ABSTRACT
Design for manufacturing (DFM) processes are critical aspects that govern the deployment of solutions in all market segments today. Vendors typically use early simulation models that they can feed their design parameters into and obtain outcomes for defects and corner conditions of usage. This data helps to understand the probabilities of different outcomes in a process and to understand the impact of risk and the uncertainty in prediction. High Performance Computing (HPC) has provided solutions in this area by providing tools that greatly aid in getting the necessary data.

In this white paper, we present why the Marvell® ThunderX2® Arm®-based server processor provides significant value for end users deploying applications in the areas of manufacturing and improvement in overall process yield.

Marvell ThunderX2 – Designed for High-Performance Computing
Before we dig deeper into the ThunderX2 architecture, it is important to understand a typical way of categorizing high-performance computing (HPC) deployments. High-performance computing is broadly divided into two categories. Capability computing refers to using a large-scale HPC installation to solve a single problem in the shortest possible time, for example simulating weather models on a Tier-0 HPC system. Capacity computing refers to optimizing system efficiency to solve as many mid-size or smaller problems as possible at the same time at the lowest possible cost, for example automobile manufacturers using rented (on-demand) HPC resources to simulate numerous drive models for their products.

It is clear from the definitions above that an HPC customer must incorporate components of cost/CPU, # of CPUs and performance (execution time)/CPU. Thus, the cost of an HPC application can be summarized as

\[
\text{cost} \propto \text{CPU hours}
\]

where \(\text{CPU hours} = \#\text{cores} \times \text{execution time}\)

The other important factor driving design decisions of an HPC system is the application suite running on a cluster. Although capability computing targets application runs with the lowest execution time, excessive application scaling may deliver diminishing returns in performance improvement while linearly increasing CPU-hours. This is an unacceptable scenario that leads to inefficient resource utilization. Similarly, although capacity computing targets low-cost HPC
computation, excessive slowdown of application runs may have unacceptable impact, e.g., reduction in productivity of engineers waiting for simulation results.

The reality is not all applications are created equal. Some applications scale well, and some don’t. In the field of manufacturing, QMCPACK and RMG are examples of applications with good scalability and provide a good correlation to a real-life workload. Such application variability necessitates making thorough choices in HPC system design components including the processor. The ThunderX2 architecture has been built ground-up to strike the right balance between efficiency and throughput and thus provide best in class efficiency per $ and throughput per $, making it an easy choice for HPC system architects designing next-generation clusters.

**Marvell ThunderX2 Overview**

ThunderX2 is Marvell’s second generation of Arm-based server processors targeted for the HPC, Cloud/Hyperscale and Enterprise market segments. Based on the 64-bit Armv8-A architecture, the Marvell ThunderX2 processor includes a custom core built using the Arm architectural license. Fully out-of-order, it supports simultaneous multithreading, providing ample compute for data center workloads. In addition, the Marvell ThunderX2 processors support dual socket configurations essential for scaling out applications. The processors are manufactured using a power efficient TSMC 16nm process technology and are fully compliant with Arm’s Server Base System Architecture (SBSA) standard. Key features include:

- ✓ Up to 32 cores with support for simultaneous multithreading
- ✓ DDR4 72-bit memory controllers, supporting up to 2666MT/s DRAM
- ✓ Up to 8 DDR4 memory controllers
- ✓ 56 lanes of PCIe and 14 PCIe controllers
- ✓ 2 x SATA 3.0 & USB3 for boot
- ✓ Server class virtualization & RAS features
- ✓ Extensive power management
- ✓ Socketed LGA or BGA for flexibility
Marvell ThunderX2 HPC-Focused Features

Most CPUs and GPUs have flop/s and integer op/s to fully saturate the memory subsystem, hence memory bandwidth – not floating-point capability - is currently the gating factor for many HPC workloads. With 8 memory channels (as opposed to six for Intel Xeon Skylake), ThunderX2 provides a 33% greater memory bandwidth capability to effectively utilize more cores and achieve a higher per core utilization. The resulting higher operational floating-point efficiency explains why the shorter dual per-core 128-bit vector units on the ThunderX2 cores can compete so effectively against the wider dual per-core Intel Skylake AVX-512 vector units on floating-point performance. ThunderX2 SoCs can deliver over 1 Tflop/s of double-precision and over 2 Tflop/s of single-precision performance in a dual socket configuration.

