Characterizing Compiler Performance for the AMD Opteron Processor on a Parallel Platform

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Introduction

• Cray & Sandia National Labs (SNL) have chosen the Portland Group (PGI) C, C++, and Fortran compiler suite as the nominal compilers for SNL’s Red Storm

• This study takes a look at the Pathscale compiler suite by comparing it against the PGI suite on applications of interest to SNL and the ASC program

• There are other excellent Opteron compilers available, but this study is an outcome of a collaboration with Pathscale to help the maturation of their product
  - However, neither company was consulted for tuning advice
  - The companies respective literature and white papers were consulted

• In addition to single processor performance, we looked at scaled (weak-scaling) problem sets and make inferences about the applications ability to hide parallel overheads and hence take advantage of compiler optimizations at scale
Fractional Speedup

• Total fraction of time before optimization is defined as
  \[ F(N) = f_c(N) + f_o(N) = 1 \]
  – where \( f_c \) is computational fraction and \( f_o \) is the fraction of overhead

• Total fraction of time after optimization is defined as
  \[ F_s(N) = f_c(N) \times f_s(N) + f_o(N) < 1 \]
  – Where \( f_s \) is the fractional speedup

• \( F_s \) is measured by the application and is defined as
  \[ F_s(N) = \frac{\text{time for faster runtime}}{\text{time for slower runtime}} \]

• And percent speedup is defined as
  \[ \text{Speedup (\%)} = \left( \frac{1}{F_s(N)} - 1 \right) \times 100 \]
Environment

• PGI Compiler Suite Version 6.0
  – -fastsse
    • -fast -Mvect=sse -Mscalarsse -Mcache_align -Mflushz
    • -fast -> -O2 -Munroll=c:1 -Mnoframe -Mlre

• Pathscale Compiler Suite Version 2.1
  – -O3 -OPT:Ofast
    • -OPT:Ofast -> -OPT:ro=2:Olimit=0:div_split=ON:alias=typed -msse2

• Red Squall Cluster
  – Dual-Processor 2.0 Ghz Opterons
  – 333 Mhz DDR DRAM
  – Quadrics QsNetII High-Speed Interconnect
  – MPICH 1.2.4 w/Quadrics extensions
  – SuSE Linux Professional 9.0 on all nodes
Applications

- **CTH**
  - Multi-material, large deformation, strong shock wave, solid mechanics code
  - Fortran 77
  - Chosen for its extensive use at SNL and its characteristic 3-D Mesh message passing traits

- **LAMMPS**
  - (Large-scale Atomic/Molecular Massively Parallel Simulator) is a classical molecular dynamics code designed for simulating molecular and atomic systems on parallel computers using spatial-decomposition techniques
  - Fortran 90
  - FFTW is implemented in C
  - Chosen for its extensive use at SNL and well characterized behavior

- **PARTISN**
  - LANL Developed Code
  - Neutron transport solutions on orthogonal meshes with adaptive mesh refinement (AMR) in one, two, and three dimensions
  - Chosen for its irregular memory transfer characteristics
• Shape Charge problem set derived from a real calculation.
• Reports “grind time”, which halves as the problem doubles in size.
• Unable to use -O3 on Pathscale compiler, so -O2 -OPT:Ofast was used.
• Relatively constant advantage for the PGI compiler as the problem scales. Indicates that $f_c$ and $f_o$ remain constant with scale.
• This implies that the parallel inefficiency is due to algorithmic issues and that the total time for computation and overhead increases as the problem scales.
LAMMPS

- Indifferent as to which compiler to use
- Unable to characterize applications ability to take advantage of compiler optimizations

![Lammps Stouch Study](image)
PARTISN

• Three metrics measured
  – Transport Grind Time
  – Diffusion Grind Time
  – Solver Iteration Time
• Single node anomaly for Pathscale result
• Pathscale advantage from 2 to 128 nodes
  – Overhead ~ constant as scale increases
• Solver Iteration result at 128 nodes may be due to the Red Squall network architecture
Different Optimization Settings for PARTISN on a Single Node

PGI
- -fastsse
- -fastsse -Mnontemporal
- -fast -Mcache_align
- -O3 -Munroll=c:1 -Mnoframe -Mlre -Mcache_align (-fast w/03 and -Mcache_align)

Pathscale
- -O3 -OPT:Ofast
- -O3 -msse2
- -O2
PARTISN Continued

- Used -O2 with Pathscale
- Left PGI at -fastsse
- Improved Pathscale single node performance
- However, overall Pathscale performance advantage reduced
- Performance dependent on scale – 8, 32 and 128 node anomalies (?)
Summary and Conclusions

- The PGI Compiler provided the best results for CTH.
- The Pathscale Compiler provided the best results for PARTISN.
- LAMMPS was indifferent.
- Each ended the season with a record of 1-1-1.
- Both compilers can be tweaked with numerous switches and it is most likely possible that excellent run time results can be obtained with either compiler.
- However, it seems beneficial to the application developer to have multiple compilers to choose from, as one may provide a more optimal result for a given application without significant “fishing” for the right options.
- Compilers can be a significant monetary investment, but after taking into account increased efficiency of the platforms resources over an extended period of time, it may be worth it.
Questions?