ANALYSIS OF BLIS MULTITHREADED GEMM AND HPC WORKLOADS

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AMD

AGENDA

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◢ BLIS DGEMM Multi-threaded performance analysis on the AMD EPYC^{TM} processor
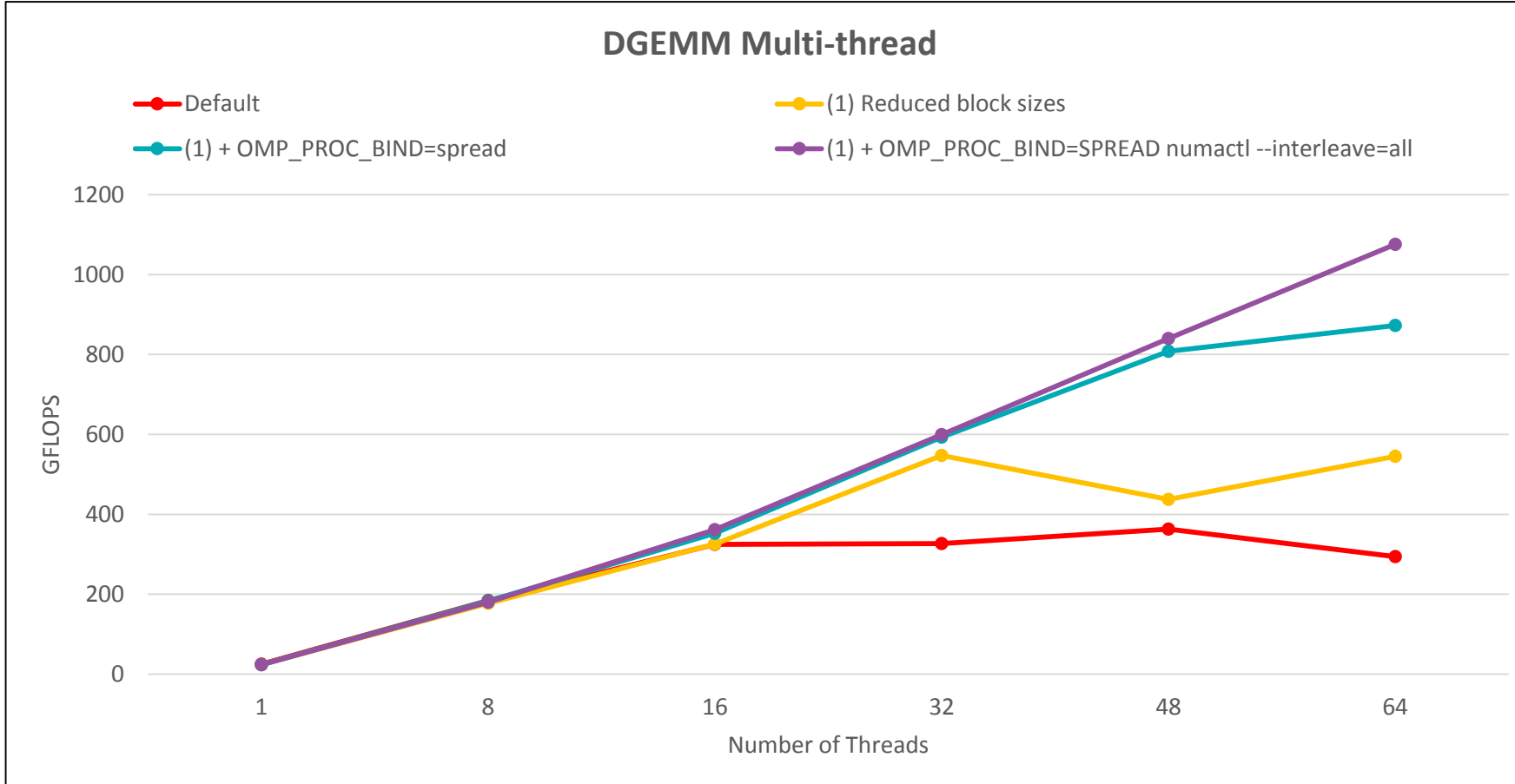
◢ BLIS overheads in HPC workloads

