STORAGE AND MEMORY HIERARCHY IN HPC: NEW PARADIGM AND NEW SOLUTIONS WITH INTEL

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WE ARE IN A DATA-CENTRIC WORLD
TODAY ALL DATA MUST BE STORED, PROCESSED, ANALYZED & MONETIZED

DATA IS STORED BY DIFFERENT TIERS

- **HOT DATA**
  - Higher Cost
  - Lower Delay

- **WARM DATA**
  - Lower Cost
  - Higher Delay

- **COLD DATA**
  - Lower Cost
  - Lower Delay
STORAGE TRENDS

TREND 1
EVOlUTION OF NAND

“BULK STORAGE”
LOWER COST & HIGHER DENSITY

TREND 2
NEW NON-NAND MEDIA

“WORKING STORAGE”
HIGHER PERFORMANCE

Trend 1: Evolution of NAND
- Higher Performance

Trend 2: New Non-NAND Media
- Lower cost & higher density

“Bulk Storage”
- Lower cost & higher density

“Working Storage”
- Higher performance

Diagram showing the evolution of NAND technology and the introduction of new non-NAND media, highlighting trends in cost and delay.
HIGH CAPACITY TRADEOFFS
COST AND DENSITY FOR ENDURANCE AND PERFORMANCE

TREND 1
EVOLUTION OF NAND

"BULK STORAGE"
LOWER COST & HIGHER DENSITY

7.5X DENSER FROM 2D MLC - 3D TLC GEN 2
2.5X
1.5X
2X

2D MLC
3D MLC
3D TLC
3D TLC Gen 2

“Bulk Storage”
Lower cost & higher density

Source: Intel internal analysis of areal density of die sizes measured at Gb/mm2
OEM PLATFORM INNOVATION
ENTERPRISE DATACENTER SSD FORM FACTORS (EDSFF)

1PB IN 42U
WITH 2 TB HDDs

1PB IN 1U
WITH INTEL® 3D NAND SSDs
INTEL® OPTANE™ TECHNOLOGY

PERFORMANCE AND ENDURANCE FOR DENSITY AND COST/GB

ENDURANCE

QoS

THROUGHPUT (IOPS)

LATENCY

TREND 2
NEW NON-NAND MEDIA

“WORKING STORAGE”
HIGHER PERFORMANCE & ENDURANCE
World's Most Responsive Data Center SSD

Delivering an industry leading combination of low latency, high endurance, QoS and high throughput, the Intel® Optane™ SSD is the first solution to combine the attributes of memory and storage. This innovative solution is optimized to break through storage bottlenecks by providing a new data tier. It accelerates applications for fast caching and storage, increasing scale per server and reducing transaction cost. Data centers based on the latest Intel® Xeon® processors can now also deploy bigger and more affordable datasets to gain new insights from larger memory pools.

1. Responsiveness defined as average read latency measured at queue depth 1 during 4k random write workload. Measured using FIO 2.15. Common configuration - Intel 2U PCSD Server ("Wildcat Pass"), OS CentOS 7.2, kernel 3.10.0-327.el7.x86_64, CPU 2 x Intel® Xeon® E5-2699 v4 @ 2.20GHz (22 cores), RAM 396GB DDR @ 2133MHz. Intel drives evaluated - Intel® Optane™ SSD DC P4800X 375GB, Intel® SSD DC P3700 1600GB, Intel® SSD DC P4600 1600GB. Samsung drives evaluated – Samsung® SSD PM1725a, Samsung® SSD PM1725, Samsung® PM963, Samsung® PM953. Micron drive evaluated – Micron® 9100 PCIe® NVMe™ SSD. Toshiba drives evaluated – Toshiba® ZD6300. Test – QD1 Random Read 4K latency, QD1 Random RW 4K 70% Read latency, QD1 Random Write 4K latency using fio-2.15.
Predictably Fast Service

1. Common Configuration - Intel 2U PCSD Server ("Wildcat Pass"), OS CentOS 7.2, kernel 3.10.0-327.el7.x86_64, CPU 2 x Intel® Xeon® E5-2699 v4 @ 2.20GHz (22 cores), RAM 396GB DDR @ 2133MHz.

