Migrating CUDA to oneAPI: A Smith-Waterman Case Study

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IWBBIO
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Agenda

- Motivation and Goal
- oneAPI
- Smith-Waterman
- Experimental Work
- Experimental Results
- Conclusions

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Motivation

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CPUs

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VPUs

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Data Parallel C++ (DPC++)

- C++
- SYCL

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Same source code on different architectures

Data Pa
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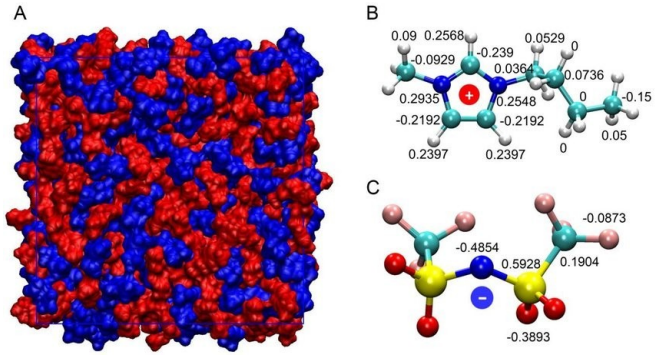
Molecular dynamics



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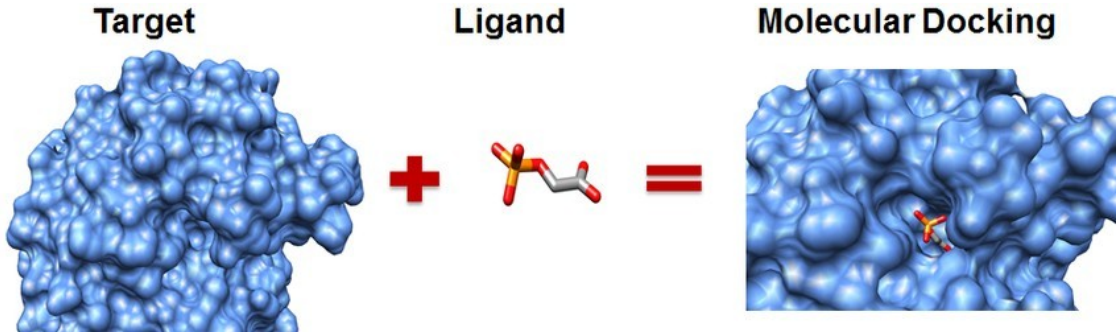
Molecular docking



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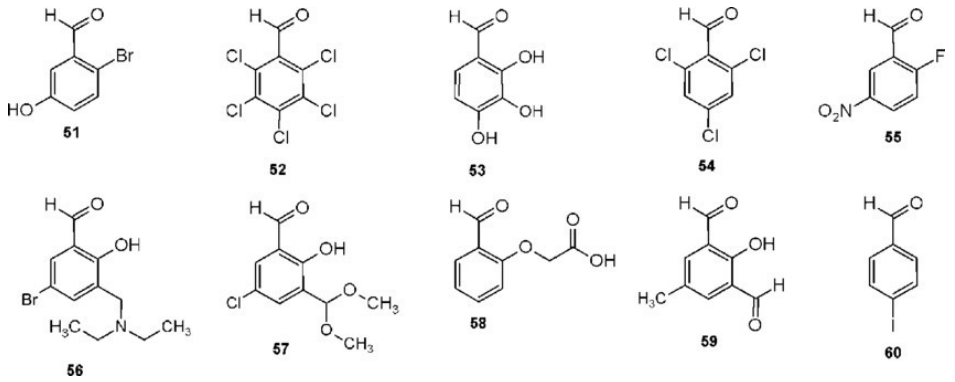
Prediction and searching of molecular structures



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Sequence alignment

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One of the most widely used implementations

Sequence alignment

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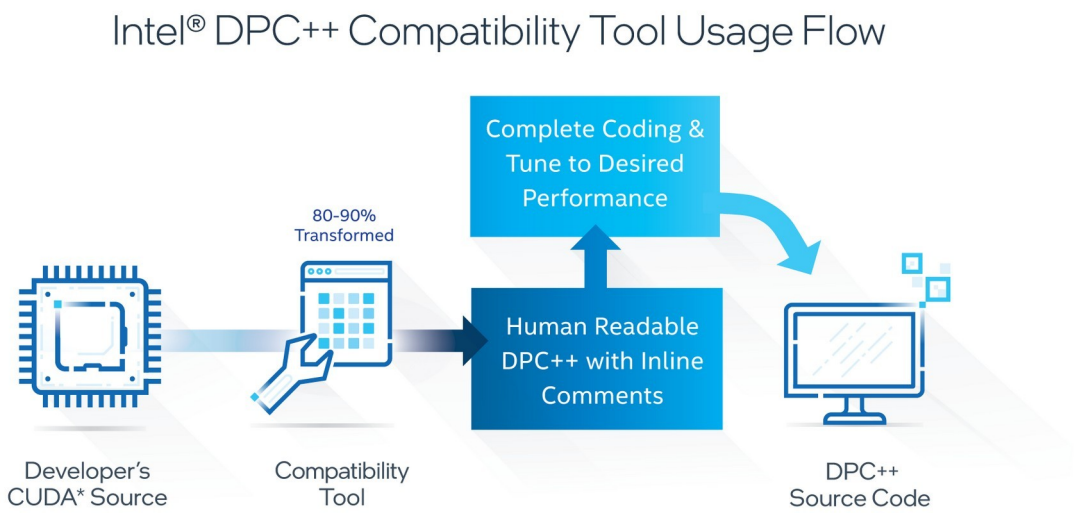
GPUs ca… …hile
CUDA is … …them
nowadays.

Bioinform…
exploiting GPUs for more than two decades.

❌ Difficulty in porting the code to other architectures.

oneAPI - DPCT

oneAPI facilitates the migration to the SYCL-based DPC++ programming language through the DPCT tool.



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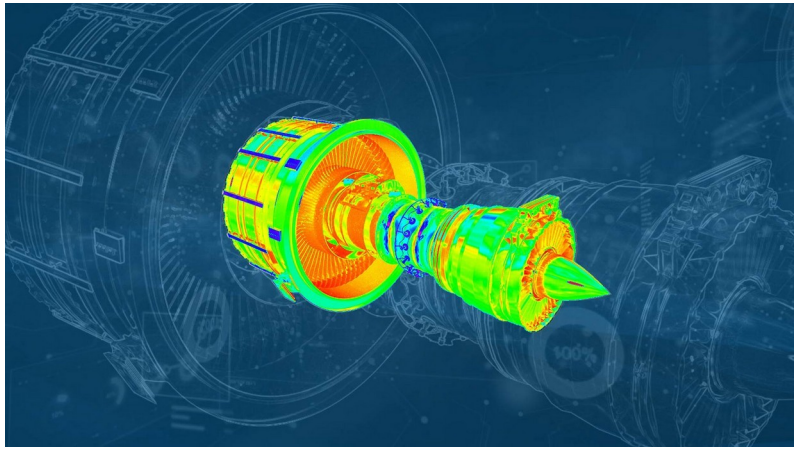
Simulation



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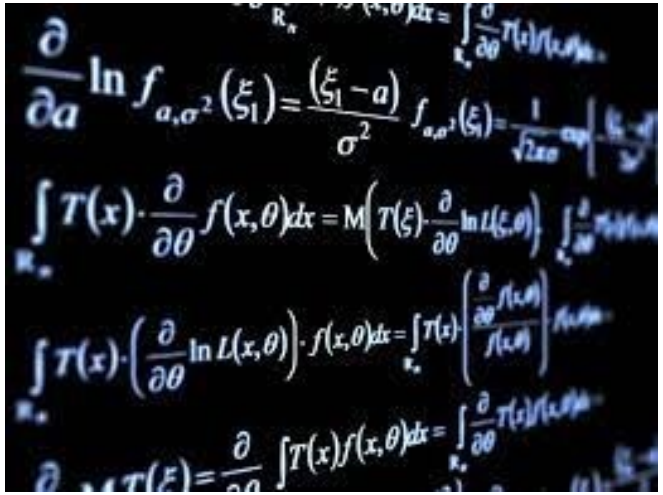

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No study has assessed their utility in Bioinformatics

Goal

To present our experiences porting a biological software tool to DPC++ using dpct

SW#db: *a CUDA-based, memory efficient implementation of the Smith-Waterman algorithm*

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- ➔ An analysis of the dpct effectiveness for CUDA code migration
- ➔ An analysis of the DPC++ code's portability, considering different target platforms and vendors (CPU and GPUs).
- ➔ A comparison of the performance on different hardware architectures (CPU and GPUs).

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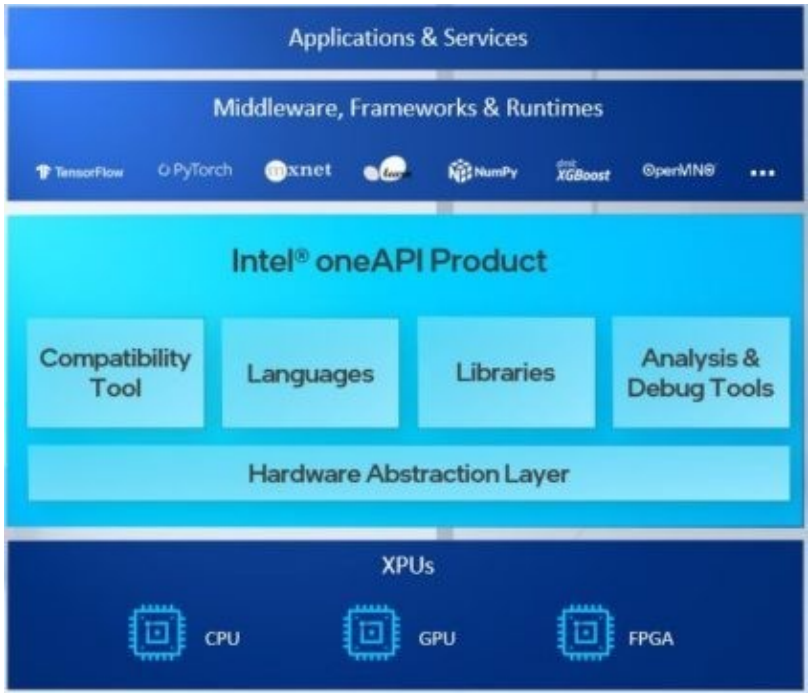
Technologies - oneAPI

oneAPI is a programming ecosystem, which provides a unified programming model for a wide range of hardware architectures



Technologies - SYCL & DPC++

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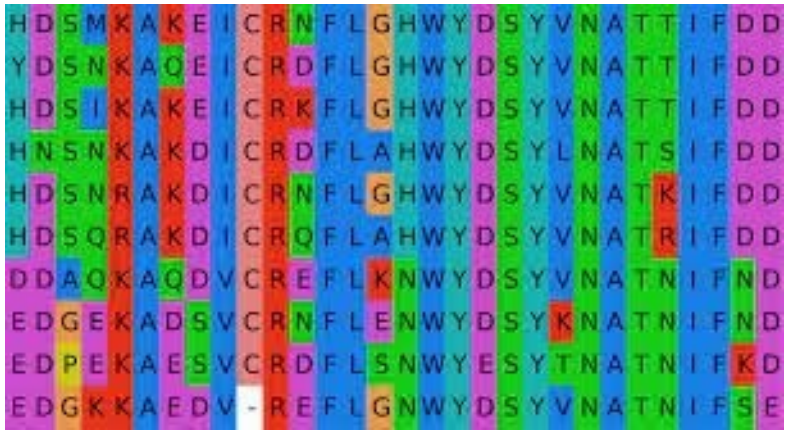
Smith-Waterman

Obtains the optimal local alignment between two biological sequences.



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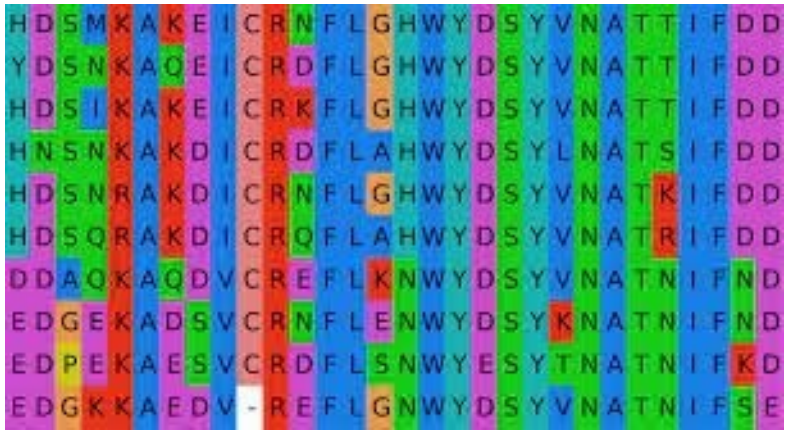

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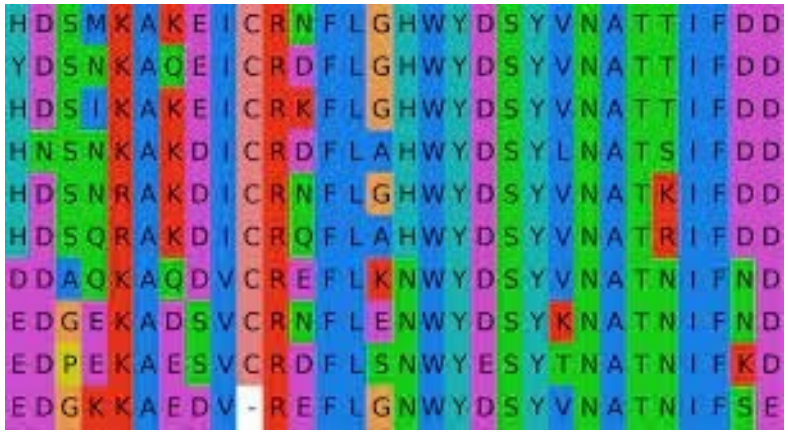


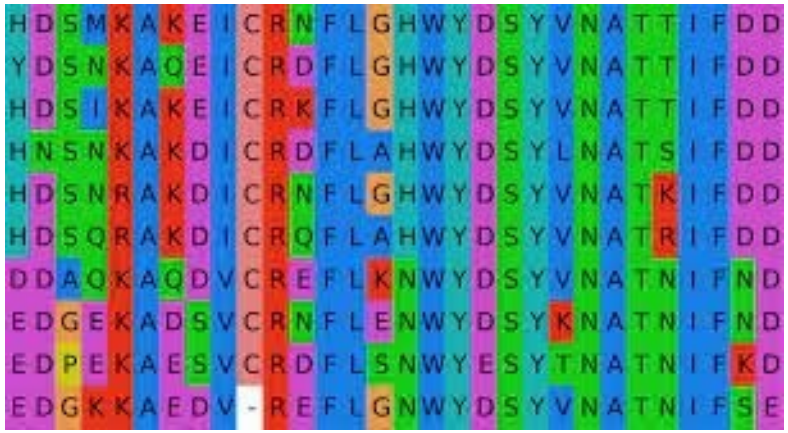
Smith-Waterman

Obtai gical
sequ

It has orithms

SW# is a CUDA tool for computing biological sequence alignments that works with both protein and DNA sequences.