◢ Q & A

BLIS DGEMM Multi-threaded performance on the AMD EPYC™ processor

TUNING PARALLEL DGEMM PERFORMANCE

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MATRIX SIZE-5000X5000

DGEMM Multi-thread

Legend:
- Default
- (1) Reduced block sizes
- (1) + OMP_PROC_BIND=spread
- (1) + OMP_PROC_BIND=SPREAD numactl --interleave=all

Y-axis: GFLOPS (0, 200, 400, 600, 800, 1000, 1200)
X-axis: Number of Threads (1, 8, 16, 32, 48, 64)

1. **Reduce block sizes**
    - Each thread works on smaller blocks
2. **OpenMP settings**
    - OMP_PLACES = cores
    - OMP_PROC_BIND=spread
3. **numactl**
    - interleave

PARALLEL DGEMM PERFORMANCE

◢ Issue

– Memory contention increases as the number of threads increase

◢ Tuning strategy

– Reduce the block sizes

- Each thread works on smaller blocks of data

- Improved per thread cache

– Higher available bandwidth per thread achieved by dividing the threads over two sockets using

OMP_PROC_BIND=spread

– Distribute the memory across all the nodes

– Reduced CPU stalls

BLIS overheads in HPC workloads

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HPC WORKLOADS

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CP2K

- Package to perform atomistic simulations of solid state, liquid, molecular, and biological systems

GROMACS

- Molecular dynamics package mainly designed for simulations of proteins, lipids, and nucleic acids

ScaLAPACK

- Library of high-performance linear algebra routines for parallel distributed memory machines

BLIS OVERHEADS IN HPC WORKLOADS

CP2K – 26%

- Input : 128 H_2O atoms
- DGEMM (6%), packing 5.7%
- Small matrix sizes: 1 x 1, 5 x 3, 7 x 1….128 x 1152
- HERK, TRMM, TRSM – invoked but negligible

GROMACS - 63%

- Test : Covariance Analysis, size 1167x1167
- DGEMM (29%), Dotxf, Saxpyf

ScaLAPACK – 49%

- Test : xzpbllt - Symmetric or Hermitian positive definite band matrix solve
- CGEMM, DGEMM, AXPY, ZAMAX
- Small matrix sizes : 1 x 1, 2 x 2, ….1023 x 1023

BLIS IN HPC WORKLOADS

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◢ BLAS functionalities have considerable overhead in most HPC workloads

◢ Operations on small matrices dominate in many such applications such as CP2K and GROMACS

◢ There is scope to optimize the smaller matrices operations further

REFERENCES & SOURCE CODE

- https://www.amd.com/en/products/epyc-server

- http://developer.amd.com/amd-cpu-libraries/

- https://github.com/amd/blis

- https://www.cp2k.org/

- http://www.gromacs.org/

- http://www.netlib.org/scalapack/

Questions

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DISCLAIMER & ATTRIBUTION

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END NOTE

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◢ Slide 4

– DGEMM performance for 5000 x 5000 matrices using AMD optimized BLIS. Testing were conducted as of 5th September 2018 on the test system comprising AMD EPYC^{TM}, 64 cores clocked at 2.5 GHz. The machine had DDR4 RAM of 256 GB, clocked at 1.2 GHz and 1 TB of Hard disk. The test system had Ubuntu operating system installed. PC manufacturers may vary configurations yielding different results

◢ Slide 8

– Testing were conducted as of 27th August 2018 on the test system comprising AMD EPYC^{TM}, 64 cores clocked at 2.5 GHz. The machine had DDR4 RAM of 256 GB, clocked at 1.2 GHz and 1 TB of Hard disk. The test system had Ubuntu operating system installed. PC manufacturers may vary configurations yielding different results