In summary, Marvell ThunderX2 can deliver competitive or superior performance on parallel and floating-point dominated HPC workloads because it:

1. Has a higher per SoC core count that translates to an overall increase in vector units since each core has two 128-bit vector units.
2. Is a balanced architecture that delivers a higher operational flop/s on real HPC applications because the memory system can better supply data to the Arm cores and dual per-core vector units. This is seen in the benchmark and optimized performance results discussed below.
3. Can better support those HPC applications that benefit from shorter 128-bit vector operations as opposed to longer 512-bit vector operations.
4. Does not underclock. Briefly, the size of the dual per-core vector units on the die means that the Marvell ThunderX2 SoC can preserve floating-point performance when using the per-core vector units rather than underclocking to keep the SoC within thermal design limits.

HPC Synthetic Benchmark Results

Synthetic benchmark results demonstrate the design choices to create a more balanced processor for HPC workloads. Specifically, ThunderX2 matches or exceeds the performance or scaling efficiency of the latest x86 processors on STREAM, HPCG, and HPL synthetic benchmarks.
The HPL benchmark shows the benefit of ThunderX2 processors’ balanced design, including the internal interconnect bus clocked at core clock rate. In contrast, Intel processors adjust their frequency according to workload. While this can provide power efficiency, an independent CERN presentation notes, “Intel processors adjust their frequency according to workload. Highly threaded, vectorized code may run in a lower frequency range. This behavior can confuse scaling studies, and it may reduce the benefit of AVX and AVX-512 vectorization.”

As a more balanced processor, Marvell ThunderX2 can deliver superior performance on many HPC workloads to compete very effectively against the latest AVX-512 powered Intel processors.

**STREAM**

The STREAM benchmark is the industry standard for measuring memory bandwidth. A 1.27x higher STREAM benchmark result (shown in Table 1) demonstrates that a pair of 32-core Marvell ThunderX2 processors can process more data per second compared to a dual-socket Intel Xeon Skylake Gold 6148. Users can verify that the Intel results reported here are consistent with those reported by third-party studies, including Colfax Research.

<table>
<thead>
<tr>
<th>Workload</th>
<th>Marvell ThunderX2</th>
<th>Intel SKL Gold 6148</th>
<th>ThunderX2 Improvement over SKL</th>
</tr>
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<tbody>
<tr>
<td>STREAM</td>
<td>251 GB/s</td>
<td>198 GB/s</td>
<td>1.27</td>
</tr>
</tbody>
</table>

Table 1: STREAM benchmark numbers. (gcc7.2 compiler on ThunderX2, icc18 compiler on SKL)

The consistency of the ThunderX2 memory subsystem performance across all aspects of the STREAM benchmark can be seen in the table below.
Table 2: Complete STREAM benchmark numbers. (gcc7.2 compiler on ThunderX2, icc18 compiler on SKL)

Comparing single and dual socket performance demonstrates the efficacy of the Marvell CCPI2™ interconnect as both single and dual socket configurations deliver high performance. The CCPI2 interconnect provides full cache coherency between the ThunderX2 processors in a dual socket system.

HPCG

The High-Performance Conjugate Gradients (HPCG) benchmark is based on an iterative sparse-matrix conjugate gradient kernel with double-precision floating-point values. HPCG is representative of HPC applications governed by differential equations, which tend to have much stronger needs for high memory bandwidth, low latency, and accessing data using irregular patterns.

The following benchmark results were independently determined by HPE.

Table 3: HPCG benchmark numbers. (gcc7.2 compiler on ThunderX2, icc18 compiler on SKL, results provided by HPE)

The rapid evolution of Arm for HPC applications, and capability of the memory system design can be seen in the HPCG results as ThunderX2 delivers effectively equivalent floating-point performance compared to a latest generation x86 processor that has a significantly higher peak-floating point capability.
The Marvell ThunderX2 processor pair was able to more effectively use all its cores and 128-bit vector units on the HPL benchmark to deliver 92% of its theoretical peak floating-point performance.

The HPL benchmark has low memory bandwidth utilization and is a flop/s dominated synthetic benchmark. Results show a ThunderX2 processor pair was able to more effectively use all its cores and 128-bit vector units to deliver 91.82% of its peak theoretical floating-point performance on HPL without underclocking or dynamic clock scaling. As a result, ThunderX2 was able to deliver 1.077 TF/s of HPL performance on the HPL benchmark.

In contrast, the Intel Xeon Skylake Gold 6148 processor was only able to deliver 72% efficiency using its dual per-core AVX-512 vector units as measured independently by Fujitsu. The Fujitsu results confirm that other processors in the Intel Xeon Scalable Processor family deliver lower HPL efficiency than ThunderX2.

