Transforming Irregular Algorithms for Heterogeneous Computing - Case Studies in Bioinformatics

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Invent the Future

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Irregular Algorithms

- Characterized by …
  - Operate on **irregular data structures** - trees, graphs, linked lists, priority queues
  - Data are processed in variable-iteration loops
  - Both memory access and control flow are **irregular** and **unpredictable**

- Emerging data intensive applications have increasing irregularity in memory access and control flow over massive data set
  - Bioinformatics applications
    - Human genome: 3.2 billion letters (3.2 Gb)
  - Social network analysis, graph algorithms
    - Twitter (June-Dec 2009) - 17 million users, 476 million tweets (6Gb)

Heterogeneous Computing Systems

- Heterogeneous computing systems can offer massively parallel computation with high power efficiency and throughput
  - **GPU, AMD APU**
  - **Intel Xeon Phi**
  - FPGA, DSP, …
- But, designed for regular programs, relying on data locality and regular computation to tolerate access latencies
  - Thousands of smaller (weak), more efficient (simple) cores
  - Limited cache size, i.e., short cache line lifetimes

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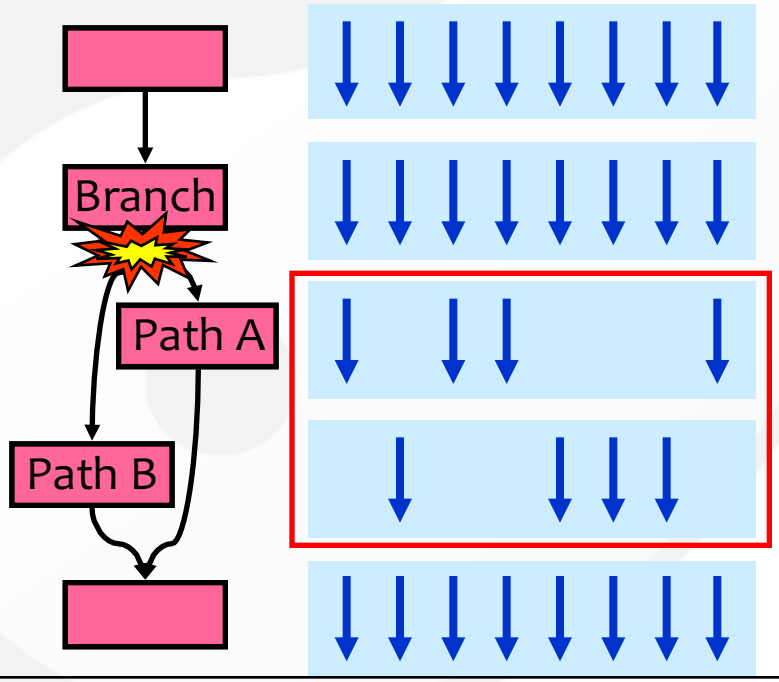
  - FPGA, DSP, …

- But, designed for regular programs, relying on data locality and regular computation to tolerate access latencies
  - Thous… …es, which… …on, etc.
  - Limite…

It is very challenging to map irregular algorithms on heterogeneous computing systems!

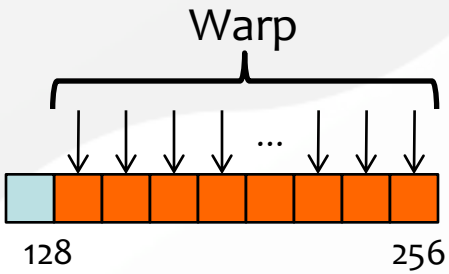
Impacts of Irregularity on GPU Performance

- Irregular control flow
  - Branch divergence
    - Occurs when threads inside warps branches to different execution paths
    - Waste computational resource

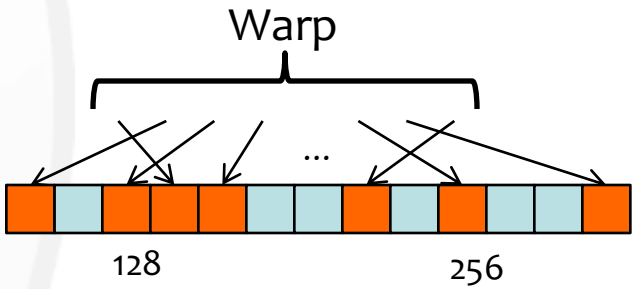


Impacts of Irregularity on GPU Perf (cont'd)

- Irregular memory access
  - Uncoalesced memory access
    - Lower memory bus utilization



One segments
A single 128-byte transaction
Coalesced Memory Access



Cross N segments
N 32-byte transaction
Uncoalesced Memory Access

Irregular Algorithms Optimizations on GPU

- Irregular control flow
  - Kernel fission
  - Sorting work
  - Warp-centric execution

  ……
- Irregular memory access
  - Memory access reordering
  - Exploiting memory hierarchy
  - Data structure adaptation

  ……

Case Study: Mapping BLASTp on GPU*

- BLAST - Basic Local Alignment Search Tool
  - Find most similar sequences from database for a query sequence
  - Use ***heuristic*** algorithms, which have significant irregularities in both memory access and control flow

