Making Effective Use of Compilers at NERSC

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Introduction

- Description of the Hopper compiling environment.
- Strengths and weaknesses of each compiler.
- Advice on choosing the most appropriate compiler for your work.
- Comparative results on benchmarks and other codes.
- How to use the compilers effectively.
- Carver compiling environment.
- Plans for the new Cray Cascade system (NERSC 7) compiling environment.
- Your feedback.

Why So Many Compilers on Hopper?

- NERSC5 (Cray Franklin XT) was delivered in 2006 with the only commercially available compiler, PGI.
- GNU compilers were on Franklin, but at that time GNU Fortran optimization was poor.
- Next came Pathscale because of superior optimization for Franklin's AMD Opteron processors.
- Cray ported their well optimized compiler to the Opteron so it was added next.
- Intel was popular on Carver, and it produced highly optimized codes on Hopper.
- PGI is still the default, but this is not a NERSC recommendation. Cray's current out of the box compiler is the Cray compiler, but we kept PGI as the default to avoid disruption.

How to Change Compilers on Hopper

- Use the Cray wrappers ftn, cc, and CC to invoke the compiler to get the proper libraries and not the compiler specific invocation, e.g. gcc, pgf90, ifort.
- By default PGI will be used with the wrappers.
- To use other compilers simply swap in the appropriate PrgEnv module:
  - module swap PrgEnv-pgi PrgEnv-cray
  - module swap PrgEnv-pgi PrgEnv-intel
  - module swap PrgEnv-pgi PrgEnv-gnu
- Nothing else needs to be done to use the new compiler to build codes.

PGI

- Strengths
  - Available on a wide variety of platforms making codes very portable.
  - Because of its wide usage, it is likely to compile almost any valid code cleanly.
  - Very well supported. Bugs are fixed relatively quickly and there are frequent bugfix releases.
- Weaknesses
  - Does not optimize as well as compilers more narrowly targeted to AMD architectures.
- Optimization recommendation:
  - -fast
  - Default optimization level: -O1

Cray

- Strengths
  - Fortran is well optimized for the Hopper architecture.
  - Uses Cray math libraries for optimization.
  - Well supported.
  - Very good at standards compliance and adoption.
- Weaknesses
  - Compilations can take much longer than with other compilers and create much larger executables.
  - Not very comfortable with C++ codes.
  - Very picky about standard compliance.
- Optimization recommendations:
  - Compile with no explicit optimization arguments. The default level of optimization is very high.

Intel

- Strengths
  - Optimizes C and Fortran codes very well.
  - Supports C++ very well.
- Weaknesses
  - Occasional problems in porting codes to this compiler.
  - -fast optimization level can be problematic.
    - Can take a very long time or fail.
    - Occasionally has produced incorrect results.
- Optimization recommendations:
  - Compile with no explicit optimization arguments. The default level of optimization is very high.

GNU/GCC

- Strengths
  - Available on a wide variety of platforms for free.
  - Exposure to a wide variety of codes, so any given code is likely to compile cleanly.
  - Very good at C++ optimization.
  - Optimizes Fortran codes as well as PGI on the average.
- Weaknesses
  - Not a commercial product, so no guarantee of bug fixes.
  - Does not optimize as well as architecture targeted compilers like Intel and Cray.
- Optimization recommendation:
  - -O3 -ffast-math

Pathscale

- **This compiler is no longer supported by Cray.**
- Contact consultants for assistance in converting to a different compiler (consult@nersc.gov).
- Strengths
  - Good optimization, generally not as good as Intel or Cray.
- Weaknesses
  - Support level and future of the product are questionable.
  - Cray is withdrawing library support for this compiler.
- Optimization recommendation:
  - -O3
  - Default optimization is -O2.

Fortran Standards Compliance

- Fortran 2003 - Object Oriented extensions.
  - Cray and Intel almost fully compliant.
  - PGI and GNU mostly compliant.
  - See http://fortranwiki.org/fortran/show/Fortran+2003+status for status.
- Fortran 2008 - Coarray support.
  - No one close to being fully compliant.
  - Cray, Intel, GNU have many features, PGI comparatively few.
  - Status at http://fortranwiki.org/fortran/show/Fortran+2008+status.

Which Compiler to Use?

- Porting a code to Hopper.
  - Use the existing compiler if it is on Hopper, since relatively minor changes should be necessary to the Makefile or configure script.
- Developing a code on Hopper.
  - For C++ use Intel or GNU.
  - Targeted for Cray systems? The Cray Fortran and Intel compilers are likely to produce the fastest code.
  - Will it be ported to other systems? GNU will produce relatively fast code and can be ported more easily to other architectures.