Is often employed as a benchmark when comparing different alignment techniques



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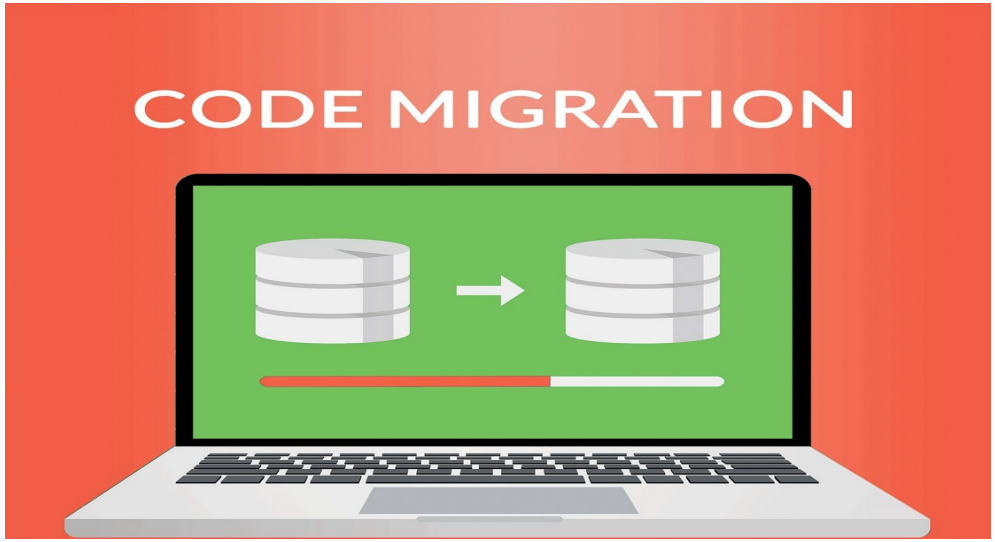

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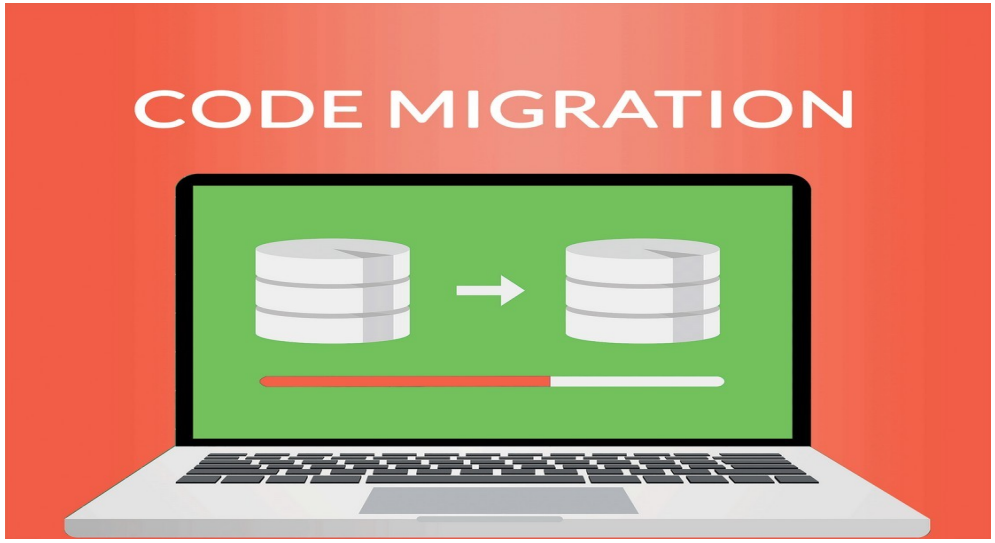

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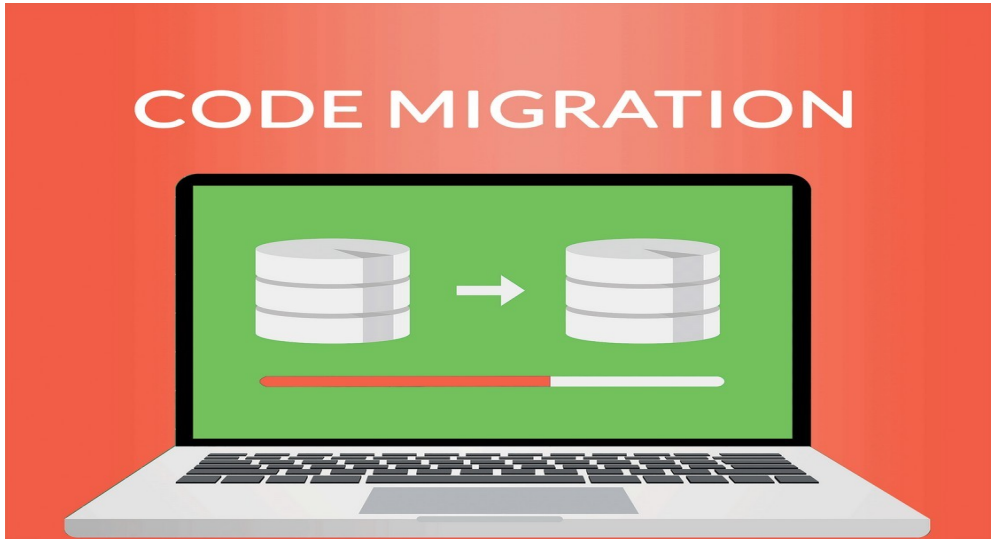
2. Based on the DPCT alerts, modify the resulting code (Stage 2).



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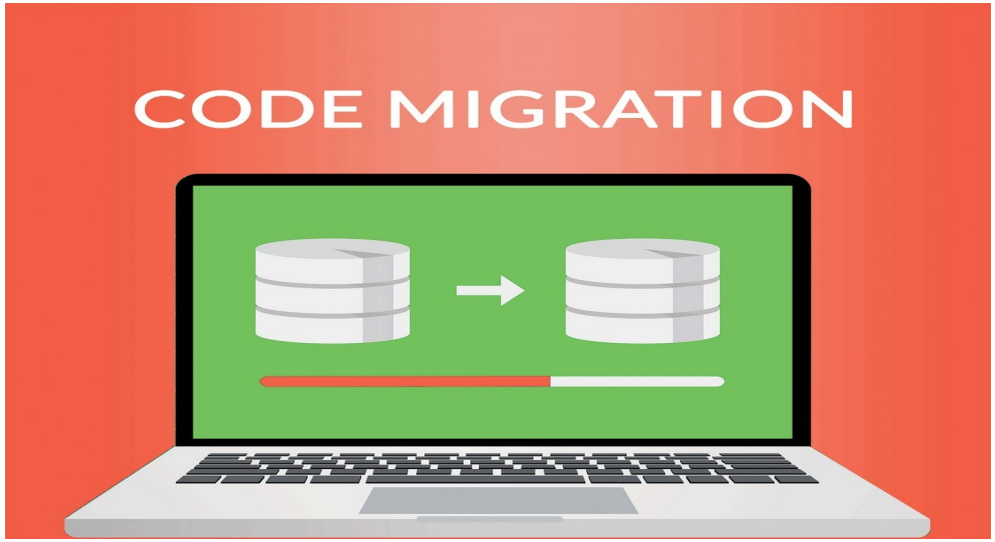

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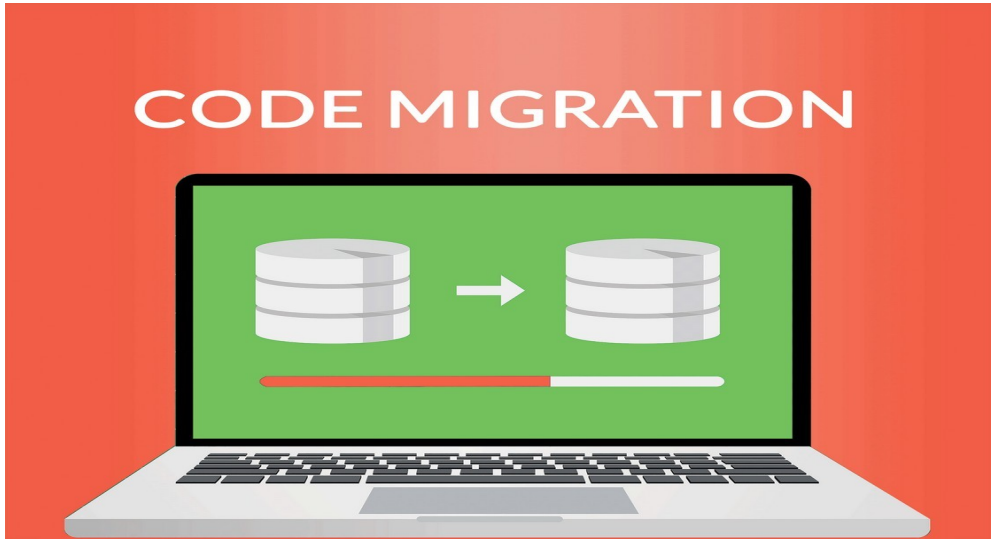
4. Verify that the results are correct (Stage 4).



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Generate first version of DPC++ code using DPCT tool

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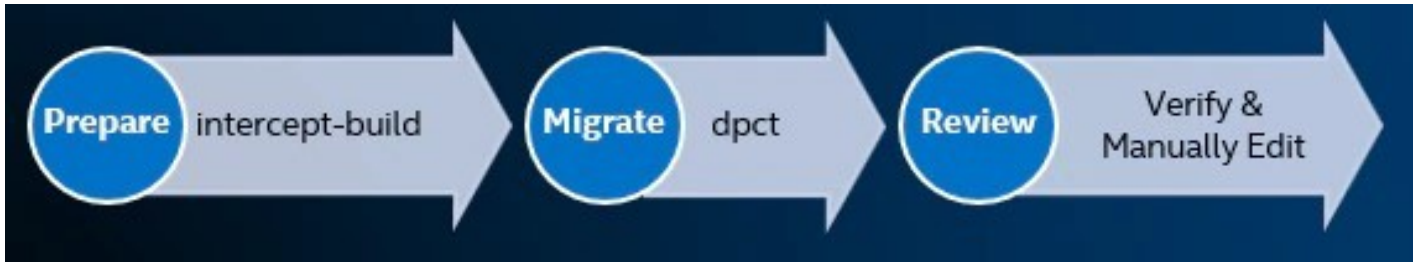

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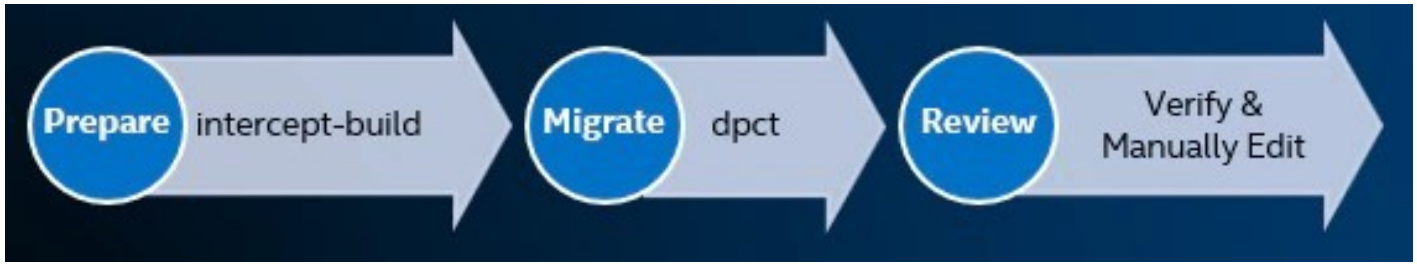
Generate first version of DPC++ code using DPCT tool

1. *intercept-build make*

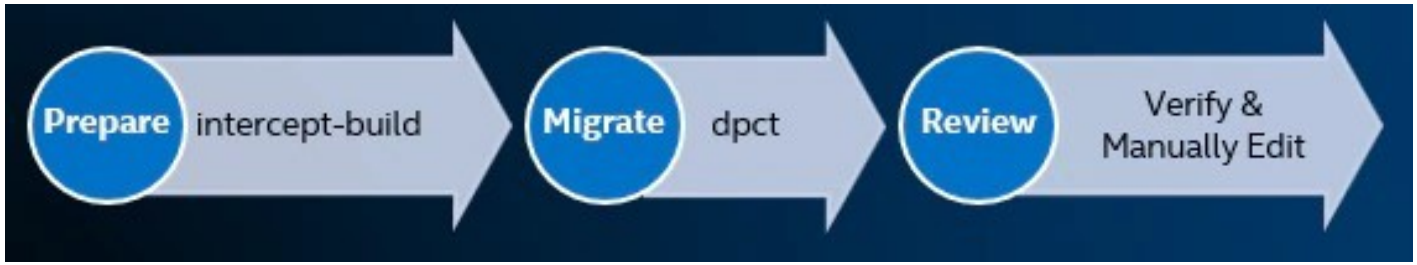


Experimental Work - Stage 1

Generate first version of DPC++ code using DPCT tool

1. *intercept-build make*

2. *dpct -p compile_commands.json -in-root=$PROJ_DIR*



Experimental Work - Stage 2

DPCT1003: Migrated API does not return error code. (, 0) is inserted. You may need to rewrite this code*

DPCT1009: SYCL uses exceptions to report errors and does not use the error codes. The original code was commented out and a warning string was inserted. You need to rewrite this code.

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DPCT uses Unified Shared Memory (USM) model by default

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2
3
4
5
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1   cudaDeviceProp properties;
2   cudaGetDeviceProperties(
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5
6   bool major = properties.major < 2;
7   int threads = major ? 64 : 128;
8   int blocks = major ? 360 : 480;
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8   int blocks = major ? 360 : 480;
```

(a) CUDA

```
1   dpct::device_info properties;
2
3   dpct::dev_mgr::instance()
4       .get_device(card)
5       .get_device_info(properties);
6
7   bool major = false;
8   int threads = major ? 64 : 128;
9   int blocks = major ? 360 : 480;
```

(b) oneAPI

Experimental Work - Stage 2

DPCT1049: The workgroup size passed to the SYCL kernel may exceed the limit. To get the device limit, query info::device::max_work_group_size. Adjust the workgroup size if needed.

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```
1   solveShort<<<blocks, threads>>>(...);
```

(a) CUDA

```
1   dpct::get_default_queue()
2       .submit([&](sycl::handler &cgh) {
3    ...
4   cgh.parallel_for(
5     sycl::nd_range<3>
6       (sycl::range<3>(1, 1, blocks) *
7       sycl::range<3>(1, 1, threads),
8       sycl::range<3>(1, 1, threads)),
9     [=](sycl::nd_item<3> item_ct1) {
10      solveShort(...);
11    });
12  });
```

(b) oneAPI

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(b) oneAPI

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DPCT1065: Consider replacing sycl::nd_item::barrier() with sycl::nd_item::barrier(sycl::access::fence_space::local_space) for better performance if there is no access to global memory.