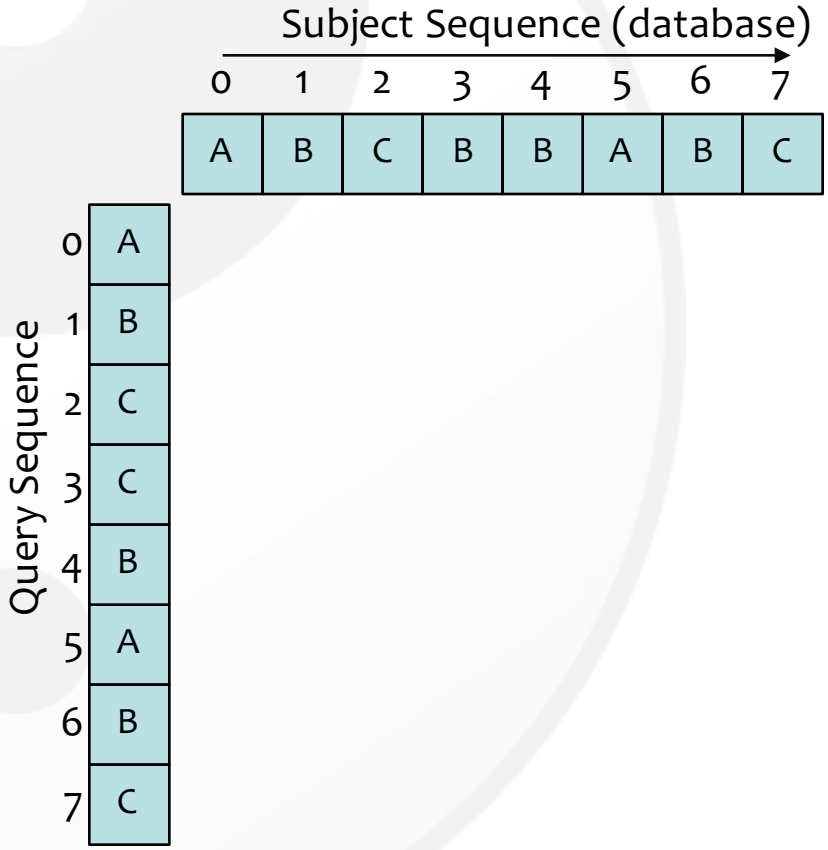
- P is for protein sequence; N is for nucleotide sequence

*: J. Zhang, H. Wang, H. Lin, W. Feng, "*cuBLASTP: Fine-Grained Parallelization of Protein Sequence Search on a GPU*", IPDPS 2014

BLAST Algorithm

Four stages in BLAST

1. Hit detection
2. Ungapped extension
3. Gapped extension
4. Final extension



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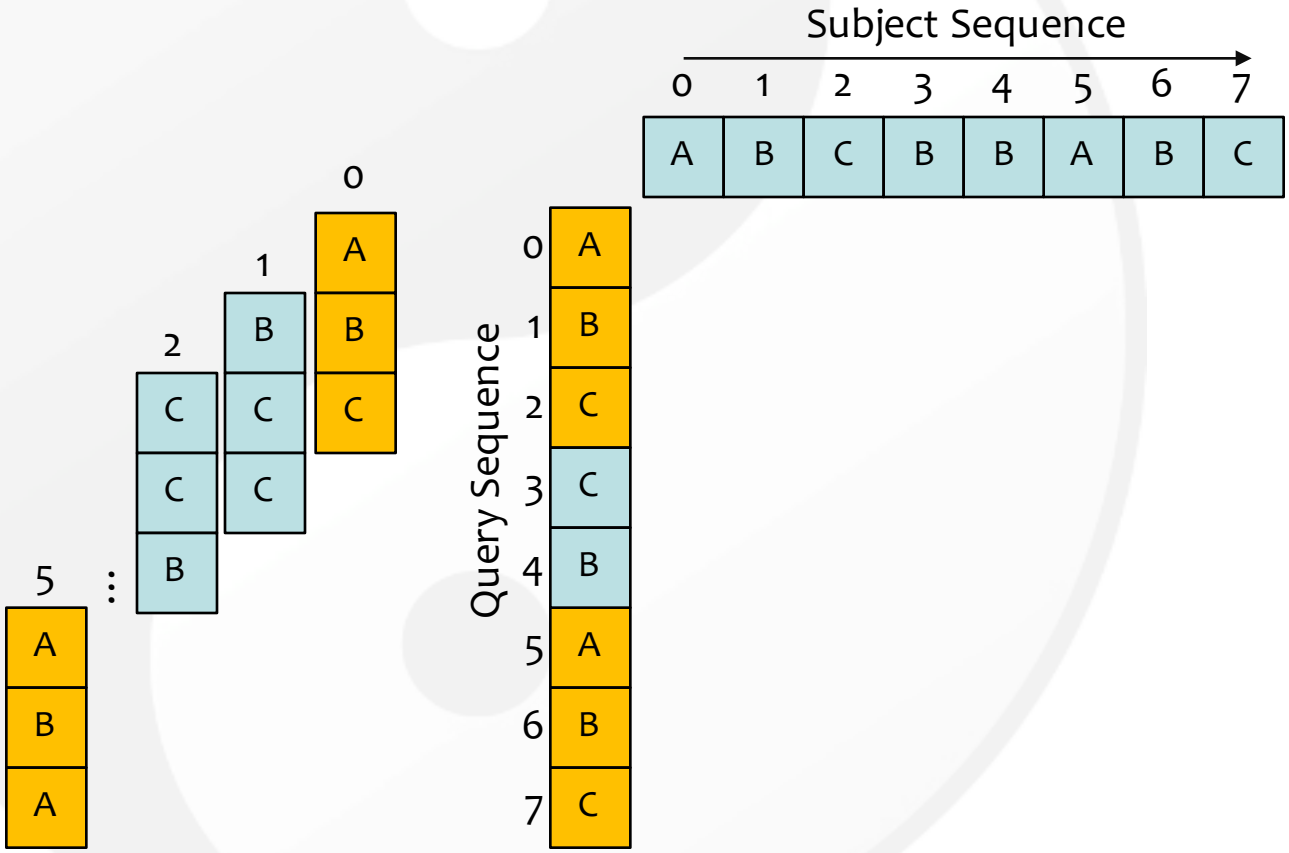

