

The Cray Compiler Environment: Introduction and Intial Results

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Outline



- Introduction to the Cray compiler
- Example
 - GTC
 - Overflow
 - PARQUET

Cray Compiler Environment (CCE): Brief History of Time

- Cray has a long tradition of high performance compilers
 - Vectorization
 - Parallelization
 - Code transformation
 - More...
- Began internal investigation leveraging an open source compiler called LLVM
- Initial results and progress better than expected
- Decided to move forward with Cray X86 compiler
- 7.0 released in December 2008
- 7.1 will be released Q2 2009

Technology Sources





Cray Opteron Compiler: How to use it



- Make sure it is available
 - module avail PrgEnv-cray
- To access the Cray compiler
 - module load PrgEnv-cray
- To target the Barcelona chip
 - module load xtpe-quadcore
- Once you have loaded the module "cc" and "ftn" are the Cray compilers
 - Recommend just using default options
 - Use –rm (fortran) and –hlist=m (C) to find out what happened
- man crayftn



- Excellent Vectorization
 - Vectorize more loops than other compilers
- OpenMP
 - 2.0 standard
 - Nesting
- PGAS: Functional UPC and CAF available today.
- Excellent Cache optimizations
 - Automatic Blocking
 - Automatic Management of what stays in cache
- Prefetching, Interchange, Fusion, and much more...

Cray Opteron Compiler: Future Capabilities



- C++ Support
- Automatic Parallelization
 - Modernized version of Cray X1 streaming capability
 - Interacts with OMP directives
- OpenMP 3.0
- Optimized PGAS
 - Will require Gemini network to really go fast
- Improved Vectorization
- Improve Cache optimizations

Case Study: The Gyrokinetic Toroidal Code (GTC)



- Plasma Fusion Simulation
- 3D Particle-in-cell code (PIC) in toroidal geometry
- Developed by Prof. Zhihong Lin (now at UC Irvine)
- Code has several different characteristics
 - Stride-1 copies
 - Strided memory operations
 - Computationally intensive
 - Gather/Scatter
 - Sorting and Packing
- Main routine is known as the "pusher"



Case Study: The Gyrokinetic Toroidal Code (GTC)

- Main Pusher kernel consists of 2 main loop nests
- First loop nest contains groups of 4 statements which include significant indirect addressing

e1=e1+wp0*wt00*(wz0*gradphi(1,0,ij)+wz1*gradphi(1,1,ij))

e2=e2+wp0*wt00*(wz0*gradphi(2,0,ij)+wz1*gradphi(2,1,ij))

e3=e3+wp0*wt00*(wz0*gradphi(3,0,ij)+wz1*gradphi(3,1,ij))

e4=e4+wp0*wt00*(wz0*phit(0,ij)+wz1*phit(1,ij))

Turn 4 statements into 1 vector shortloop

ev(1:4)=ev(1:4)+wp0*wt00*(wz0*tempphi(1:4,0,ij)+wz1*tempphi(1:4,1,ij))

- Second loop is large, computationally intensive, but contains strided loads and computed gather
 - CCE automatically vectorizes loop

Case Study: GTC





Case Study: GTC



GTC performance 3200 MPI ranks and 4 OMP threads





- Overflow is a NASA developed Navier-Stokes flow solver for unstructured grids
- Subroutines consist of two or three simply-nested loops
- Inner loops tend to be highly vectorized and have 20-50 Fortran statements
- MPI is used for parallel processing
 - Solver automatically splits grid blocks for load balancing
 - Scaling is limited due to load balancing at > 1024
- Code is threaded at a high-level via OpenMP

Overflow Scaling using only MPI vs MPI & OMP





- Materials Science code
- Scales to 1000s of MPI ranks before it runs out of parallelism
- Want to use shared memory parallelism across entire node
- Main kernel consists of 4 independent zgemms
- Want to use multi-level OMP to scale across the node



```
!$omp parallel do ...
do i=1,4
```

```
call complex_matmul(...)
```

enddo

```
Subroutine complex_matmul(...)
```

enddo



ZGEMM 1000x1000



Parallel method and Nthreads at each level

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Case Study: PARQUET



ZGEMM 100x100



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Conclusions

- The Cray Compiling Environment is a new, different, and interesting compiler with several unique capabilities
- Several codes are already taking advantage of CCE
- Development is ongoing
- Consider trying CCE if you think you could take advantage of its capabilities