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2   __syncthreads();
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char v = tex1Dfetch(colTexture, 10);
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For a 1D/2D image/image array, the width must be a Value >= 1 and <= CL_DEVICE_IMAGE2D_MAX_WIDTH.

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4  cudaArray *sequencesGpu;
5  cudaChannelFormatDesc channel =
6    seqsTexture.channelDesc;
7  cudaMallocArray(&sequencesGpu,
8      &channel, sequencesCols, sequencesRows);
9  cudaMemcpyToArray(sequencesGpu, 0, 0,
10     sequences, sequencesSize, TO_GPU);
11 cudaBindTextureToArray(
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(a) CUDA

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3  seqsGpu = (int *)sycl::malloc_device(
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8   .memcpy(seqsGpu, sequences, sequencesCols *
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```

(b) oneAPI

```
1  int columnCodes = tex2D(
2    seqsTexture, colOff, j + rowOff);
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Experimental Work - Stage 4

Different tests were run to prove that the DPC++ code generates correct results

Agenda

- Motivation and Goal
- oneAPI
- Smith-Waterman
- Experimental Work
- **Experimental Results**
- Conclusions

Experimental Results - Hardware Platforms

CPU			GPU			
ID	**Processor**	**RAM (Memory)**	**ID**	**Vedor (Type)**	**Model (Architecture)**	**GFLOPS peak (SP)**
Core-i5	Intel Core i5-7400	16 GB	Titan	NVIDIA (Discrete)	Titan X (Pascal)	10970
Core-i3	Intel Core i3-4160	8 GB	RTX	NVIDIA (Discrete)	RTX 2070 (Turing)	7465
Core-i9	Intel Core i9-10920X	32 GB	Iris XE	Intel (Discrete)	Iris Xe MAX Graphics (Gen 12.1)	2534
Xeon	Intel Xeon E-2176G	65 GB	P630	NVIDIA (Integrated)	UHD Graphics P630 (Gen 9.5)	441.6

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Experimental Results - Design