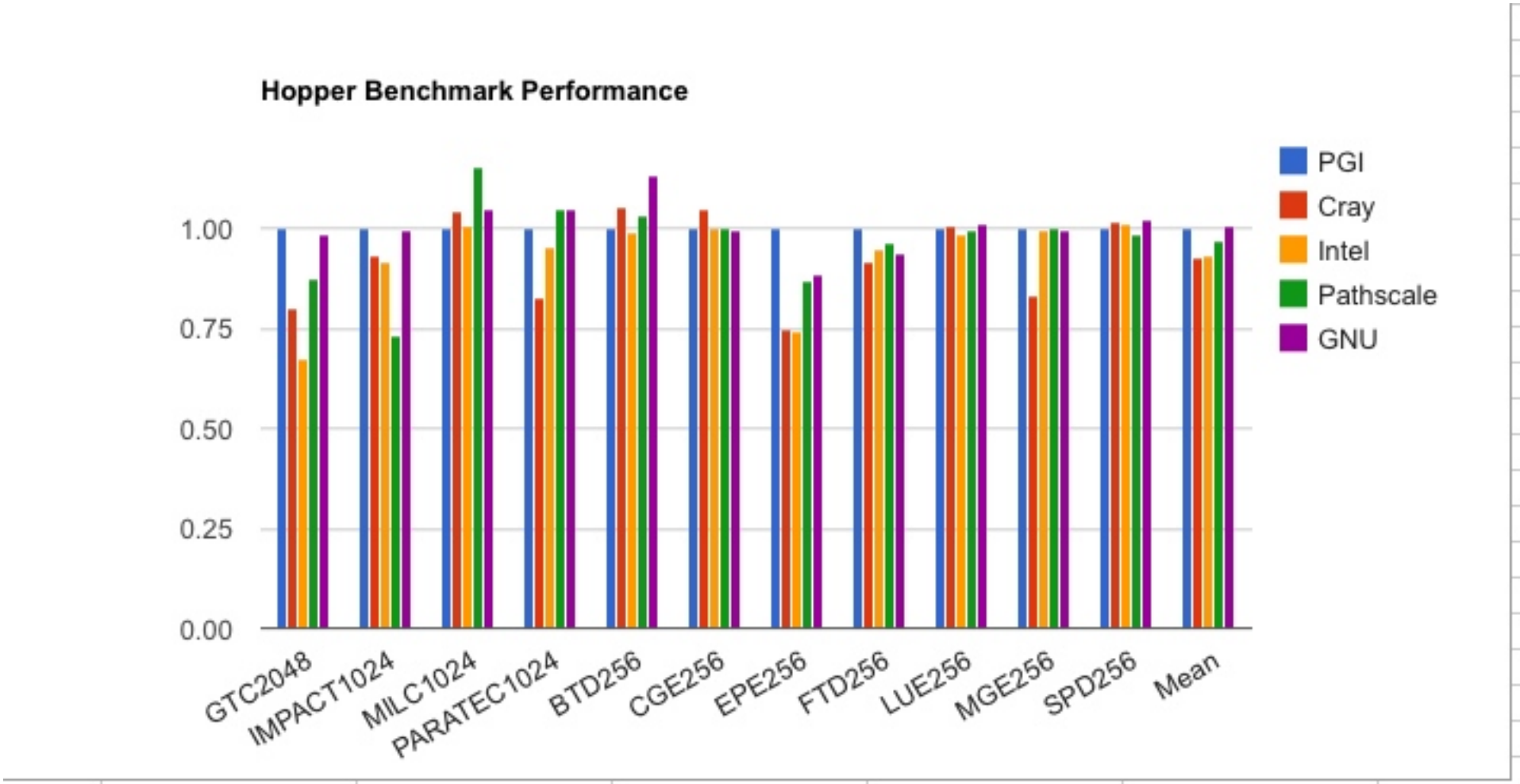
NERSC 6/7 Benchmarks

Benchmark	Science Area	Algorithm	Concurrency (Scaling)	Language
GTC	Fusion	PIC, Finite Difference	2048 (weak)	f90
IMPACT-T	Accelerator Physics	PIC, FFT	1024 (strong)	f90
MILC	Lattice Gauge Physics	Conjugate Gradient, FFT, Sparse Matrix	1024 (weak)	c, assembly
PARATEC	Material Science	DFT, FFT, BLAS	1024 (strong)	f90

3.3 NAS Parallel Benchmarks

Benchmark	Full Name	Description
BT	Block Tridiagonal	Solve a synthetic system of nonlinear PDEs using a block tridiagonal algorithm
CG	Conjugate Gradient	Estimate the smallest eigenvalue of a large sparse symmetric positive-definite matrix using the inverse iteration with the conjugate gradient method as a subroutine for solving systems of linear equation
EP	Embarassingly Parallel	Generate independent Gaussian random variates using the Marsaglia polar method
FT	Fast Fourier Transform	Solve a three-dimensional PDE using FFT
LU	Lower-Upper Symmetric Gauss-Seidel	Solve a synthetic system of nonlinear PDEs using a symmetric successive over-relaxation algorithm
MG	MultiGrid	Approximate the solution to a three-dimensional discrete Poisson equation using the V-cycle multigrid method
SP	Scalar Pentadiagonal	Solve a synthetic system of nonlinear PDEs using a scalar pentadiagonal algorithm

Hopper Benchmark Performance Normalized to PGI Performance



Wall clock time ratio, lower is better.