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<th>Workload</th>
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<th>Intel SKL Gold 6148</th>
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<tbody>
<tr>
<td>HPL</td>
<td>91.82% efficiency</td>
<td>72% efficiency</td>
</tr>
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</table>

Table 4: Comparative HPL benchmark results. (gcc7.2 compiler on ThunderX2, icc18 compiler on SKL)

Benefits of Running Manufacturing Applications Workloads on Marvell ThunderX2 Systems

Comparing datasheet specs, ThunderX2 offers higher throughput, capacity and Perf per $ compared to the volume Intel Xeon Skylake SKUs as shown in Figure 2.

Figure 2: comparison of throughput, capacity and performance per $; Marvell ThunderX2 represented in red and Intel Xeon Skylake represented in blue.
However, to prove the value of ThunderX2 in solving real manufacturing applications, we ran representative benchmarks and the results are discussed below.

**QMCPACK**

QMCPACK\(^\text{ix}\) is a modern high-performance open-source Quantum Monte Carlo (QMC) simulation code. Its main applications are electronic structure calculations of molecular, quasi-2D and solid-state systems. Variational Monte Carlo (VMC), diffusion Monte Carlo (DMC) and several other advanced QMC algorithms are implemented. Orbital space auxiliary field QMC (AFQMC) has recently been added. By directly solving the Schrodinger equation, QMC methods offer greater accuracy than methods such as density functional theory, but at a trade-off of much greater computational expense.

QMCPACK is written in C++ and designed with the modularity afforded by object-oriented programming. It makes extensive use of template metaprogramming to achieve high computational efficiency. Due to the modular architecture, the addition of new wavefunctions, algorithms, and observables is relatively straightforward. For parallelization QMCPACK utilizes a fully hybrid (OpenMP, CUDA)/MPI approach to optimize memory usage and to take advantage of the growing number of cores per SMP node or GPUs. High parallel and computational efficiencies are achievable on the largest supercomputers. Finally, QMCPACK utilizes standard file formats for input and output in XML and HDF5 to facilitate data exchange.

<table>
<thead>
<tr>
<th>Workload</th>
<th>Marvell ThunderX2</th>
<th>Intel SKL Gold 6148</th>
<th>ThunderX2 Improvement over SKL</th>
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<tbody>
<tr>
<td>QMCPACK</td>
<td>132 sec</td>
<td>154 sec</td>
<td>1.15x</td>
</tr>
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</table>

*Table 5: Comparative QMCPACK benchmark results. (gcc on ThunderX2, icc18 compiler on SKL); note that lower is better*

**RMG**

Reaction Mechanism Generator\(^x\) (RMG) is an automatic chemical reaction mechanism generator that constructs kinetic models composed of elementary chemical reaction steps using a general understanding of how molecules react. RMG is free, open-source software. To construct a mechanism, the user must specify an initial set of species and the initial conditions (temperature, pressure, species concentrations, etc.). RMG reacts the initial species in all possible ways according to its known reaction families, and it integrates the model in time. RMG tracks the rate (flux) at which each new “edge” species is produced, and species (and the reactions producing them) that are produced with significant fluxes are incorporated into the model (the “core”). These new core species are reacted with all other core species in the model to generate a new set of edge species and reactions. The time-integration restarts, and the
expanded list of edge species is monitored for significant species to be included in the core. The process continues until all significant species and reactions have been included in the model. The definition of a “significant” rate can be specified by the user by taking the following definition for a single species rate. Table 6 shows that ThunderX2 with gcc performs well relative to Intel Skylake with icc.

<table>
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<tr>
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<th>Intel SKL Gold 6148</th>
<th>ThunderX2 Improvement over SKL</th>
</tr>
</thead>
<tbody>
<tr>
<td>RMG</td>
<td>143 sec</td>
<td>178 sec</td>
<td>1.2x</td>
</tr>
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Table 6: Comparative RMG benchmark results on a single node (gcc on ThunderX2, icc18 compiler on SKL); note that lower is better

**Conclusion**

HPC deployments are driven by cost metrics that are directly proportional to the processor cost, performance and number of processors. By providing a balance of compute, throughput and efficiency, the Marvell ThunderX2 delivers best-in-class perf/$ and efficiency/$ for running HPC workloads with different scaling capabilities. For customers looking to run cost effective manufacturing applications, the Marvell ThunderX2 is an ideal processor choice.

**References**


7 Efficiency provided by Marvell.

https://qmcpack.org/about

http://reactionmechanismgenerator.github.io/RMG-Py/