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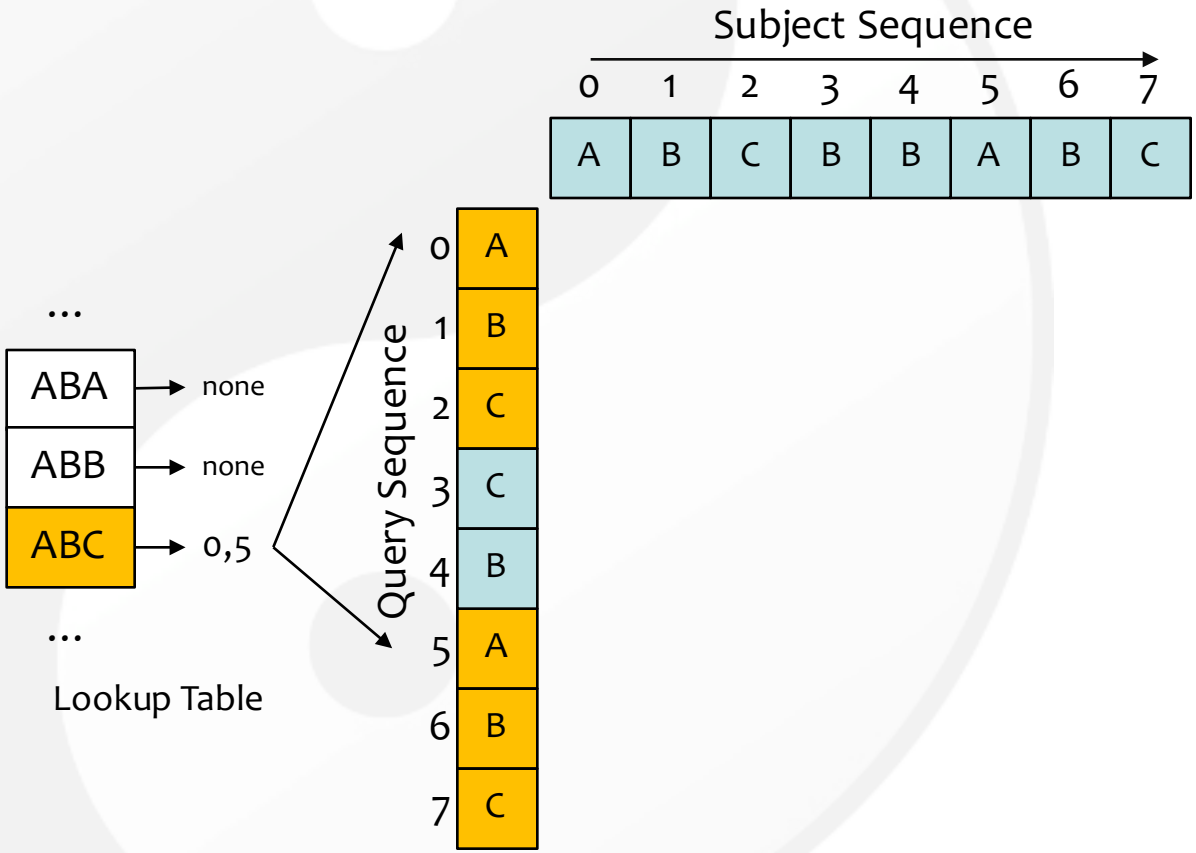

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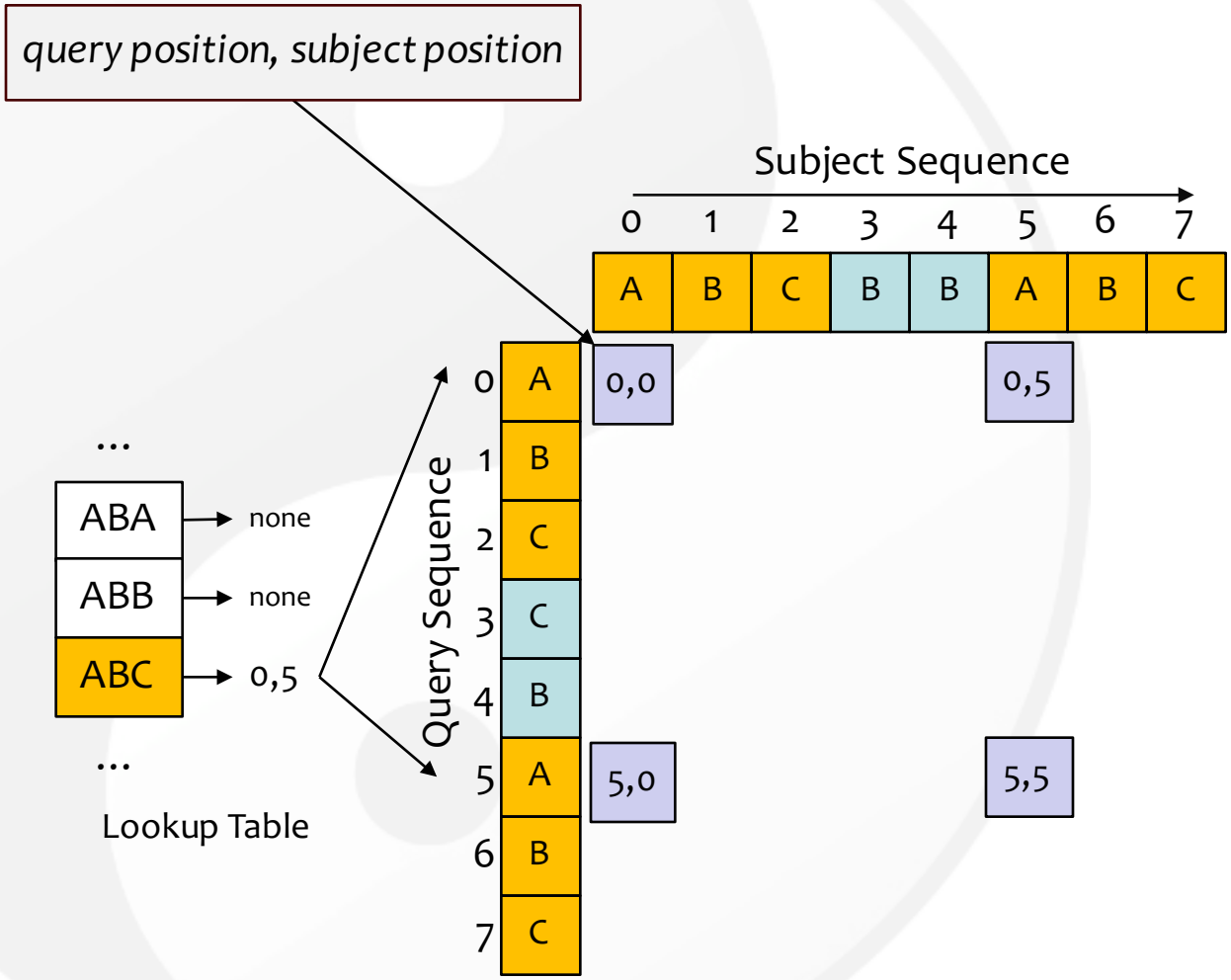