1. **UniProtKB/Swiss-Prot** database (release 2021_04) contains **204173280** amino acid residues in **565928** sequences with a maximum length of 35213
2. **20** queries with length from **144** to **5478** (accession numbers: P02232, P05013, P14942, P07327, P01008, P03435, P42357, P21177, Q38941, P27895, P07756, P04775, P19096, P28167, P0C6B8, P20930, P08519, Q7TMA5, P33450, and Q9UKN1)
3. Scoring matrix: **BLOSUM62**
   Gap insertion: **10**
   Gap extension: **2**

Experimental Results - Configuration & tests

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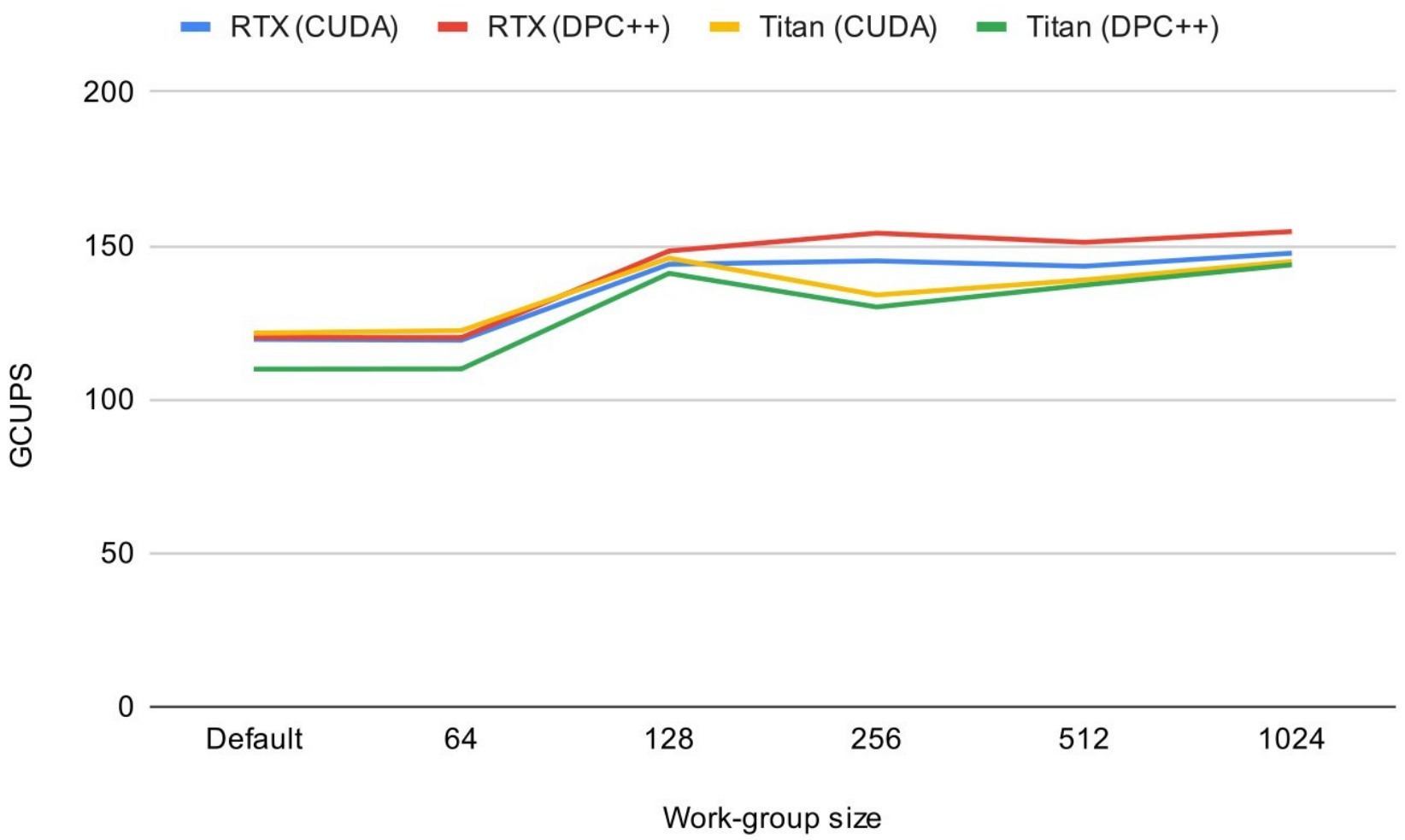
4. GCUPS as the performance metric.

$$\frac{|Q| * |D|}{t * 10^9}$$

Q ⇾ Database length
D ⇾ Sequence length
t ⇾ Execution time in seconds

Experimental Results - Varying work group size



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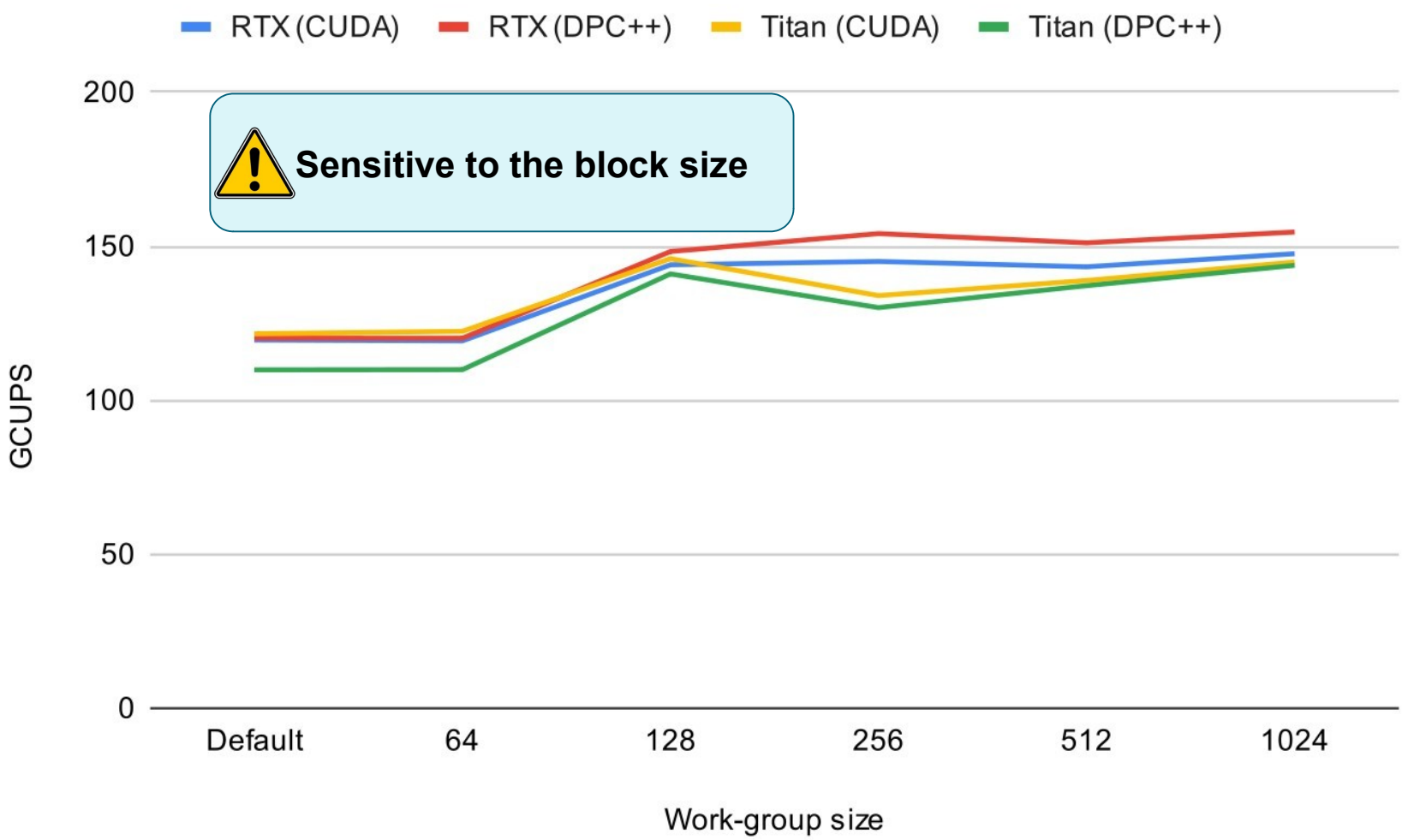

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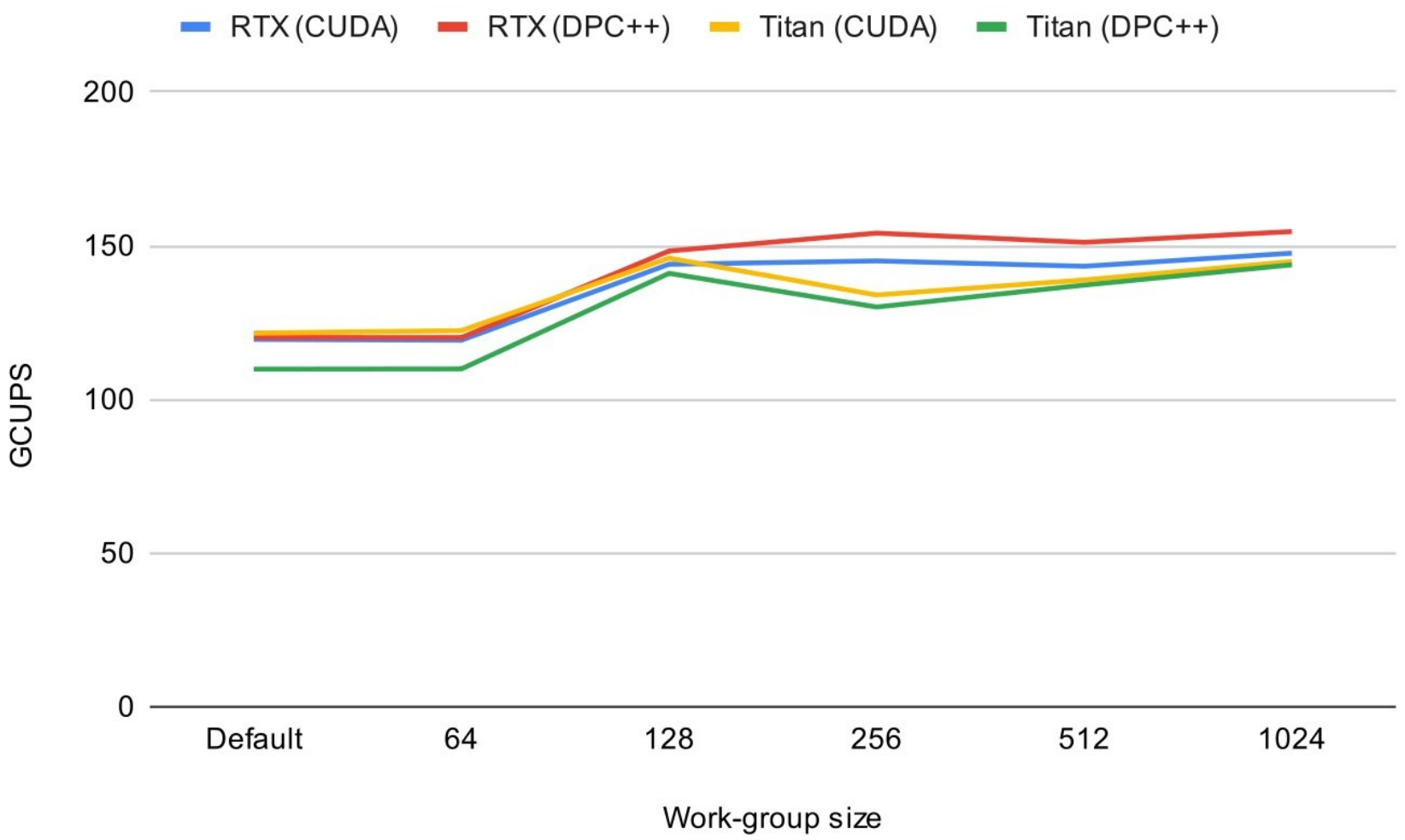