Optane Configuration – Intel® Optane™ SSD DC P4800X 375GB.

NAND Configuration – Intel® SSD DC P3700 1600GB.

QoS – measures 99% QoS under 4K 70-30 workload at QD1 using fio-2.15.
Intel® Optane™ SSD Use Cases

**Fast Storage and Cache**
- Intel® Xeon®
- DRAM
- PCIe*
- Intel® Optane™ SSD
- Intel® 3D NAND SSDs

**Extend Memory**
- Intel® Xeon®
- DDR
- PCIe
- DRAM 'memory pool'
- Intel® Optane™ SSD
- Intel® 3D NAND SSDs

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INTRODUCING INTEL® MEMORY DRIVE TECHNOLOGY

• Use Intel® Optane™ SSD DC P4800X transparently as memory

• Grow beyond system DRAM capacity, or replace high-capacity DIMMs for lower-cost alternative, with similar performance

• Leverage storage-class memory today!
  • No change to software stack: unmodified Linux* OS, applications, and programming
  • No change to hardware: runs bare-metal, loaded before OS from BIOS or UEFI

• Aggregated single volatile memory pool

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Segmented GEMM benchmark

**All DRAM**

- Original DGEMM application
  - 2,322 GFLOPS

- Optimized application
  - 2,786 GFLOPS

**DRAM + Intel® Optane™ SSD + Intel® Memory Drive Technology**

- 2,605 GFLOPS

- up to 1.1x faster matrix multiplication with optimized data locality with no changes\(^1\) in the application

- up to 0.9x near DRAM performance of the optimized application

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1. Optane + IMDT configuration – 2 x Intel® Xeon® CPU E5-2699 v4 @ 2.20GHz, Intel® Server Board S2600WT, 128GB DDR4 + 4* Intel® SSD Optane® (SSDPED1K375GA), CentOS 7.3.1611. All DRAM configuration – 2 x Intel® Xeon® CPU E5-2699 v4 @ 2.20Ghz, Intel® Server Board S2600WT, 768GB DDR4 CentOS 7.3.1611. Test – GEMM(MKL), segment size 18689, factor 22, threads 42, dataset consumed ~650GB.
LU decomposition

- Factorization of matrix $A$ into product of lower triangular ($L$) and upper triangular ($U$) matrices

- A commonly used kernel in many scientific codes:
  - Solving systems of linear equations
  - Matrix inversion
  - Computing determinants

- A kernel in LINPACK benchmark

\[ A = L \times U \]
LU decomposition

Performance results

- DDR maximum performance: 850 GFLOPs/s
- Intel® memory drive technology max performance: 1,250 GFLOPs/s
- A huge performance degradation beyond 150% RAM utilization

Can we improve these results?
LU decomposition

- Memory access pattern is by column blocks
- Nearby elements are scattered throughout different memory pages
  - 4KB page = 512 double precision numbers
  - A huge data traffic for large matrices ($2 \cdot 10^5$ and above)
- There are tiled LU algorithms (e.g. PLASMA)
LU decomposition

- Memory access pattern is by column blocks
- Nearby elements are scattered throughout different memory pages
  - 4KB page = 512 double precision numbers
  - A huge data traffic for large matrices ($2 \cdot 10^5$ and above)
- There are tiled LU algorithms (e.g. PLASMA)
- We used a simple implementation from *hetero-streams* code base
- Little performance degradation beyond 100% RAM usage
Fast Fourier transformation

- A common used kernel in physics and material science
- Compute bound, but AI grows very slow with problem size
- $O(N \log N)$ time complexity
- “Butterfly” memory access pattern – complex but predictable
Fast Fourier transformation