BLAST Algorithm

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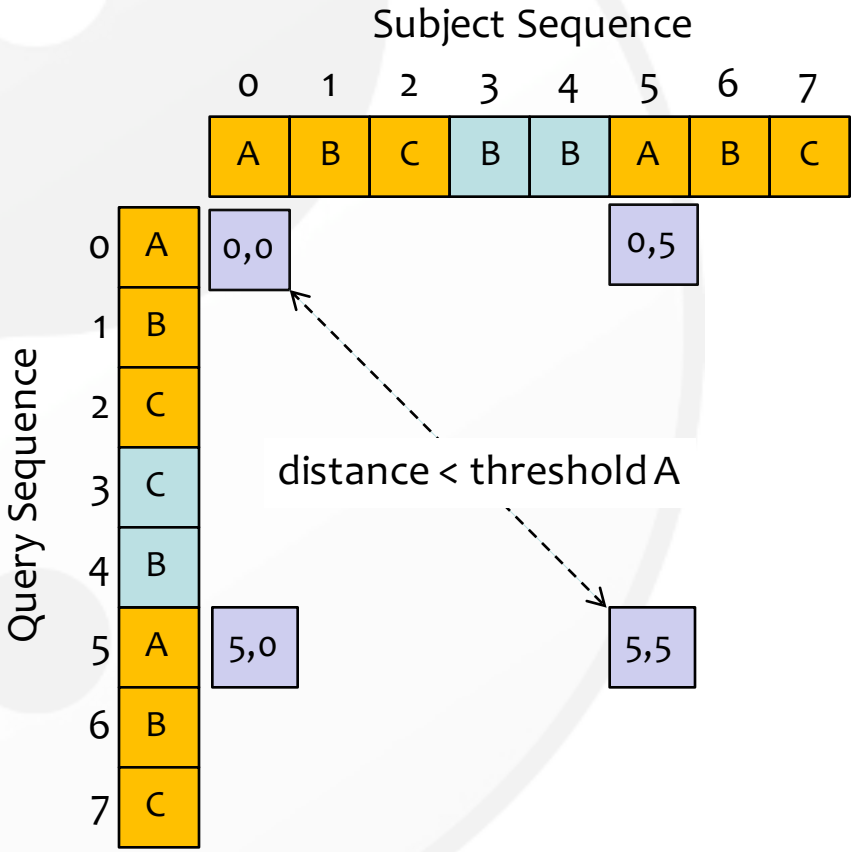

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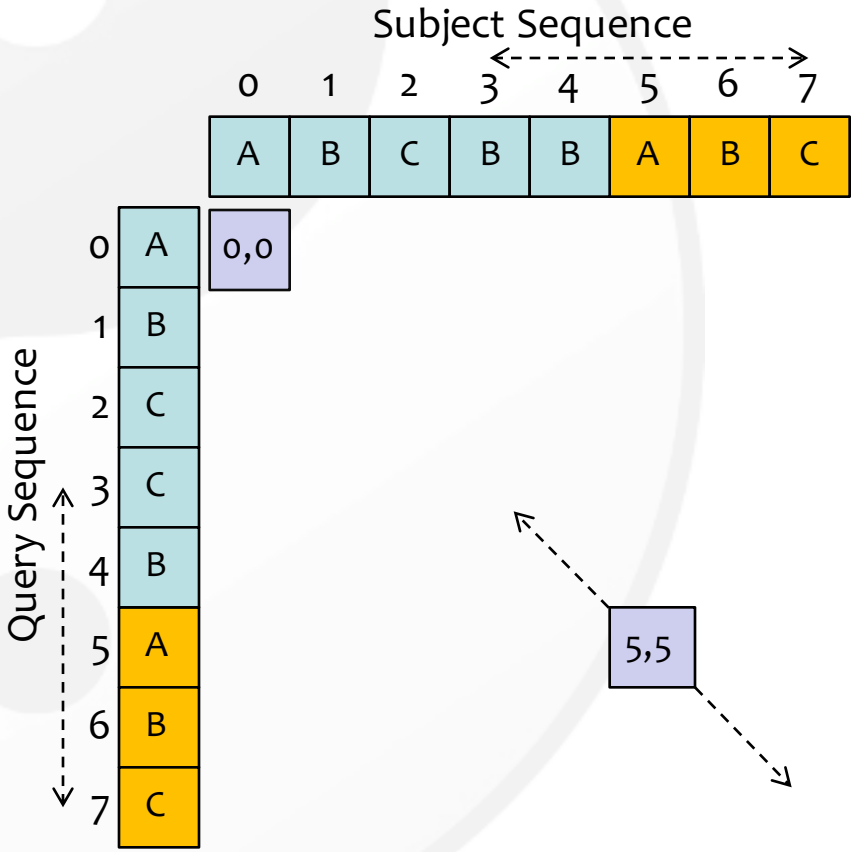

BLAST Algorithm

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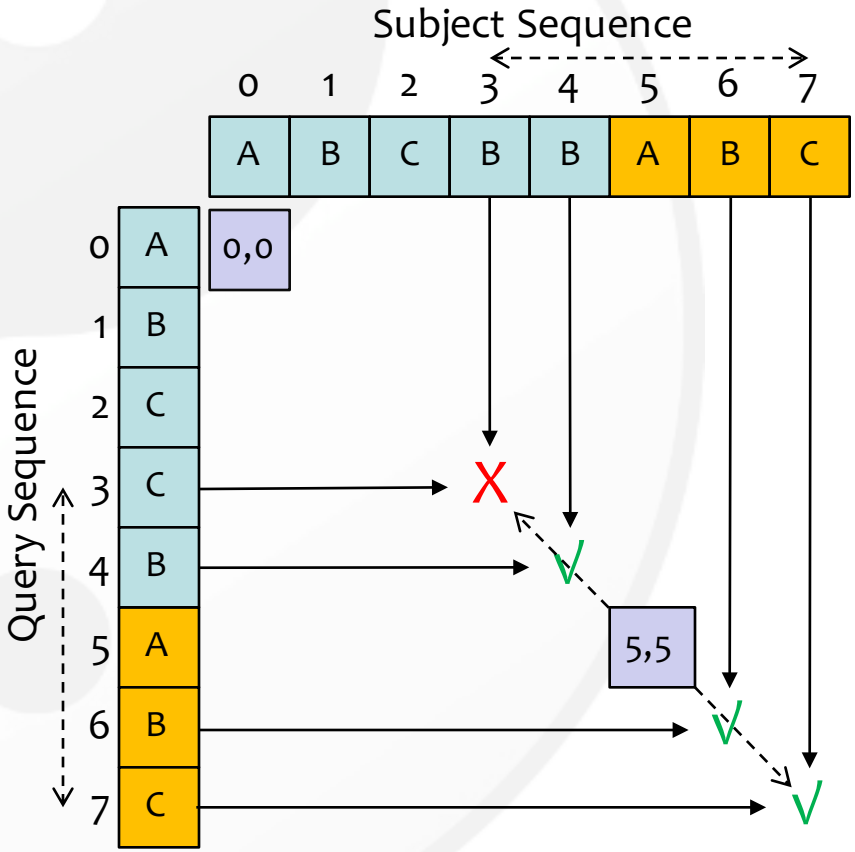