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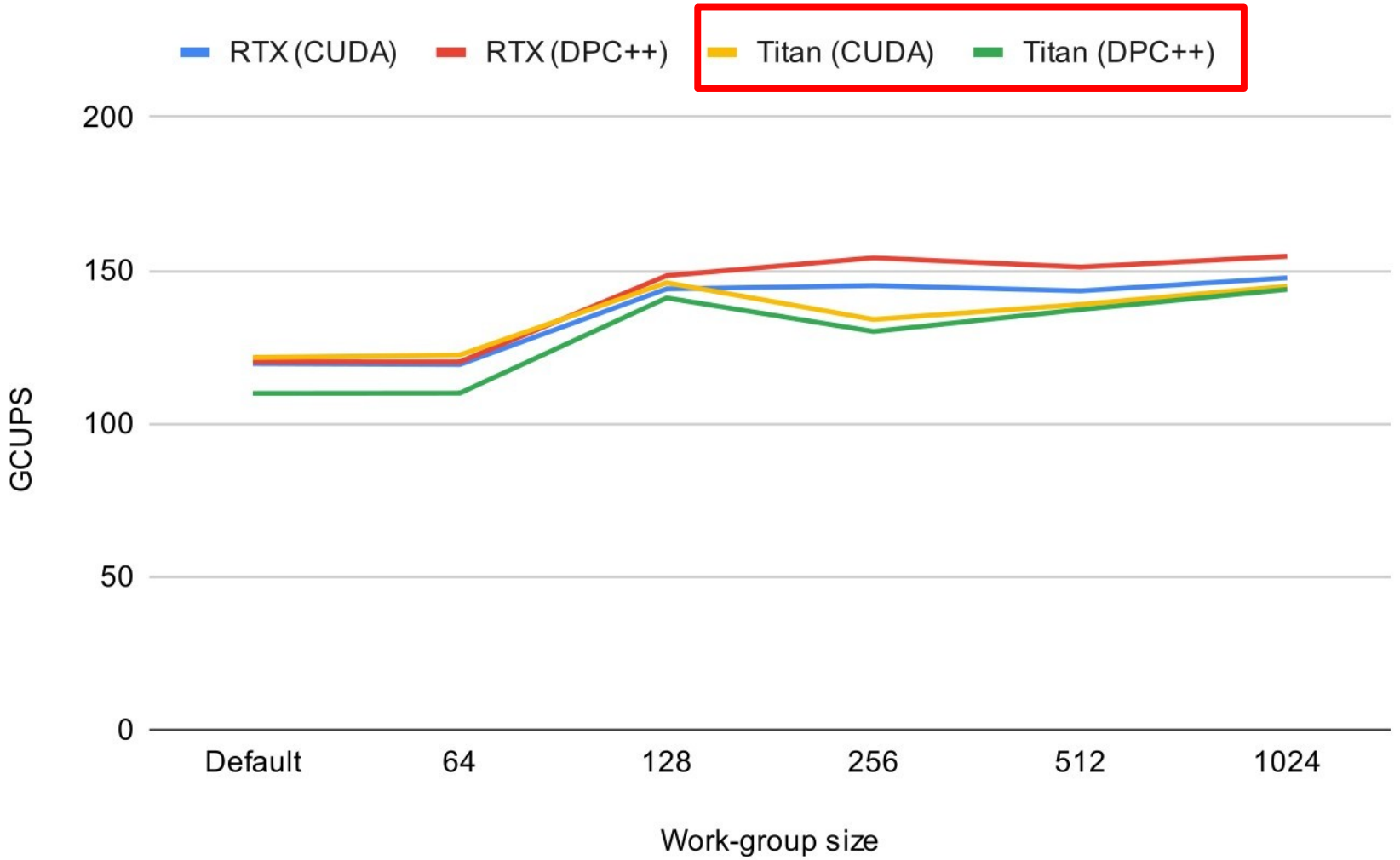

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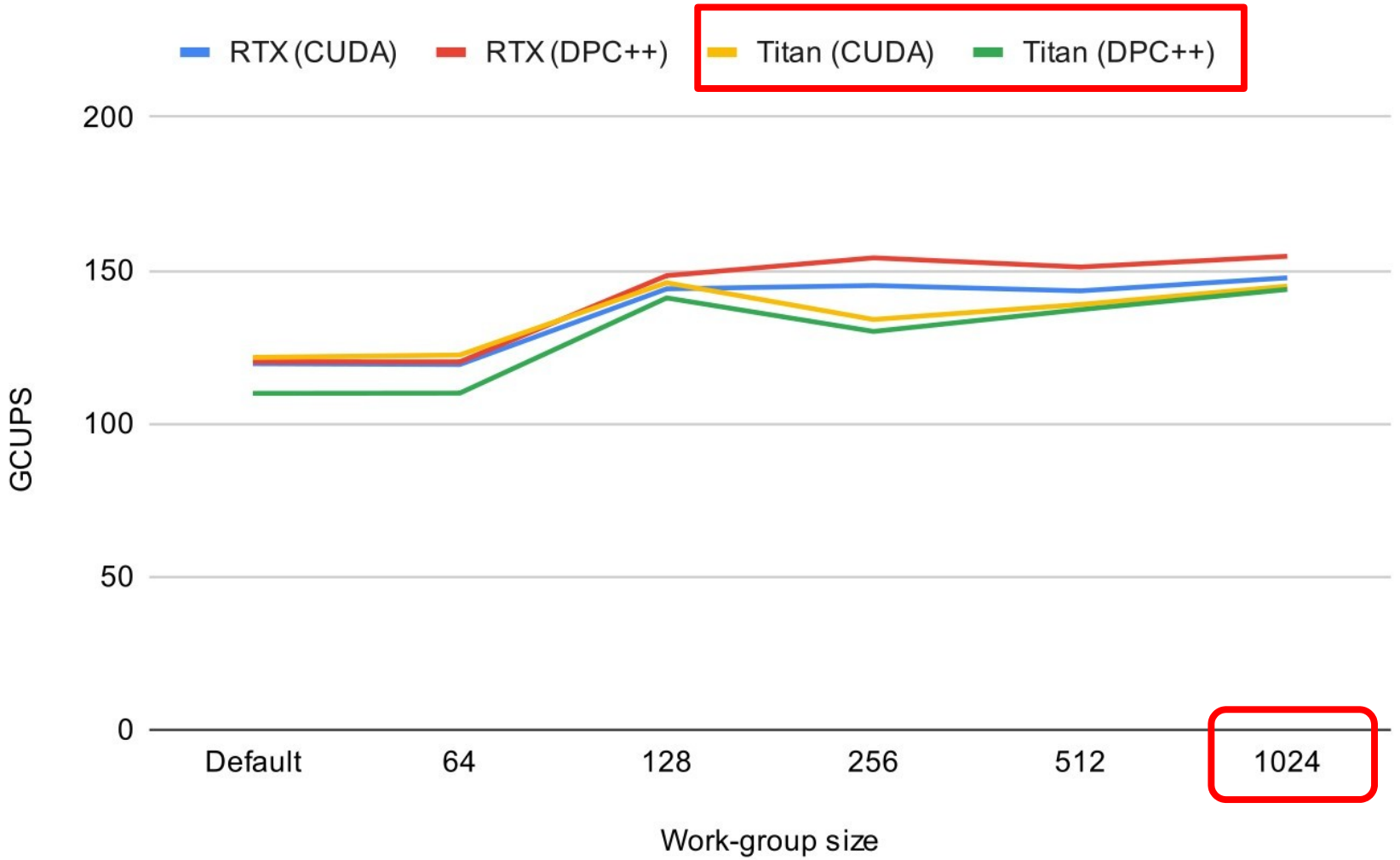

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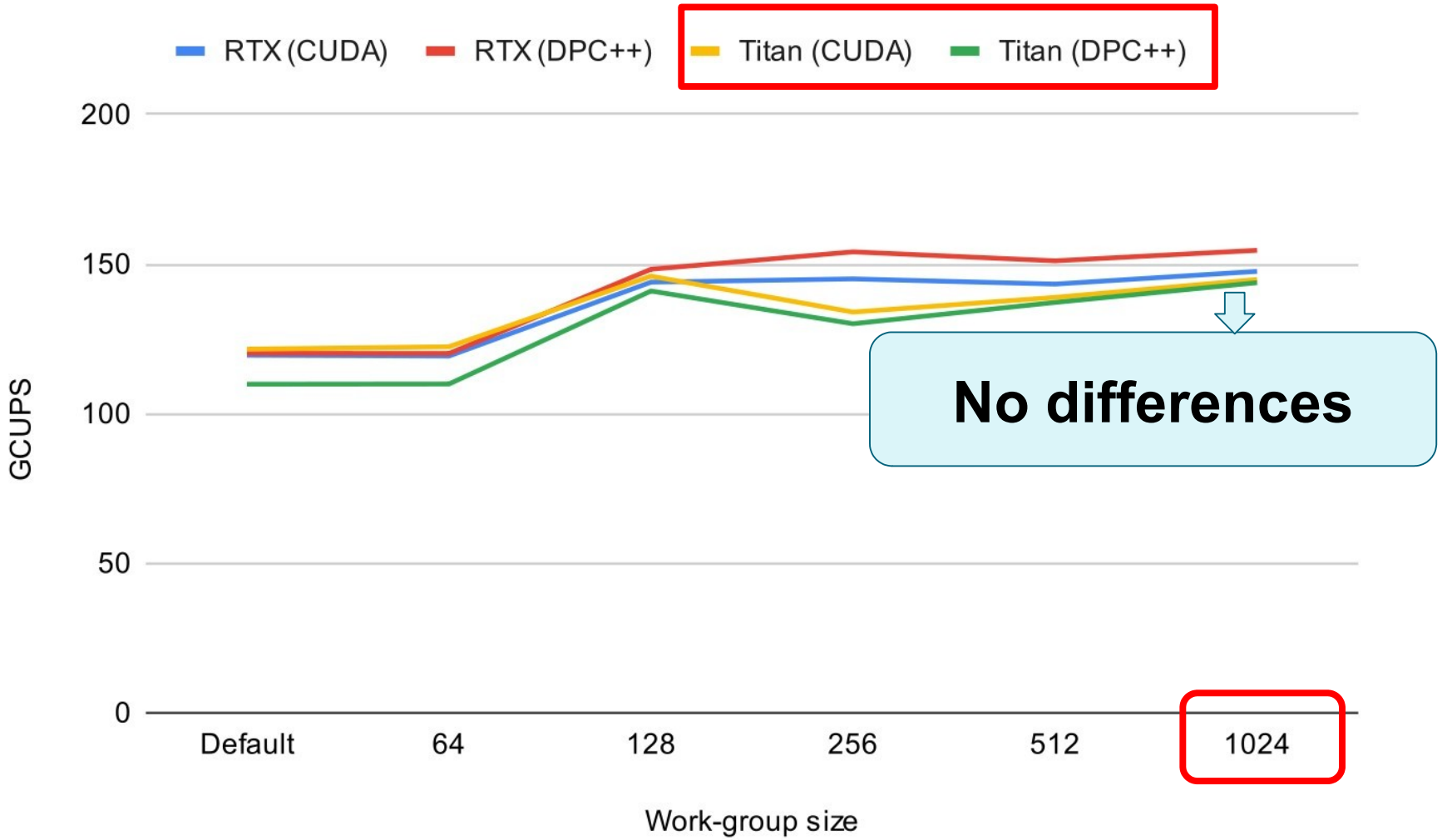

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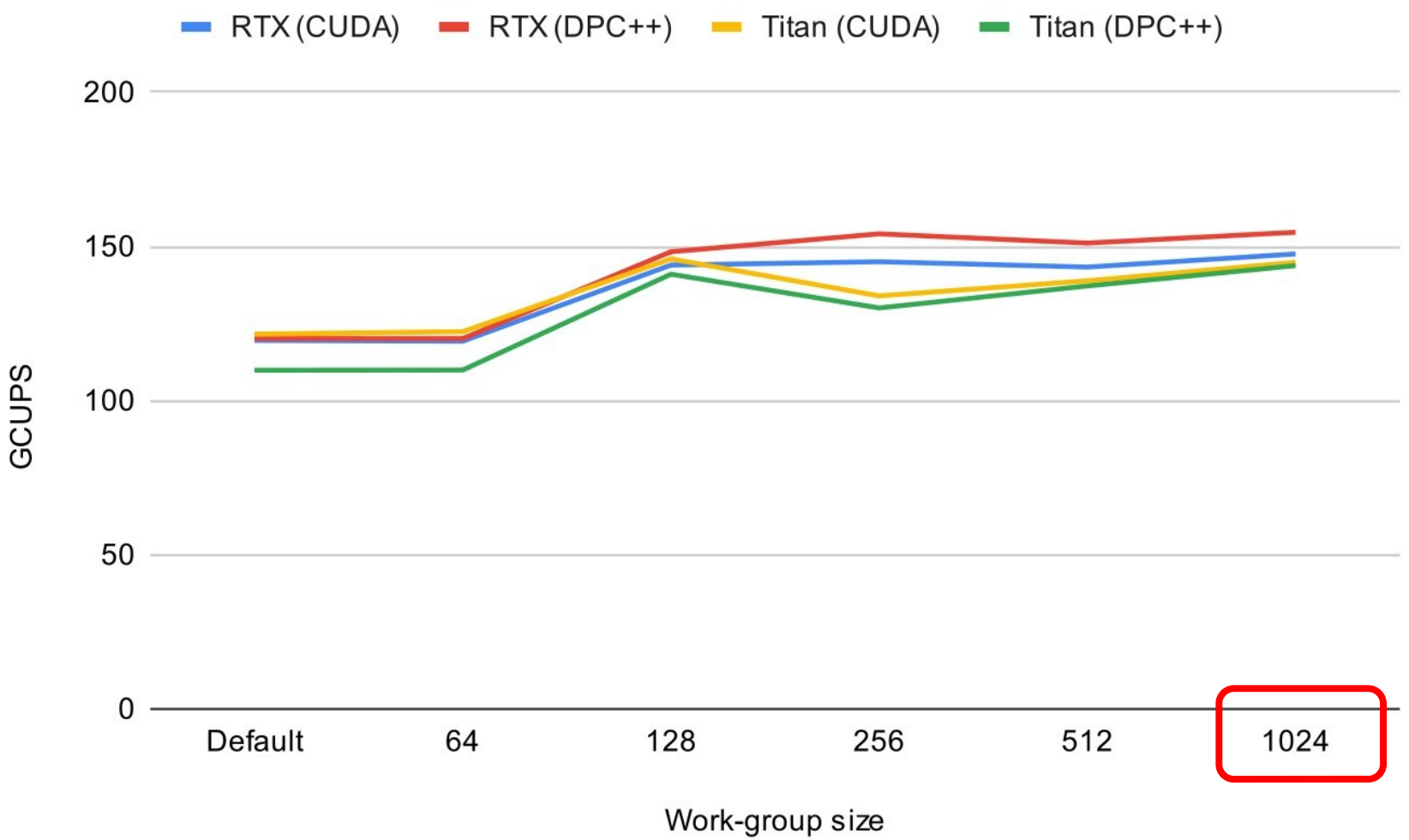

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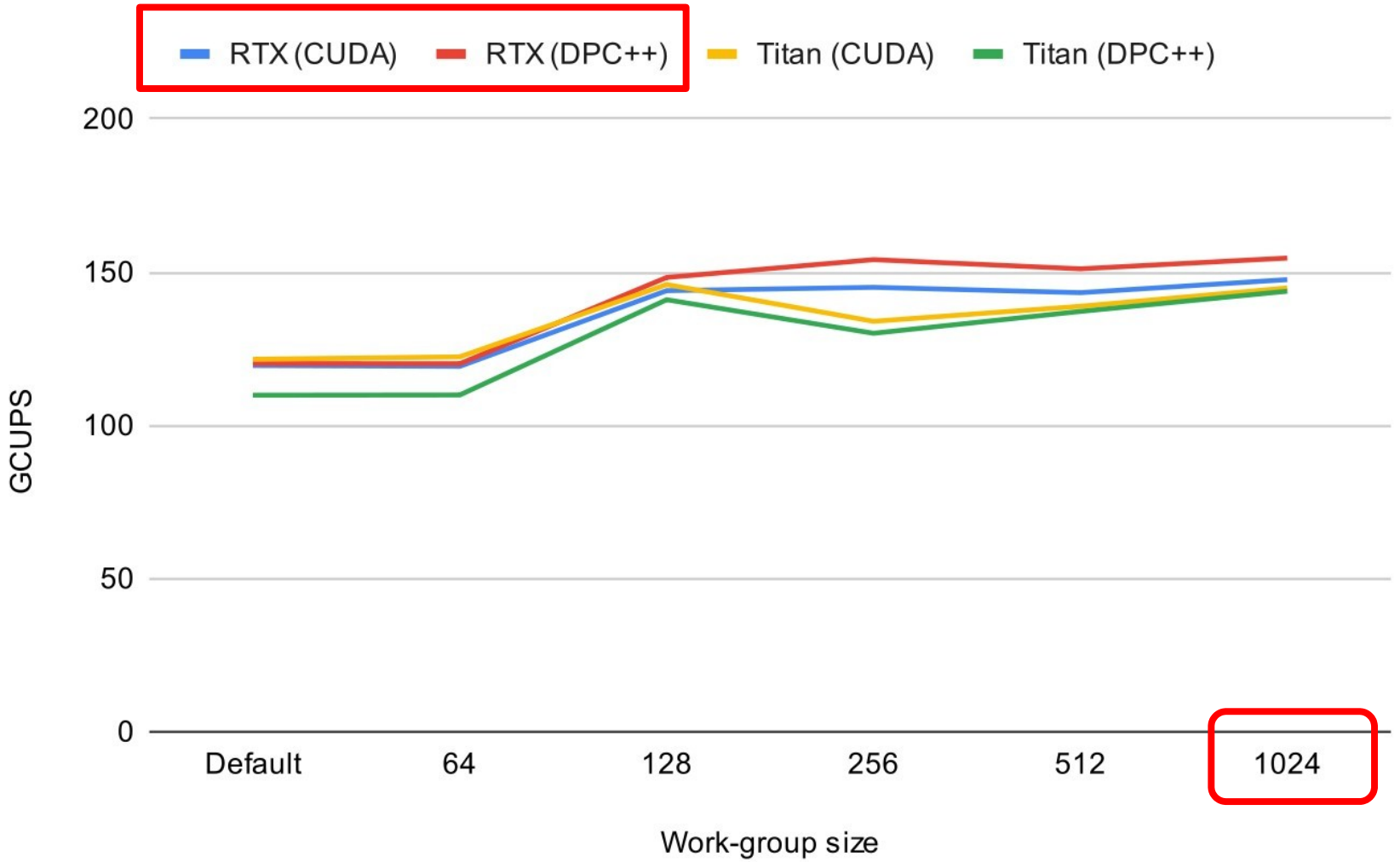

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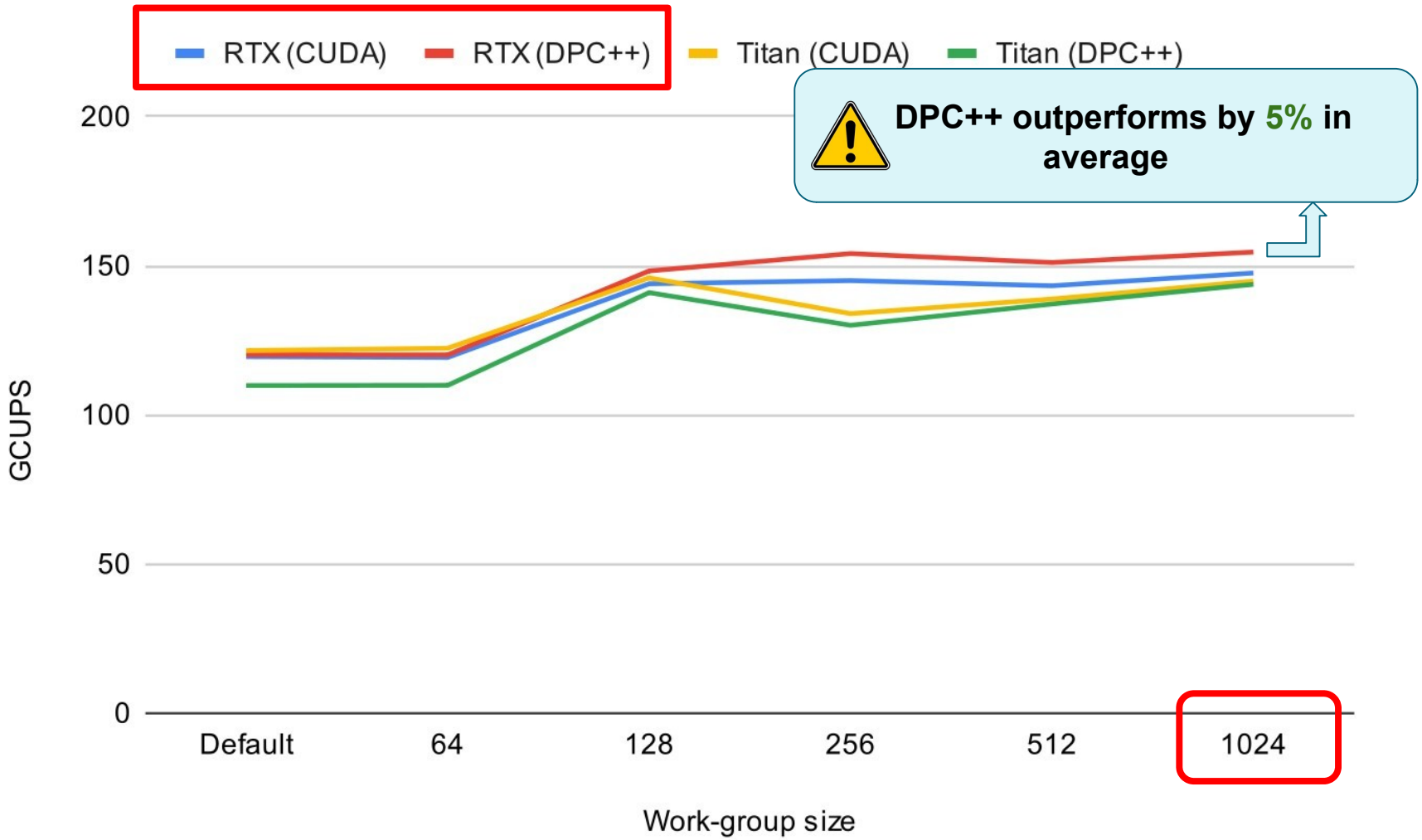
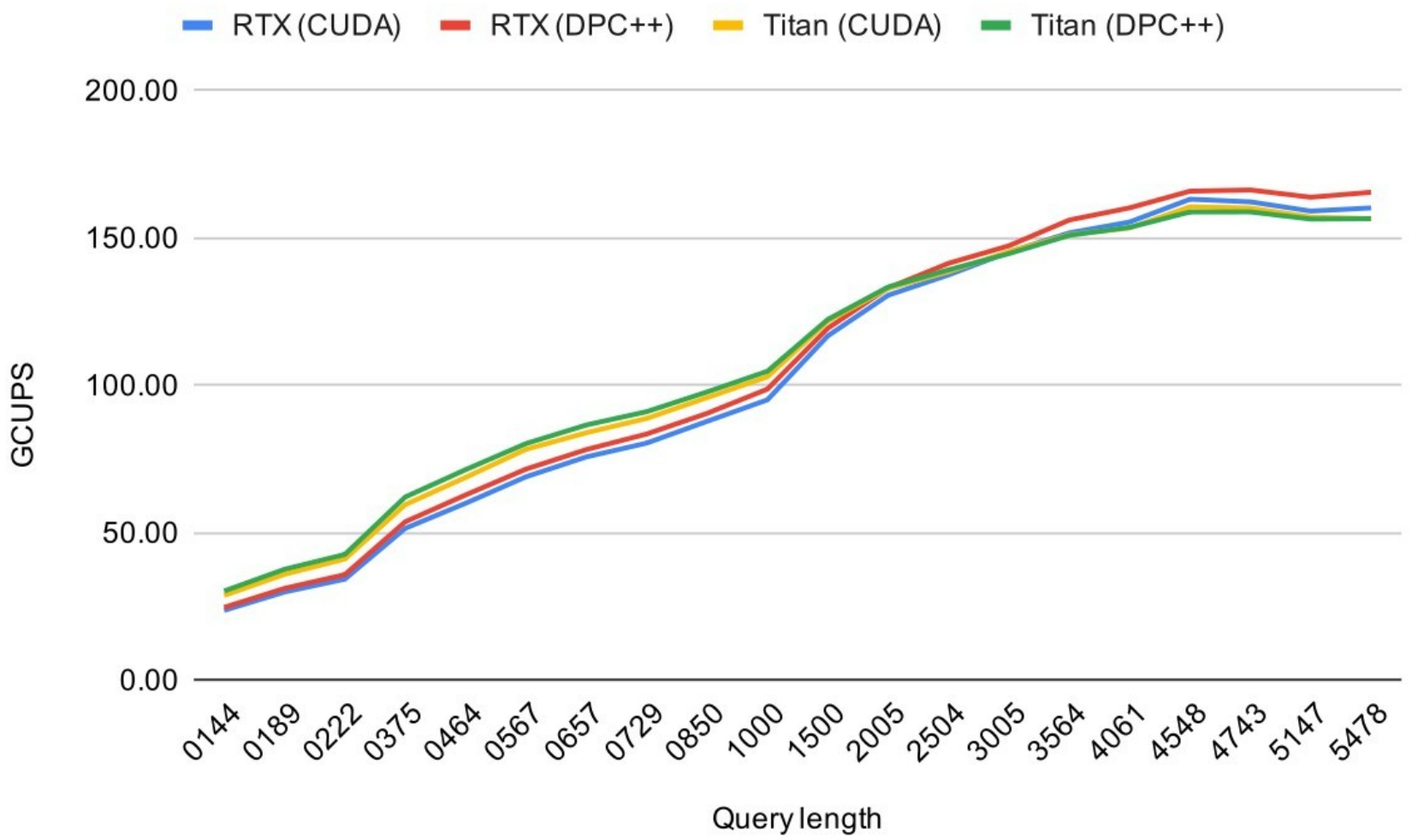


Experimental Results - Varying query length



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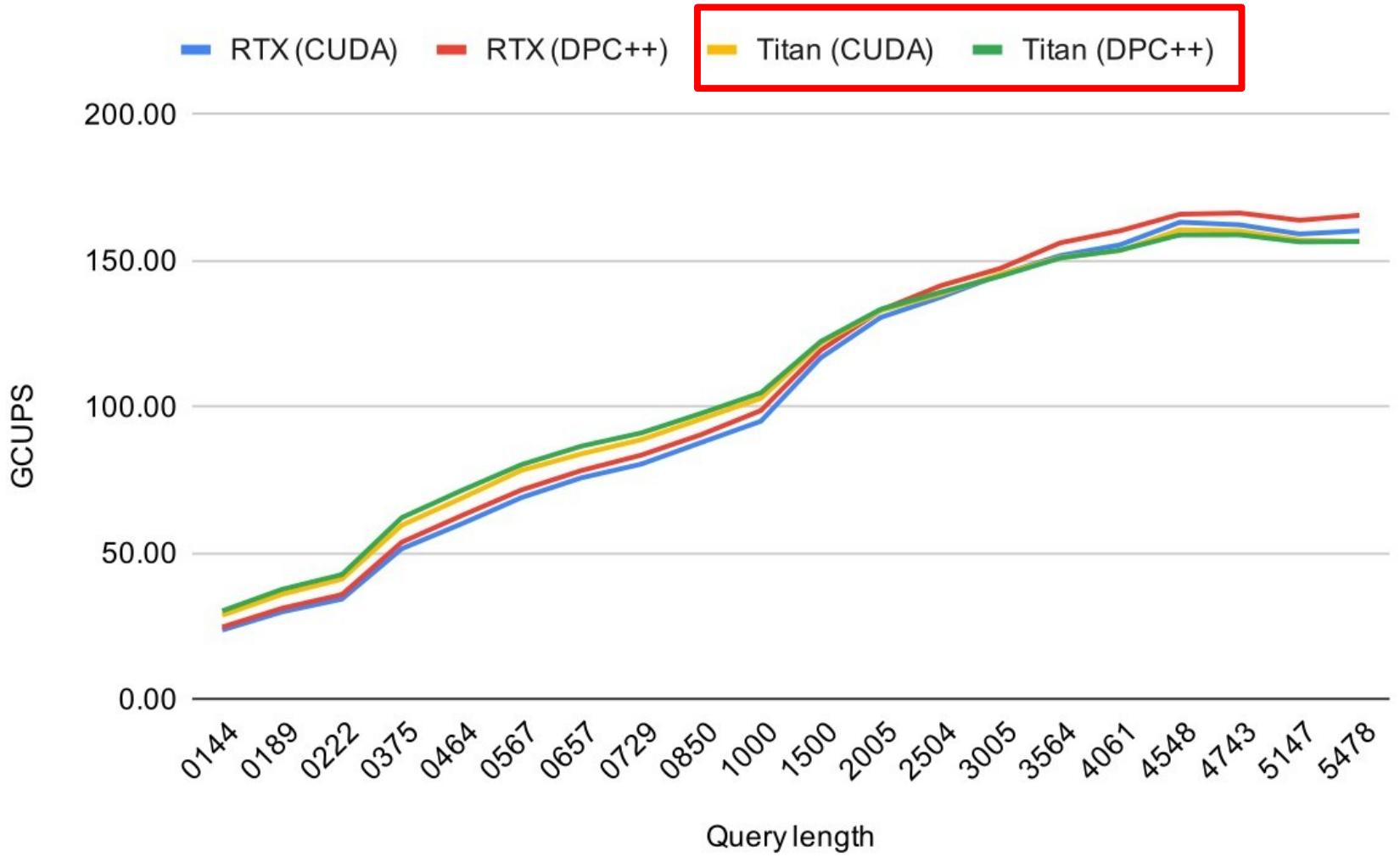

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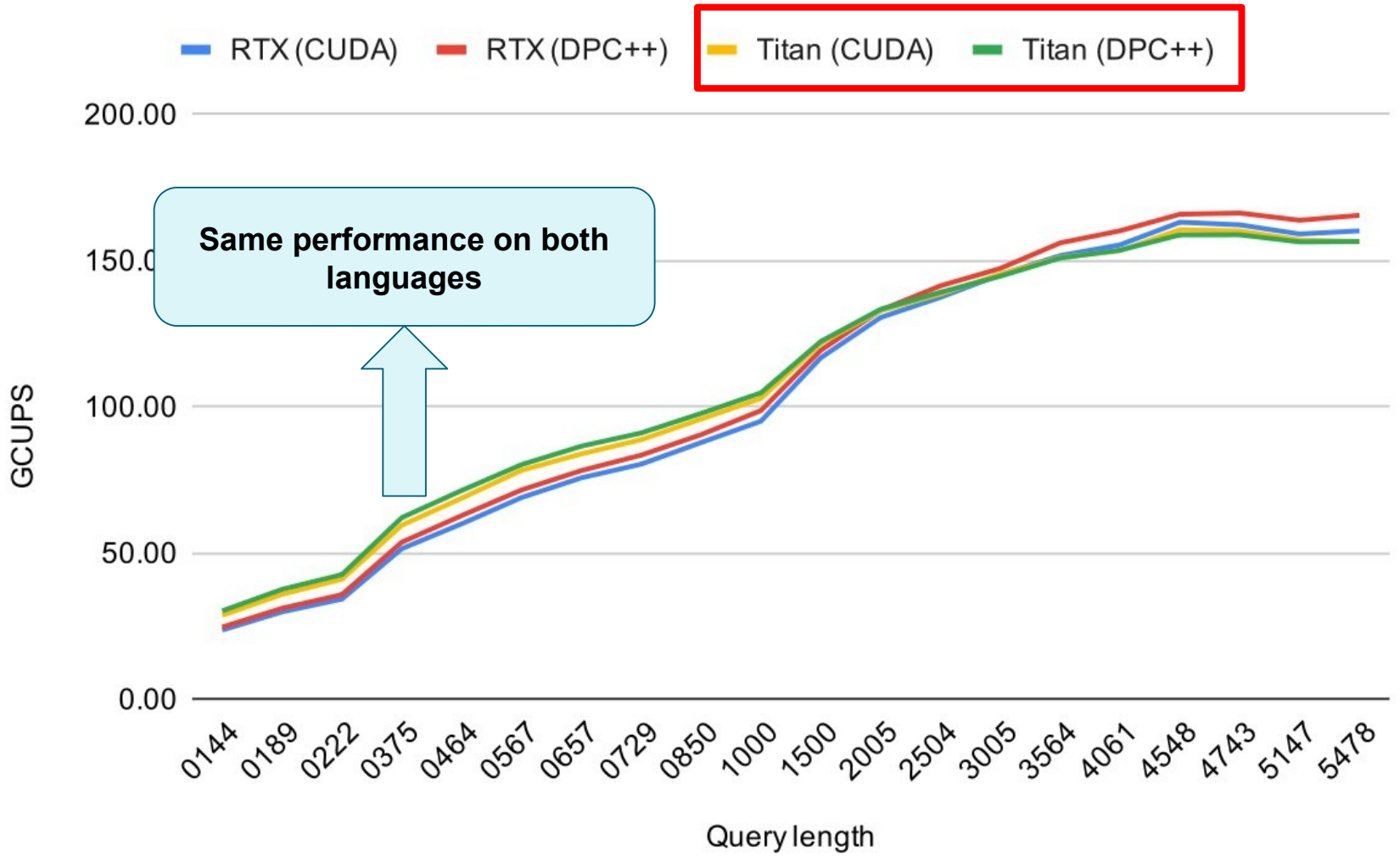

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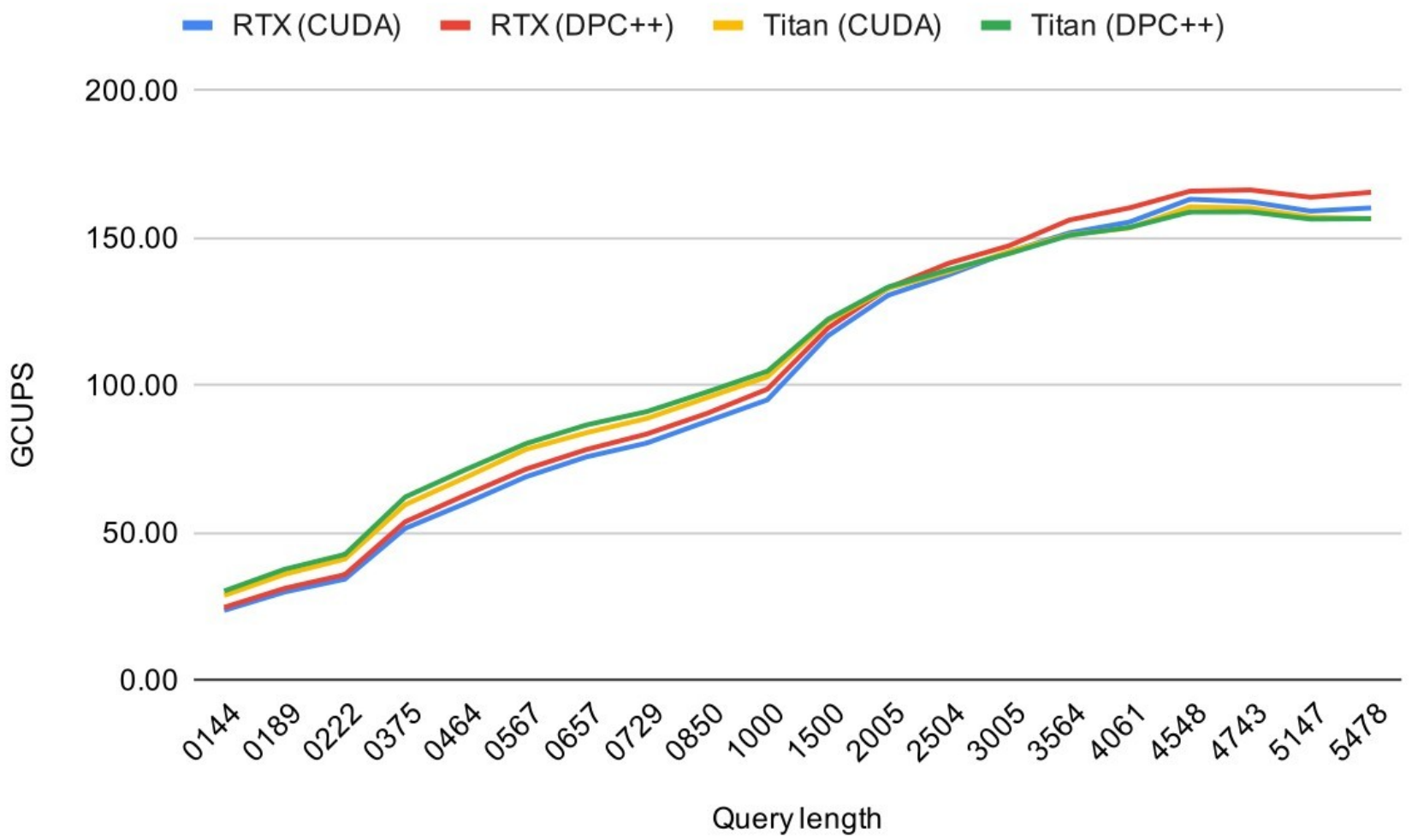

