Single Node Optimization on Hopper

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Introduction

- Why are there so many compilers available on Hopper?
- Strengths and weaknesses of each compiler.
- Advice on choosing the most appropriate compiler for your work.
- Comparative benchmark results.
- How to compile and run with OpenMP for each compiler.
- Recommendations for running hybrid MPI/OpenMP codes on a node.

Why So Many Compilers on Hopper?

- Franklin was delivered with the only commercially available compiler for Cray Opteron systems, PGI.
- GNU compilers were on Franklin, but at that time GNU Fortran optimization was poor.
- Next came Pathscale because of superior optimization.
- Cray was finally legally allowed to port their 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 default is the Cray compiler, but we kept PGI to avoid disruption.

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.
- Weaknesses
  - Does not optimize as well as compilers more narrowly targeted to AMD architectures.
- Optimization recommendation:
  - -fast

Cray

- Strengths
  - Fortran is well optimized for the Hopper architecture.
  - Uses Cray math libraries for optimization.
  - Well supported.
- Weaknesses
  - Compilations can take much longer than with other compilers.
  - Not very good optimization of C++ codes.
- 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.
- 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.
- Optimization recommendation:
  - -O3 -ffast-math

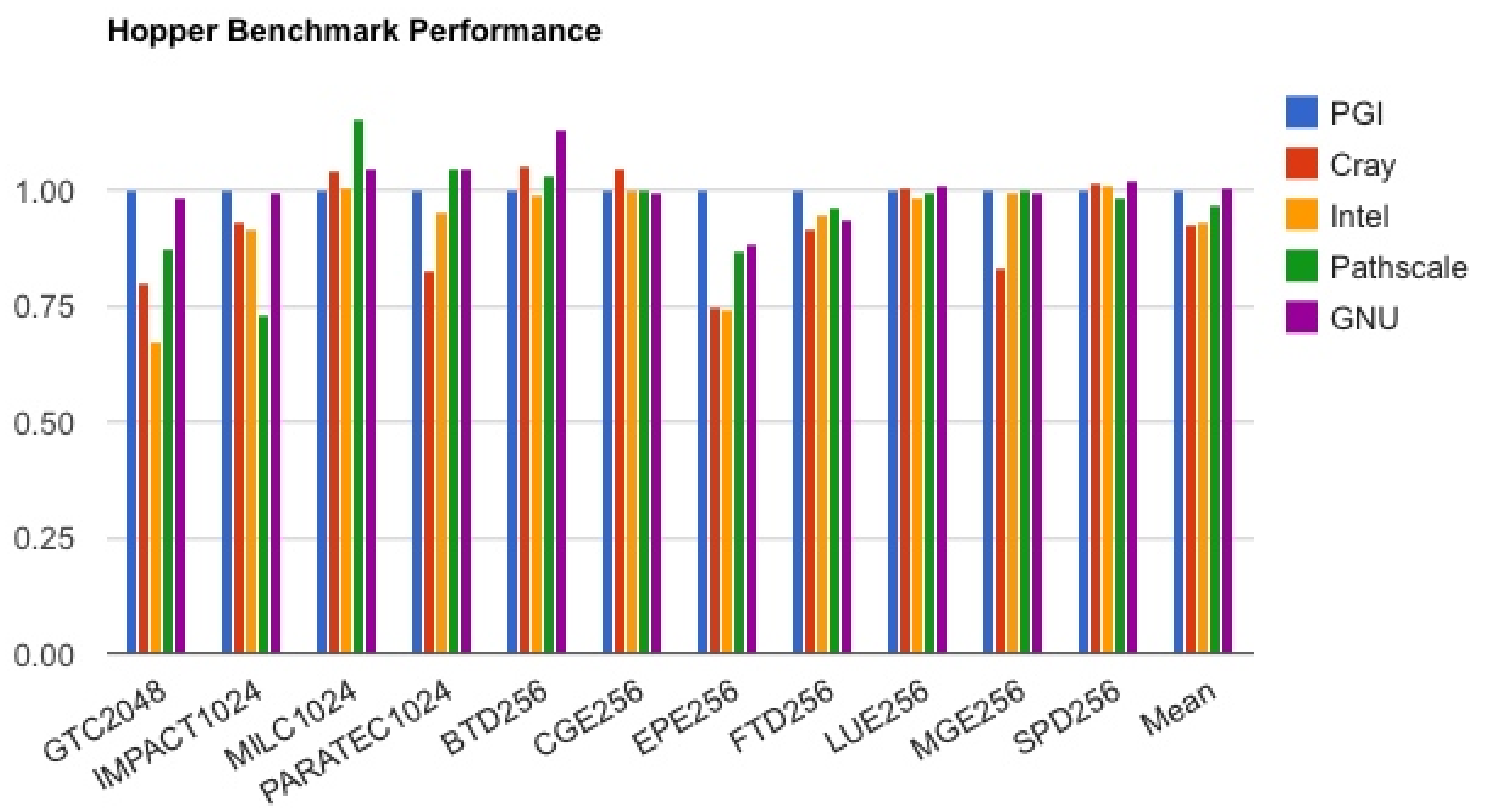
Pathscale

- Strengths
  - Good optimization.
- Weaknesses
  - Support level and future of the product are questionable.
  - Cray is withdrawing library support for this compiler.
- Optimization recommendation:
  - -O3

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.
  - Will it only run on Hopper? The Cray Fortran and Intel compilers are likely to produce the fastest code.
  - Will it be ported to other systems? GNU and PGI will produce relatively fast code and can be ported more easily to other architectures.

Hopper Benchmark Performance



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 nodes and use their local memory
- Single node parameters:
  - export OMP_NUM_THREADS=6
  - aprun -d 6 -N 4 -S 1 -ss ....

Questions?