- Intel® Math Kernel Library DFT kernel
- 3D FFT benchmark, $N \times N \times N$ grid
- Results:
  - 80-130% of DDR performance up to 200% of DDR utilization
  - 40% efficiency over 250% DDR utilization
- 3D FFT can be optimized for NUMA and MDT in a similar way to the LU decomposition
  - by dividing the total memory worked on by all threads at a given time
Lessons learned from benchmarks with Intel® memory drive technology

- Data moving between Intel® Optane™ SSDs and RAM is very expensive (10 GB/s max):
  - Reuse data as much as possible
    - Arithmetic intensity on DRAM↔MDT level should be ≥500 FLOPs/byte
  - Redesign data structures in your program for locality
  - Work with large data chunks
  - Think about DRAM as a large L4 cache for MDT

- Same optimization principles as on NUMA architectures

- Data-oriented programming is a must
  - It also favors modern hardware architectures
Scientific applications

Computational chemistry:
- LAMMPS* (molecular dynamics)
- GAMESS (two-electron integral kernel)

Astrophysics:
- AstroPhi* (hyperbolic partial differential equation solver)

Sparse linear algebra problems:
- Intel® Math Kernel Library PARDISO

Quantum computing simulator:
- Intel-QS, formerly known as qHipster
Popular molecular dynamics package

- Mostly used in material science
- Force-field based molecular dynamics
  - Partitions the simulation domain (spatial-decomposition) into small 3d sub-domains, each assigned to a CPU
  - Processors communicate and store *ghost* atom information for atoms that border their subdomain

Scaled Rhodopsin benchmark:

- Hundreds of millions atoms
- Major bottleneck is calculation of electrostatic interaction between atoms
- Reasonable efficiency up to 150% RAM
  - 50% efficiency for high memory consumption
FUTURE POSSIBILITIES
The SNIA NVM Programming Model
The Persistent Memory Development Kit
PMDK http://pmem.io

- PMDK is a collection of libraries
  - Developers pull only what they need
    - Low level programming support
    - Transaction APIs
  - Fully validated
  - Performance tuned.
- Open Source & Product neutral
Intel Persistent Memory

New Type of Memory

• Persistent, Large Capacity & Byte Addressable
  • 6 TB per two-socket system

• DDR4 Socket Compatible
  • Can Co-exist with Conventional DDR4 DRAM DIMMs

• Cheaper than DRAM

• Availability
  • Next Xeon Scalable Platform
NEW STORAGE / MEMORY SOLUTIONS FROM INTEL

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HIGHER PERFORMANCE
THANK YOU
AstroPhi

- The hyperbolic PDE engine
- Numerical 3D finite difference kernel
- Code is not currently optimized, opportunities for MDT optimization have been identified

Lagrange stage efficiency

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PARDISO

- Intel® Math Kernel Library PARDISO – Parallel Direct Sparse Solver
- Solves huge linear algebra problems: hundreds of millions variables
- Test cases:
  - Cholesky factorization of square $N \times N$ matrices
  - Matrix dimensions:
    - $N = 10 \cdot 10^7$, $20 \cdot 10^7$, $25 \cdot 10^7$
  - Number of nonzero elements: $O(N)$
Intel QS

- Quantum computing simulation
  - Application requires more memory as more qubits are simulated
  - Without MDT, scaling beyond a node's capability requires MPI on a cluster

- Test cases:
  - Quantum Fourier transform
  - $N_{qubits} = 30 - 35$

- Good performance up to $4 \times$ RAM utilization
  - 35 qubits would require > 1.5TB
  - with MDT a single node can run 35 qubits – enabling the move to HPC/HTC Cloud, instead of HPC cluster with MPI
Two-electron integrals:

- An important kernel in quantum chemistry
- Used in many quantum chemistry methods
- Different types of two-electron integrals have different efficiency on MDT
- Benchmark details:
  - Rys quadrature ERI kernel from GAMESS
  - Compute and store ERIs to memory

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