale compilers

- Pathscale compiler flags for a first start
 - Preprocessor Options:
 - -cpp runs cpp on source files
 - -ftpp runs the fortran source preprocessor
 - Optimisation Options:
 - -LNO: specify transformations performed on loop nests by the Loop Nest Optimizer
 - -OPT: controls miscellaneous optimizations
 - -ipa Inter Procedural Analysis
 - Ofast Equivalent to
 - -O3 -ipa -OPT:Ofast -fno-math-errno -ffast-math
 - Default: -O2 -mcpu=opteron -m64 -msse -msse2 -mno-sse3 -mno-3dnow
 - Start: -O3 –OPT:Ofast
- More info: man eko, man pathf95