Compiling USG Supported Applications

- VASP - performs *ab initio* quantum-mechanical molecular dynamics (MD) using pseudopotentials and a plane wave basis set. (f90)
- QE (QuantumEspresso) - an integrated suite of computer codes for electronic structure calculations and materials modeling at the nanoscale. (f90)
- NAMD - a molecular dynamics (MD) program designed for parallel computation. (C/C++)
- LAMMPS - a large scale classical molecular dynamics code. (C++)
- BerkeleyGW - calculates the quasiparticle properties and the optical responses of a large variety of materials. (f90)
- NWChem- a computational chemistry package. (f90)

Building and Running NERSC Applications

Percent Performance Decrease/Improvement over PGI

Program	Intel	GNU	Cray	Best Compiler
VASP	12% to 5%	6% to 4%	0% to 11%	Cray
QE	2%	1%	7%	Intel
NAMD	14%	18%	Failed	GNU
LAMMPS	5% to 17%	5% to 9%	6% to 4%	Intel
BerkeleyGW	0%	13%	8%	PGI/Intel
NWChem	12% to 34%	9% to 28%	Failed	Intel

Provided by Zhengji Zhao, Megan Bowling and Jack Deslippe from CUG 2012

C++ Benchmarks from http://stlab.adobe.com/performance/

Set of benchmarks to test how well a compiler optimizes C++ operations and language features. Not a test of floating point performance.

stepanov_abstraction	Sorting and summing values wrapped in curly braces.
stepanov_vector	Replacing pointers with vector iterators and using reverse iterators.
functionobjects	Instantiation of simple functors and the relative performance of function pointers, functors and inline operators.
simple_types_constant_folding	Folding constant math expressions on simple data types.
simple_types_loop_invariant	Moving loop invariant calculations out of the loop.
loop_unroll	Unrolling loops to hide instruction latency.

C++ Benchmark Performance

Benchmark	PGI	Cray	Intel	GNU
stepanov_abstraction	300.88	169.78	39.37	50.11
stepanov_vector	Did not compile.	233.44	67.99	84.97
functionobjects	36.93	38.44	31.15	31.11
simple_types_constant_folding	1413.96	7856.88	1571.74	509.68
simple_types_loop_invariant	1041.58	2366.86	863.62	889.20
loop_unroll	5014.56	1323.57	363.53	866.86

Times are in seconds, lower is better.

Compiling for OpenMP on Hopper

- Cray compiler: -Oomp (on by default)
- PGI: -mp=nonuma
- Intel: -openmp
- GNU: -fopenmp
- Pathscale: -mp

Running with OpenMP on Hopper

- Run time all compilers:
  - - set OMP_NUM_THREADS to number of threads
  - aprun -d numthreads ...
- Pathscale run time - set PSC_OMP_AFFINITY to FALSE.
- Intel run time - use "-cc none" or "-cc numa_node" arguments to aprun.

OpenMP/Hybrid Run Time Optimization

- Each 24 core Hopper compute node consists of 4 6 core "numa nodes".
- Best hybrid code performance when you allocate 1 MPI process with 6 threads to each of these numa nodes and use their local memory.
- Single node parameters:
  - export OMP_NUM_THREADS=6
  - aprun -d 6 -N 4 -S 1 -ss .....
- For more details see https://www.nersc.gov/users/computational-systems/hopper/performance-and-optimization/using-openmp-effectively-on-hopper/

OpenACC Support on Hopper

- OpenACC - A standard is designed to simplify parallel programming of heterogeneous CPU/GPU systems.
- Accomplished with #pragma's and compiler directives in the source code like OpenMP.
- Currently supported by the Cray compiler.
- Coming in verson 12.6 of the pgi compiler.

PGAS Support on Hopper

- PGAS (Partitioned Global Address Space) - allows the programmer to view a single shared partitioned address space where each variable is associated with a single processor, but can be directly read and written by any processor.
  - UPC - Unified Parallel C.
  - CAF - Coarray Fortran.
- Available with Cray, Berkeley UPC, and Intel Compilers.
- See https://www.nersc.gov/users/training/online-tutorials/introduction-to-pgas-languages/#toc-anchor-2

Carver Compiler Environment

- Default compiler is PGI for Franklin/Hopper consistency, not as a NERSC recommendation.
- Intel compiler is available as a module, and generally produces much faster code than PGI.
- GNU compiler has comparable performance to PGI.
- Optimization recommendations are the same as on Hopper:
  - Intel: default, no optimization arguments.
  - PGI: -fast
  - GNU: -O3 -ffast-math

NERSC7 Compiler Environment

- NERSC7 will be a Cray Cascade Intel Xeon based system.
- http://www.nersc.gov/news-publications/news/nersc-center-news/2012/nersc-signs-supercomputing-agreement-with-cray/
- Default compiler will be Intel.
- The Cray and GNU compilers will be available as modules.
- There are no plans to have PGI or Pathscale on the system.
- NERSC will do extensive performance analysis on benchmarks before the system becomes available to users.

Questions and Comments