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Four stages in BLAST

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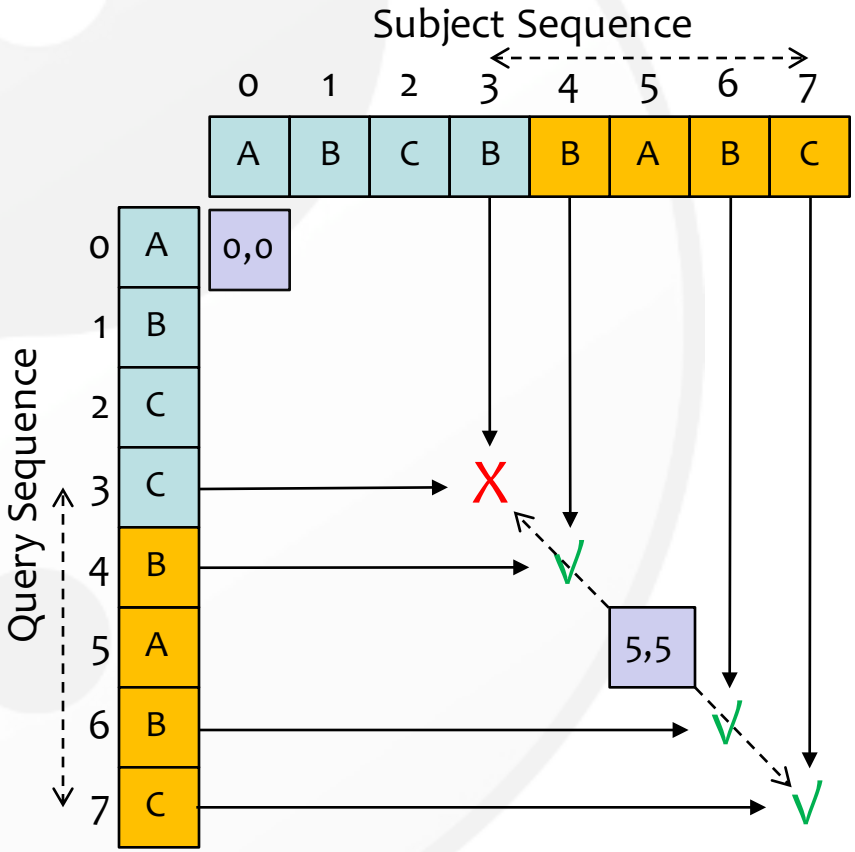

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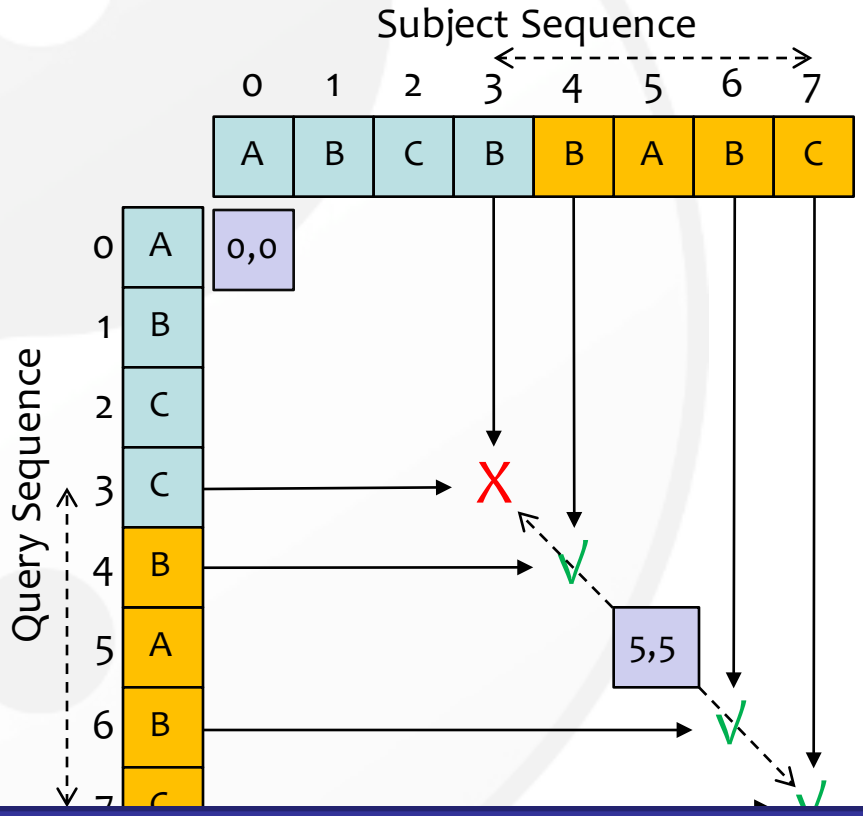
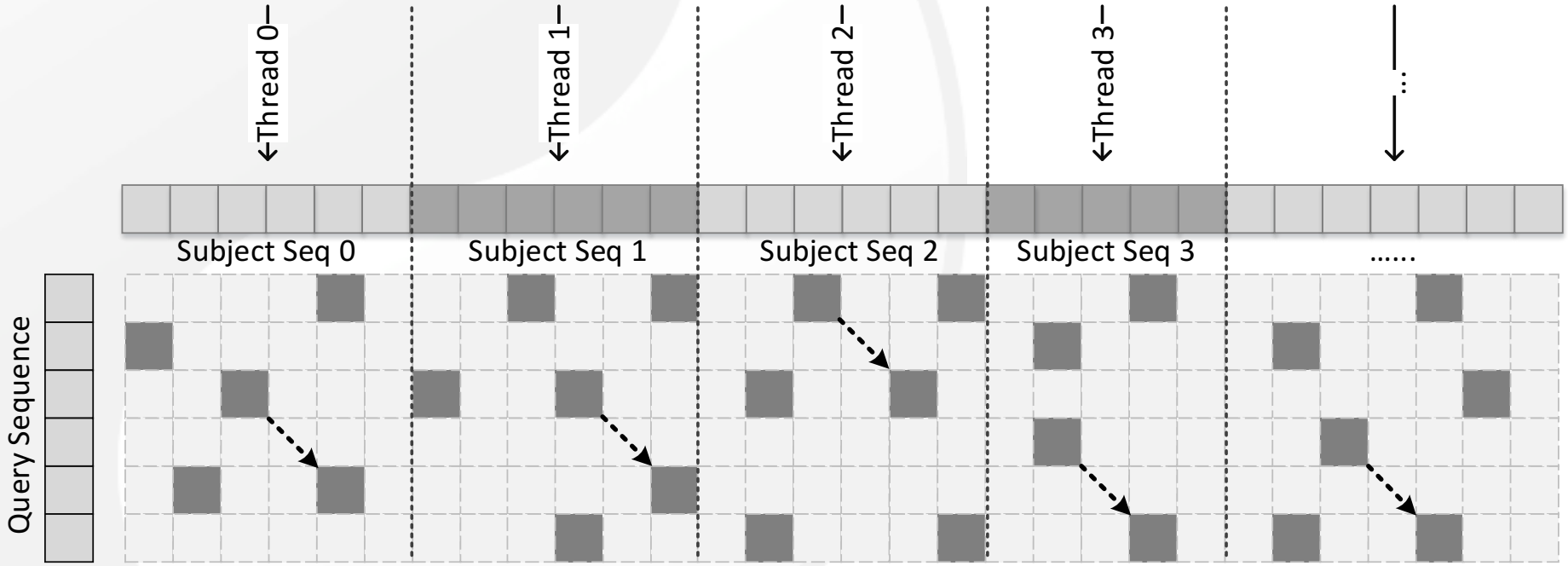