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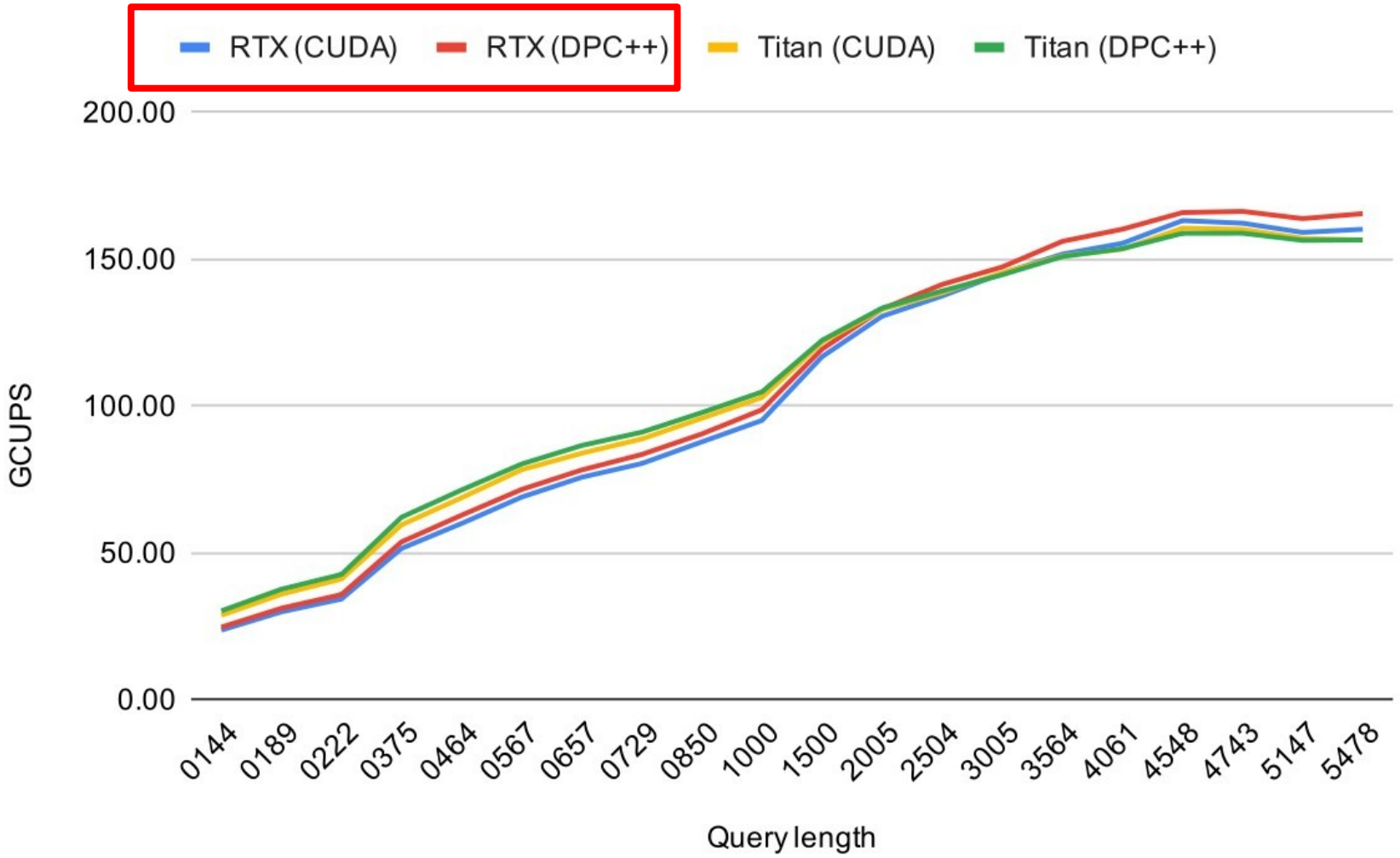

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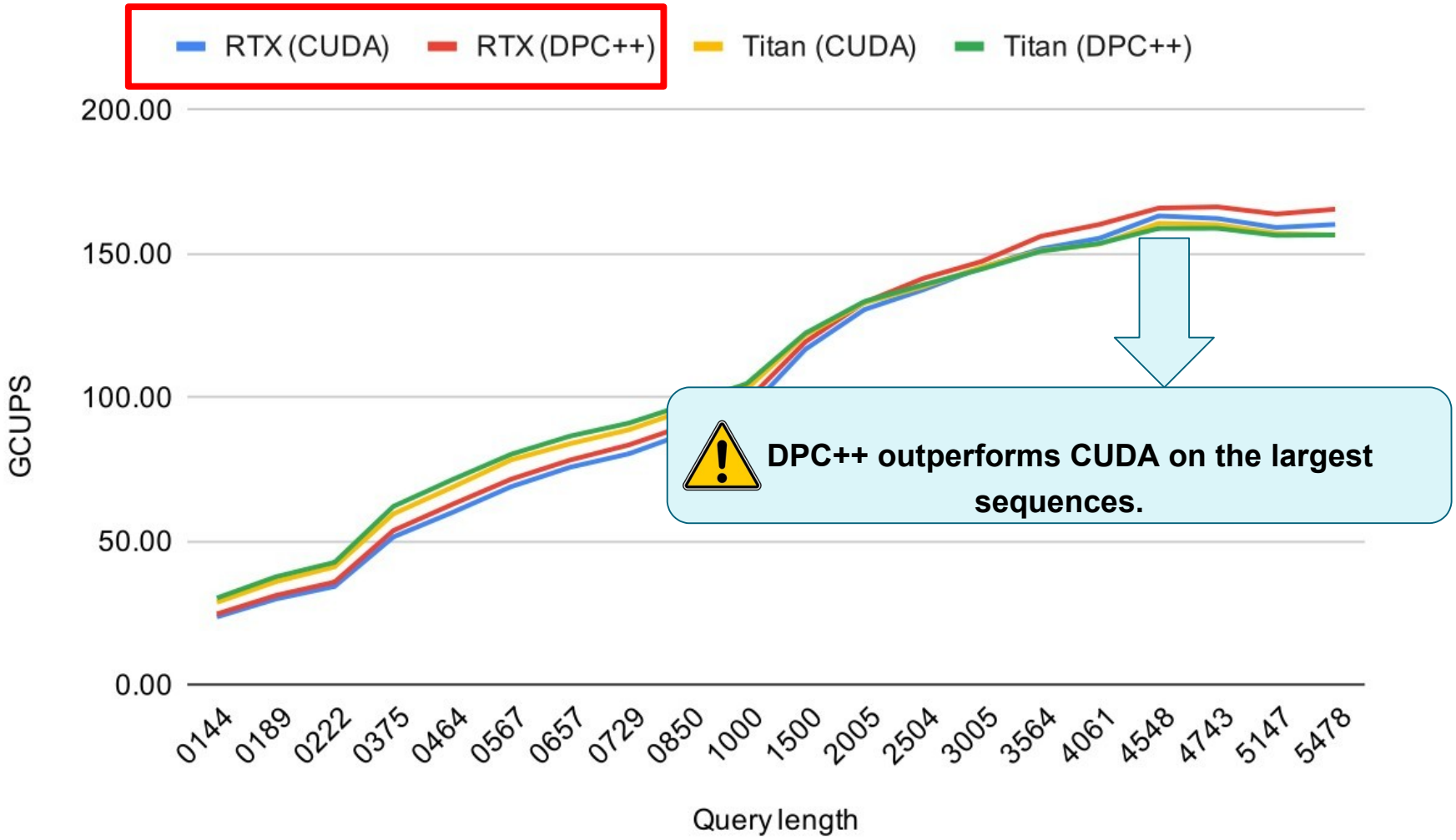
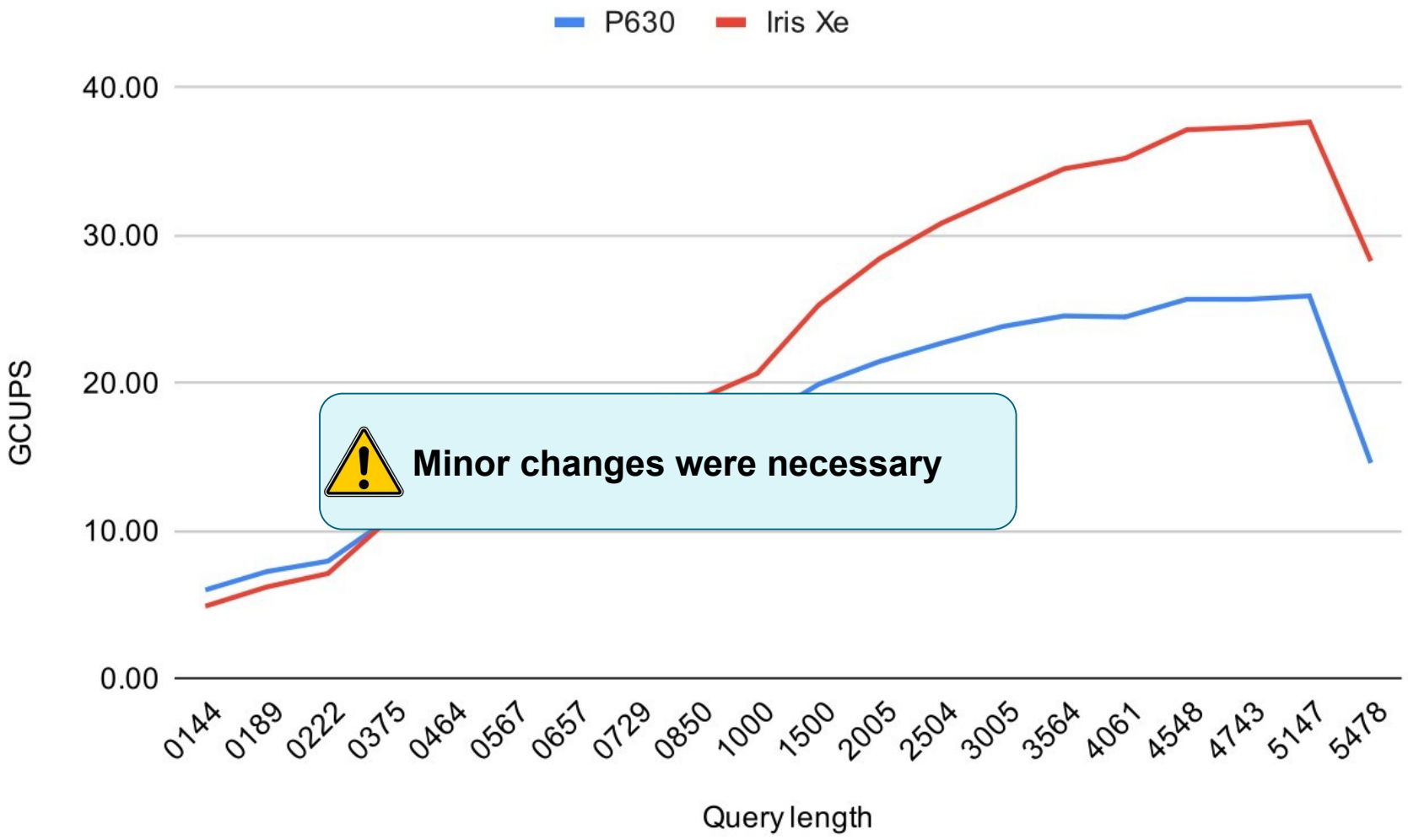


Experimental Results - Cross-GPU vendor portability



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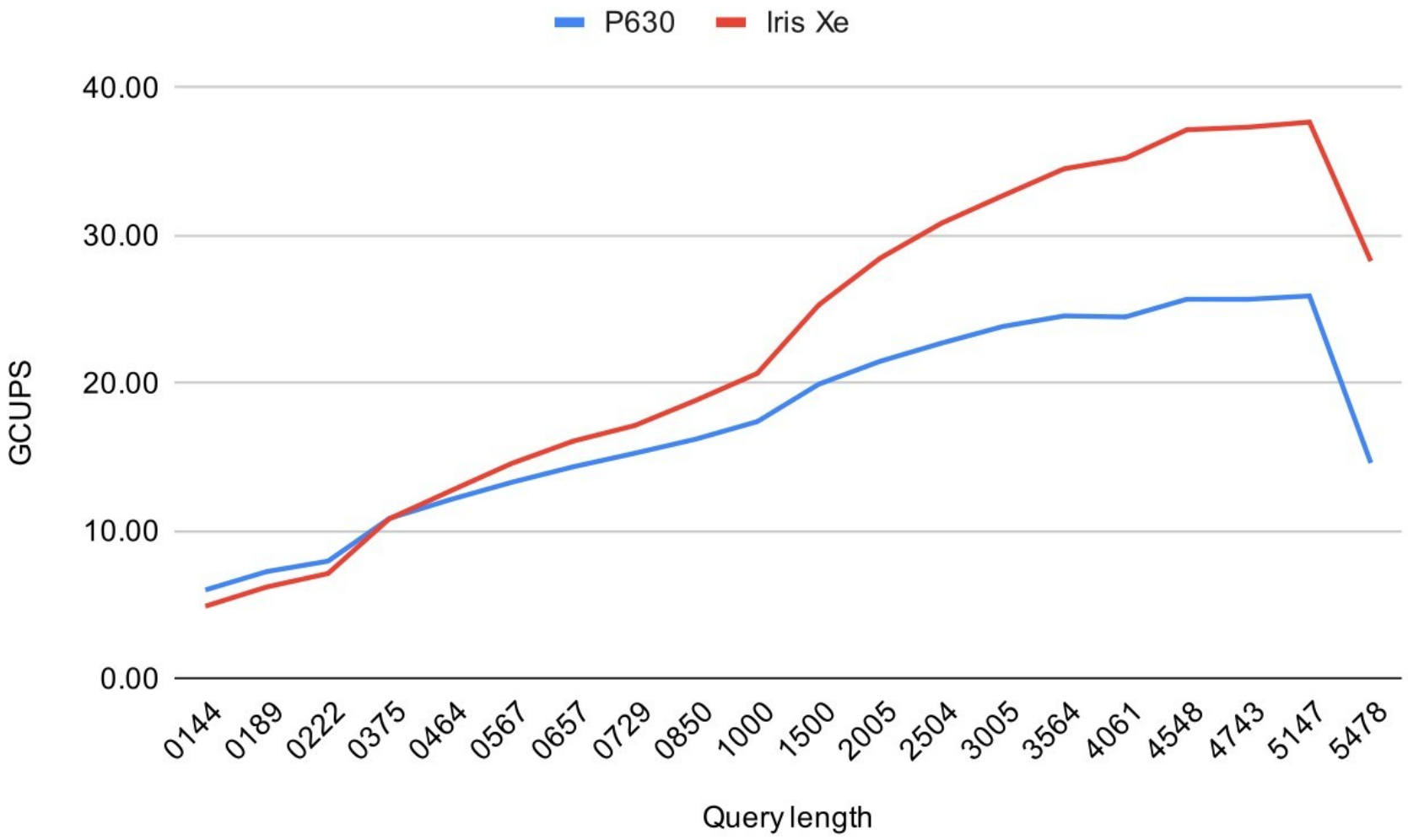

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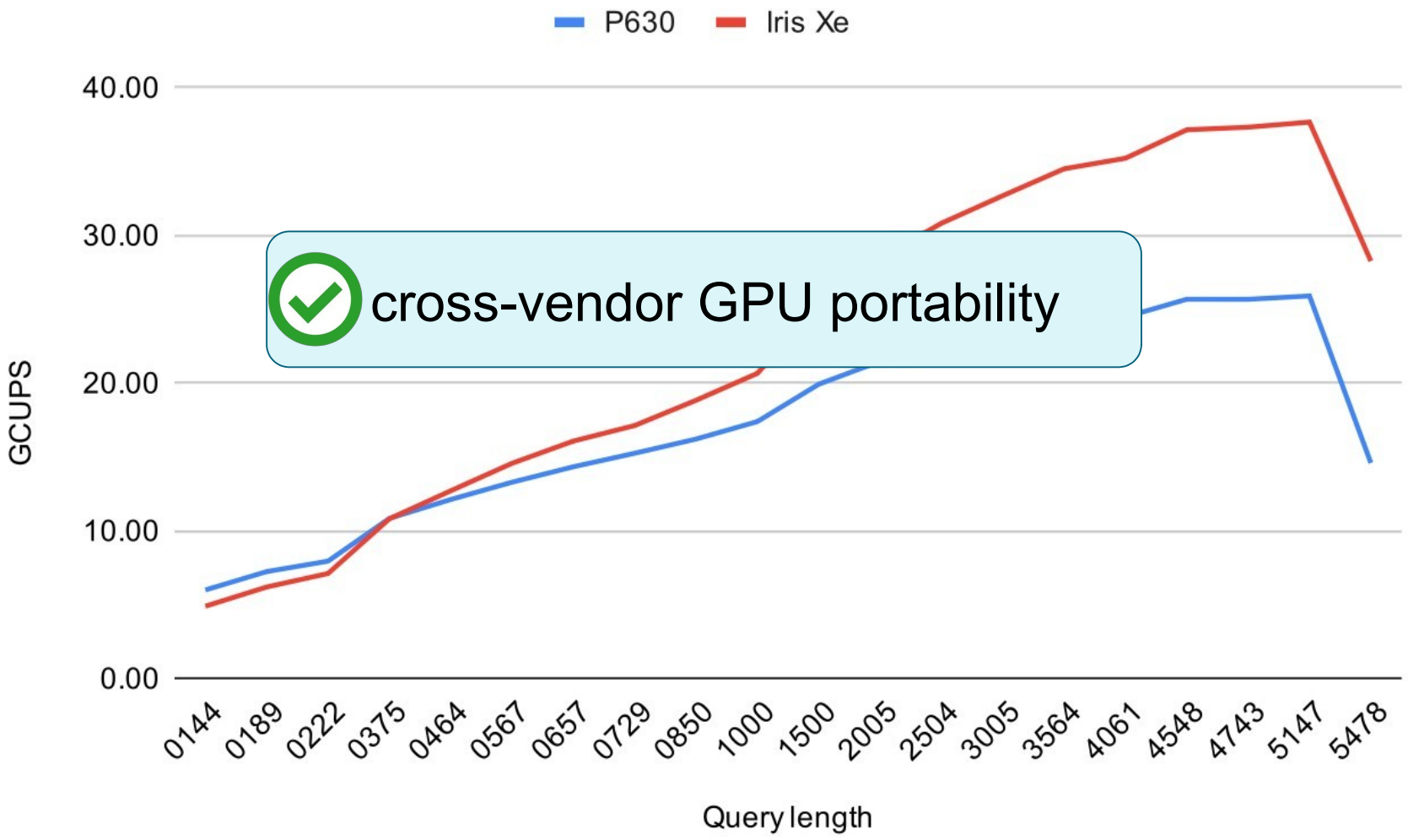
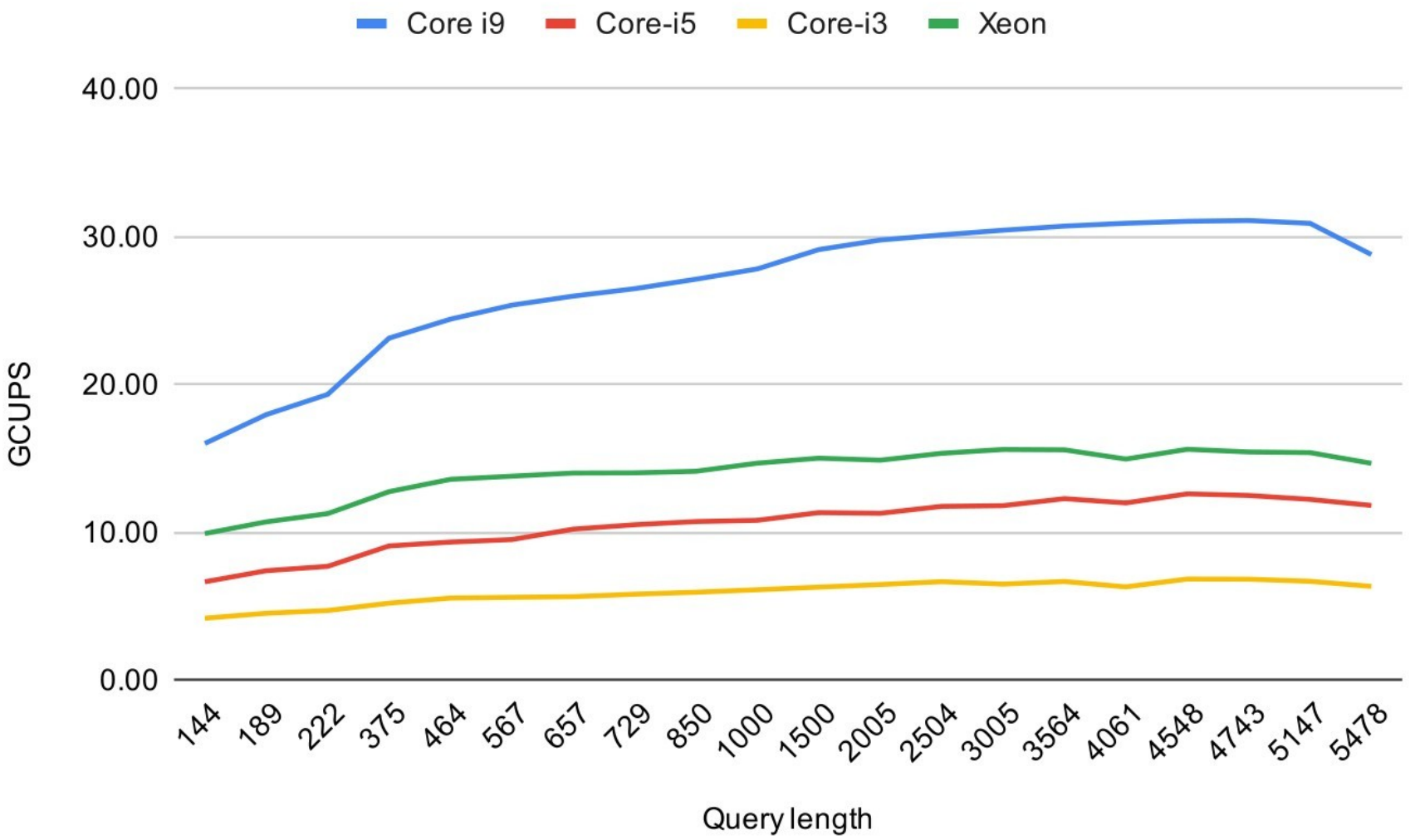


Experimental Results - Cross-architecture portability



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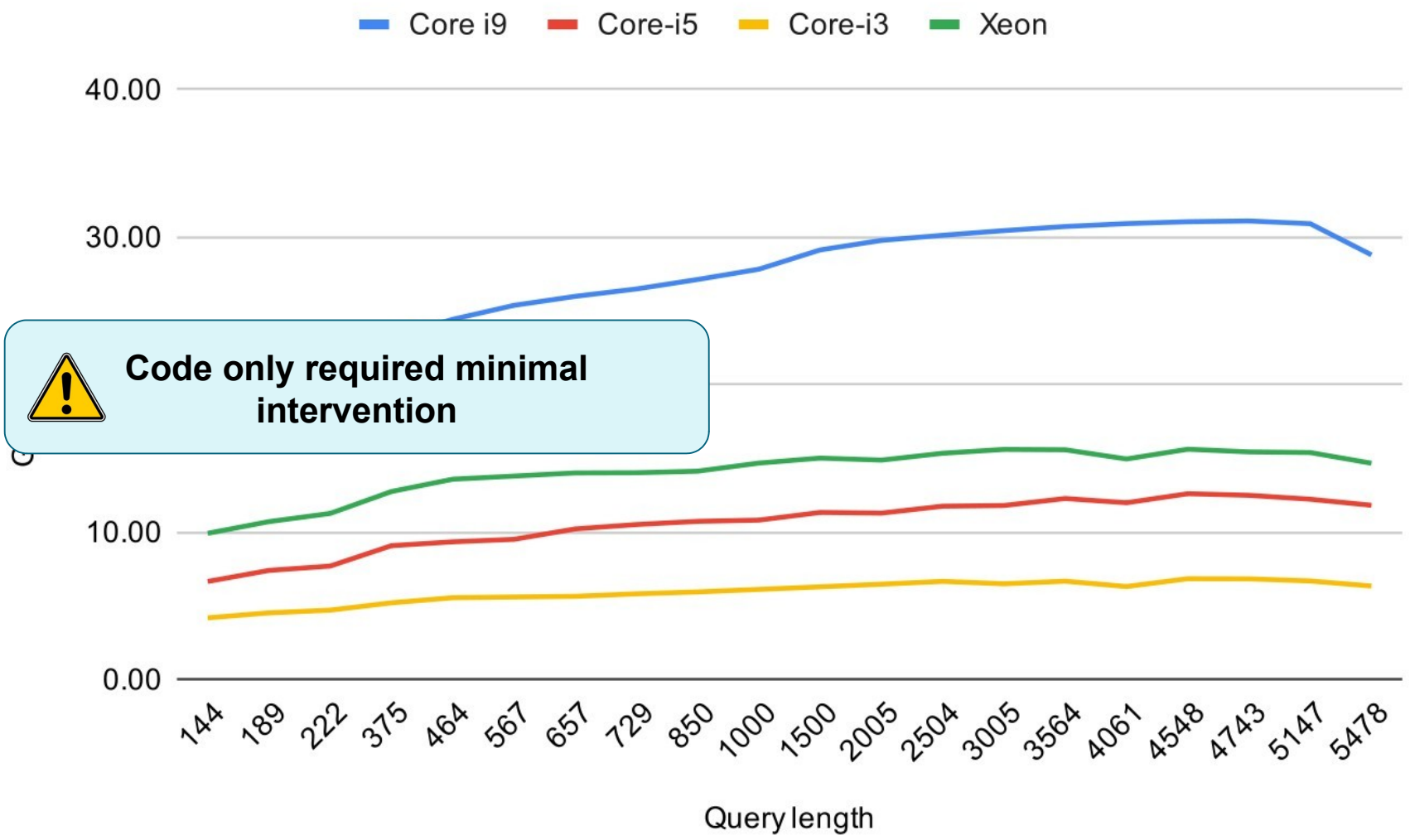

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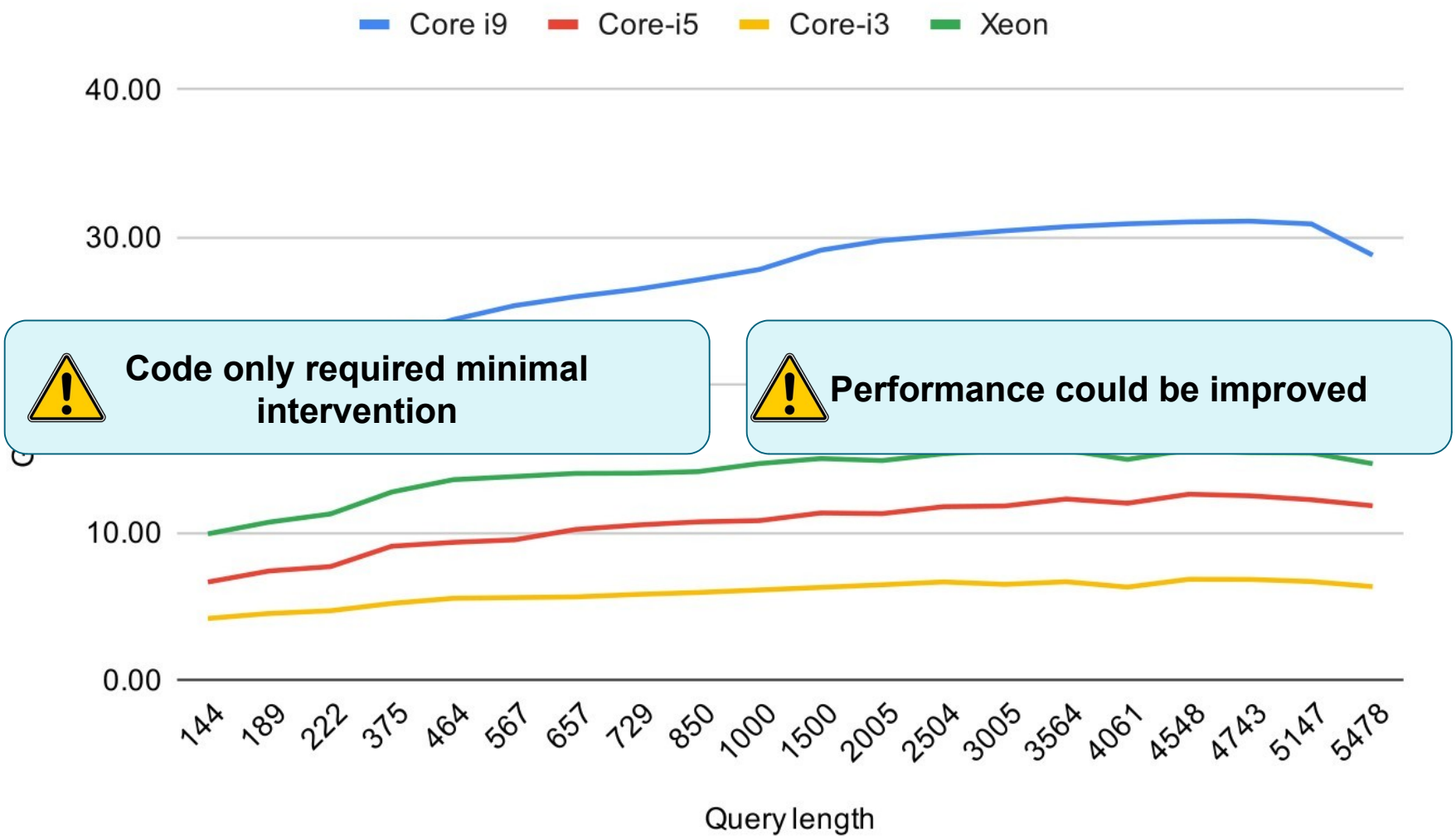

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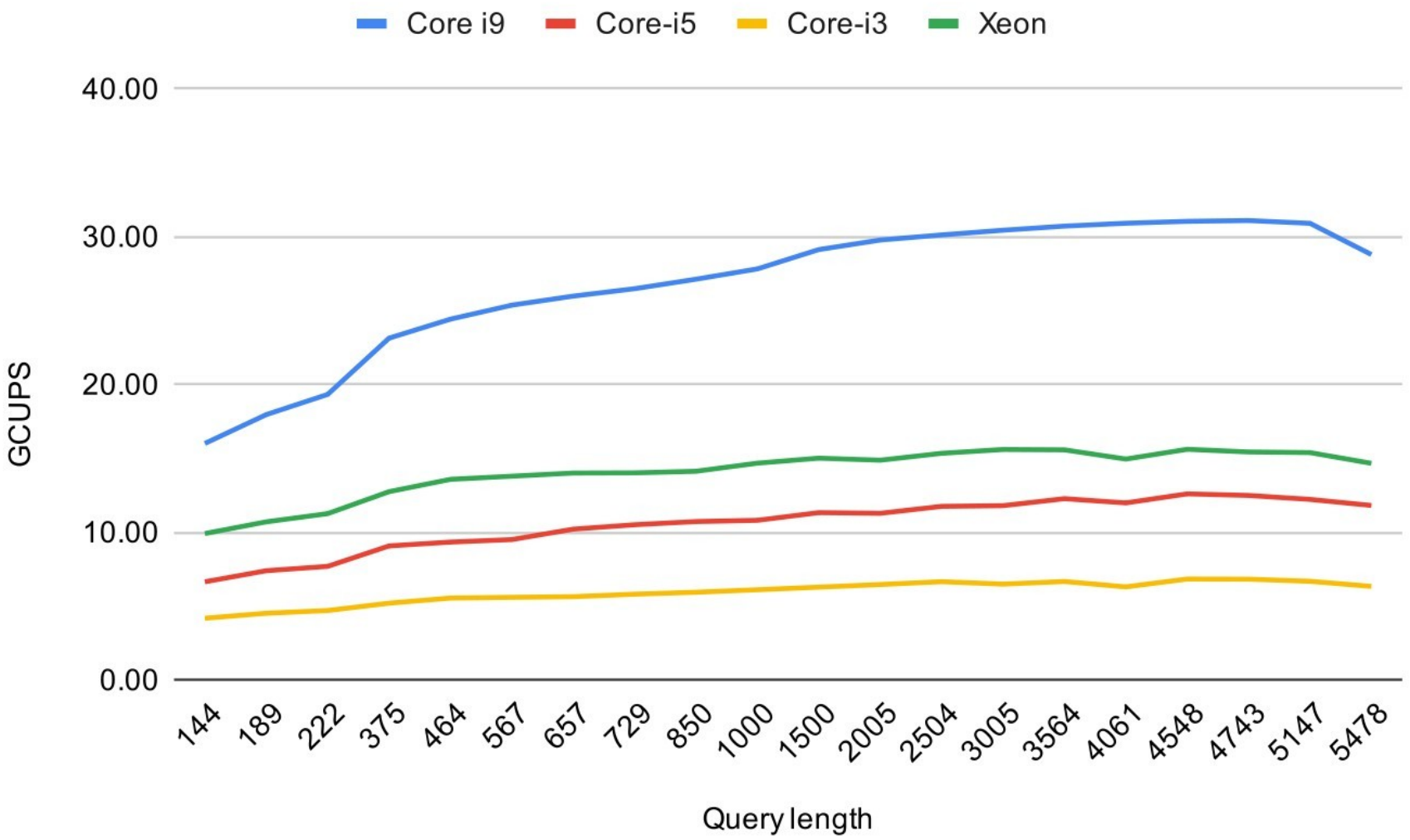

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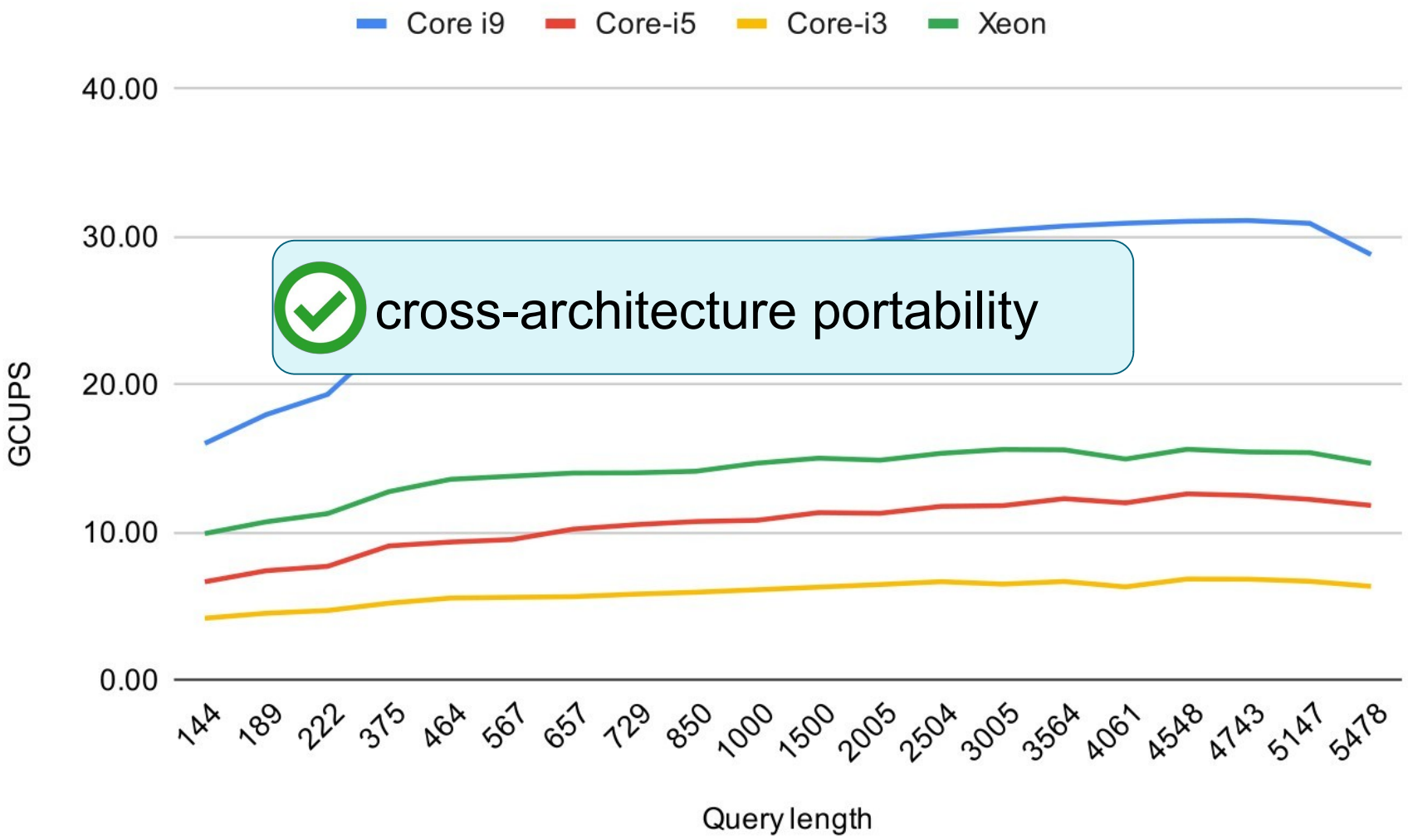

Agenda

- Motivation and Goal
- oneAPI
- Smith-Waterman
- Experimental Work
- Experimental Results
- **Conclusions**

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This paper presents our experiences migrating a CUDA-based, biological software tool to DPC++ using the oneAPI framework.

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The main contributions are:

1. DPCT proved to be an effective tool for code migration to DPC++
2. The migrated code could be successfully executed on CPUs and also GPUs from different vendors, demonstrating its cross-architecture, cross-vendor GPU portability
3. The performance results showed that the migrated DPC++ code is comparable to the original CUDA one.

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3. Running the DPC++ code on other architectures such as FPGAs, to verify its cross-architecture portability.

¡Thank you very much for your time!

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