Knowledge: "seed-and-extend" – the most widely used alignment paradigm

State-of-the-Art GPU BLAST Approaches*

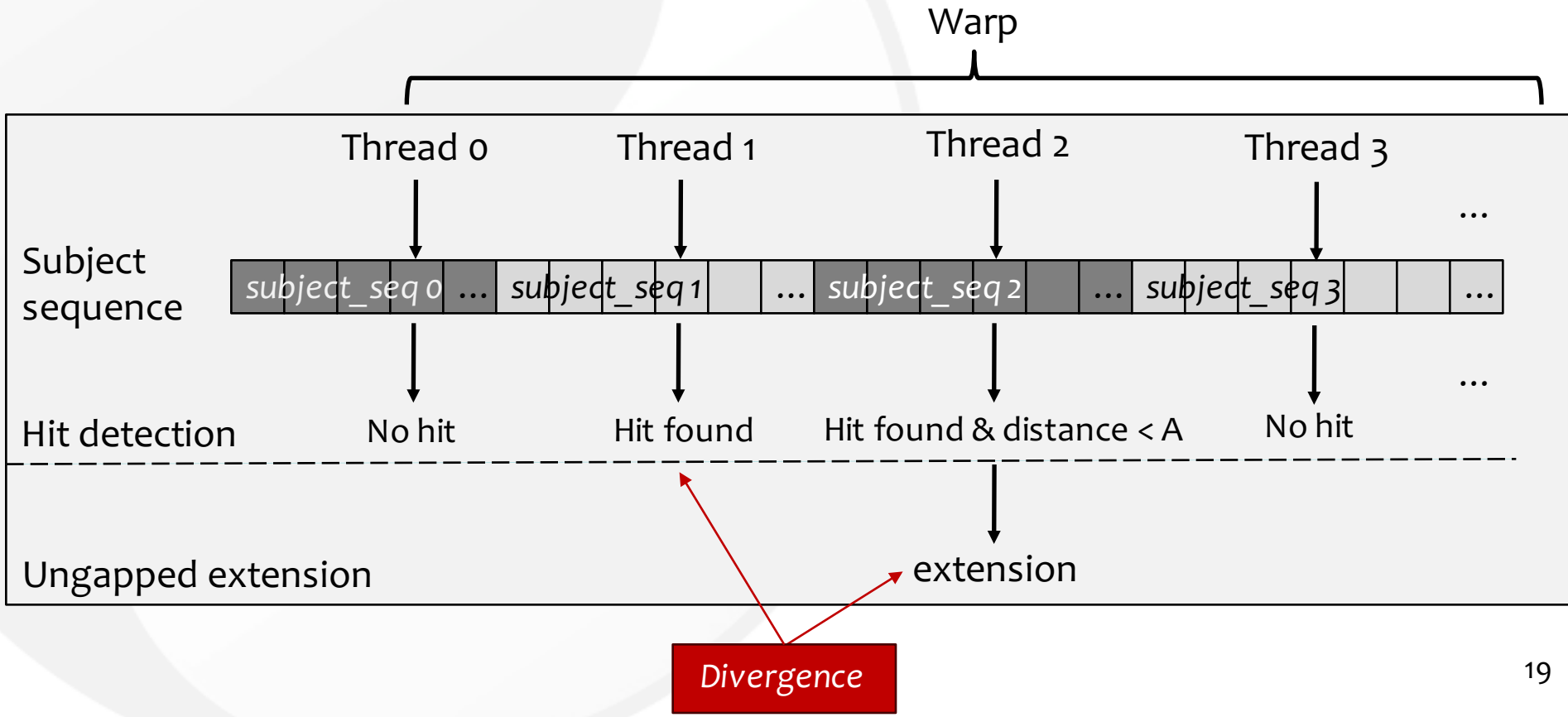
- Use intuitive parallelization - "coarse-grained parallelization", where a thread compares the query sequence to a subject sequence



*: Design and Implementation of a CUDA-compatible GPU-based Core for Gapped BLAST Algorithm (ICCS '10)
GPU- BLAST: Using Graphics Processors to Accelerate Protein Sequence Alignment CUDA-BLASTP (Binformatics)
CUDA-BLASTP: Accelerating BLASTP on CUDA-enabled Graphics Hardware (TCBB)
Accelerating Protein Sequence Search in a Heterogeneous Computing System. (IPDPS '11)

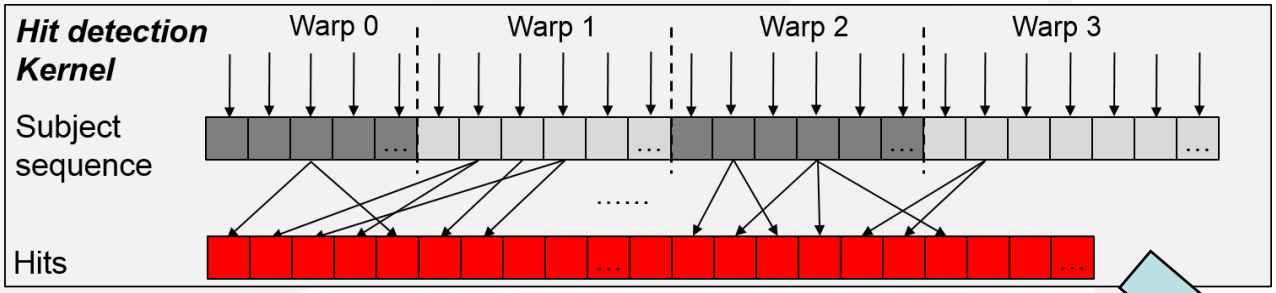
Challenge #1: Control Flow Irregularity

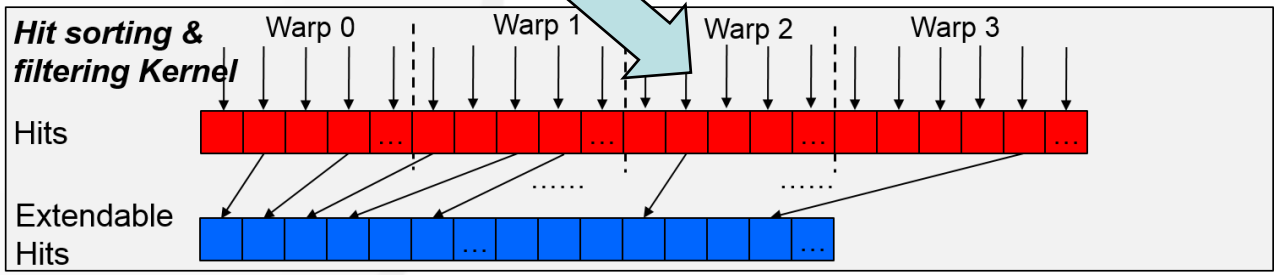
- With coarse-grained parallelism, different threads may execute across different stages

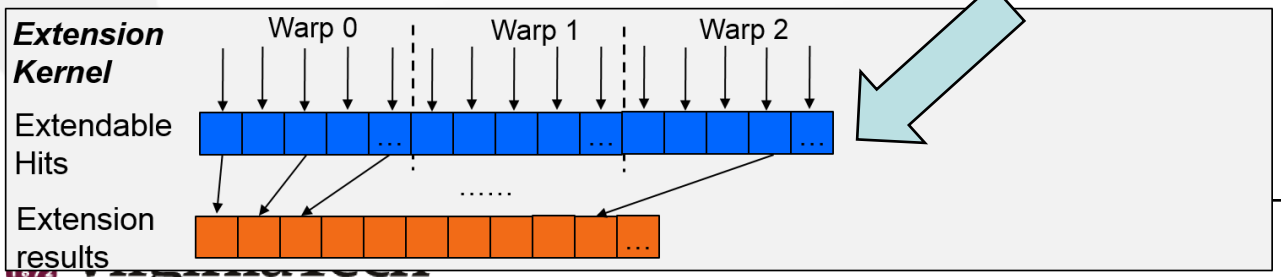


Solution: Kernel Fission

- Split hit detection and ungapped extension stage into separate kernels
- Use intermediate kernels to bridge the two stages

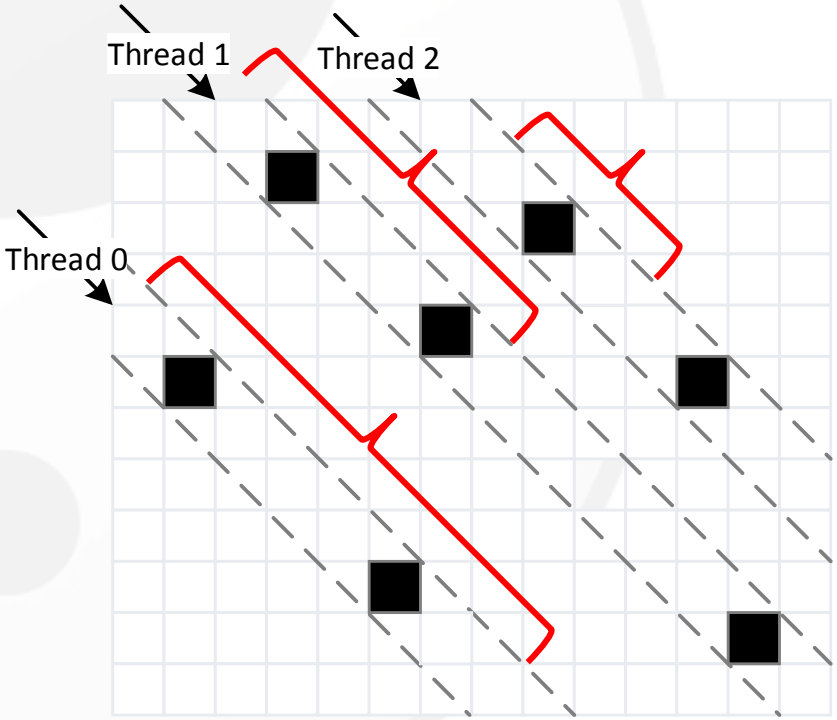






Challenge #2: Control Flow Irregularity (2)

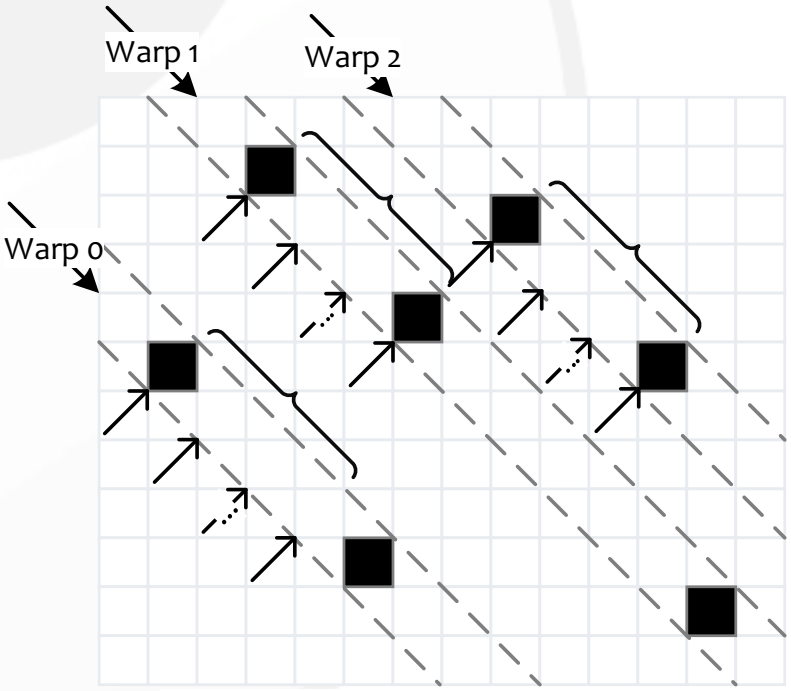
- Coarse-grained extension, where a thread is responsible for a diagonal, can result in divergence, since different diagonals could be extended to different lengths



One thread per diagonal

Solution: Warp-centric Extension

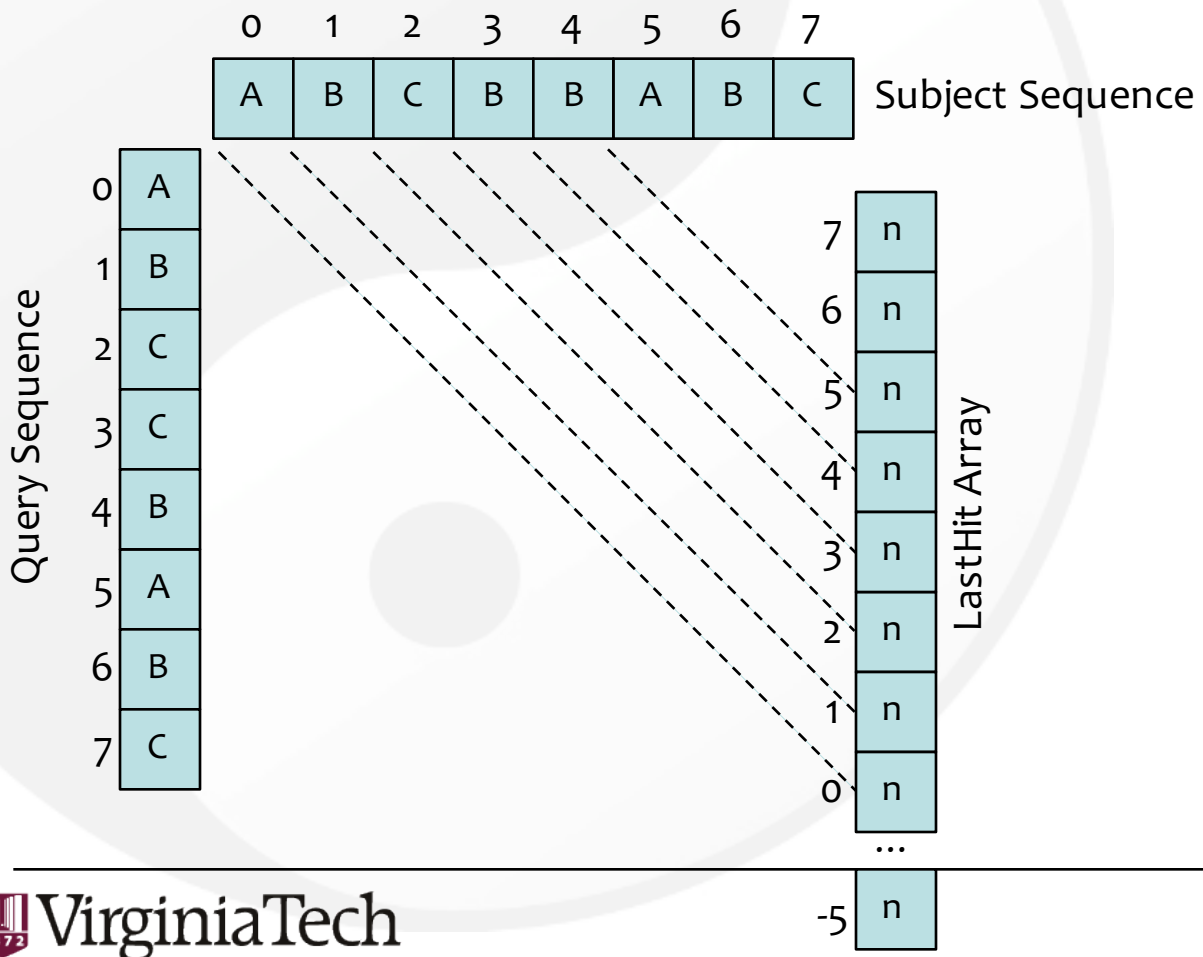
- Map a warp of threads to one diagonal
- Threads in a warp checks different positions concurrently



Warp-based Extension

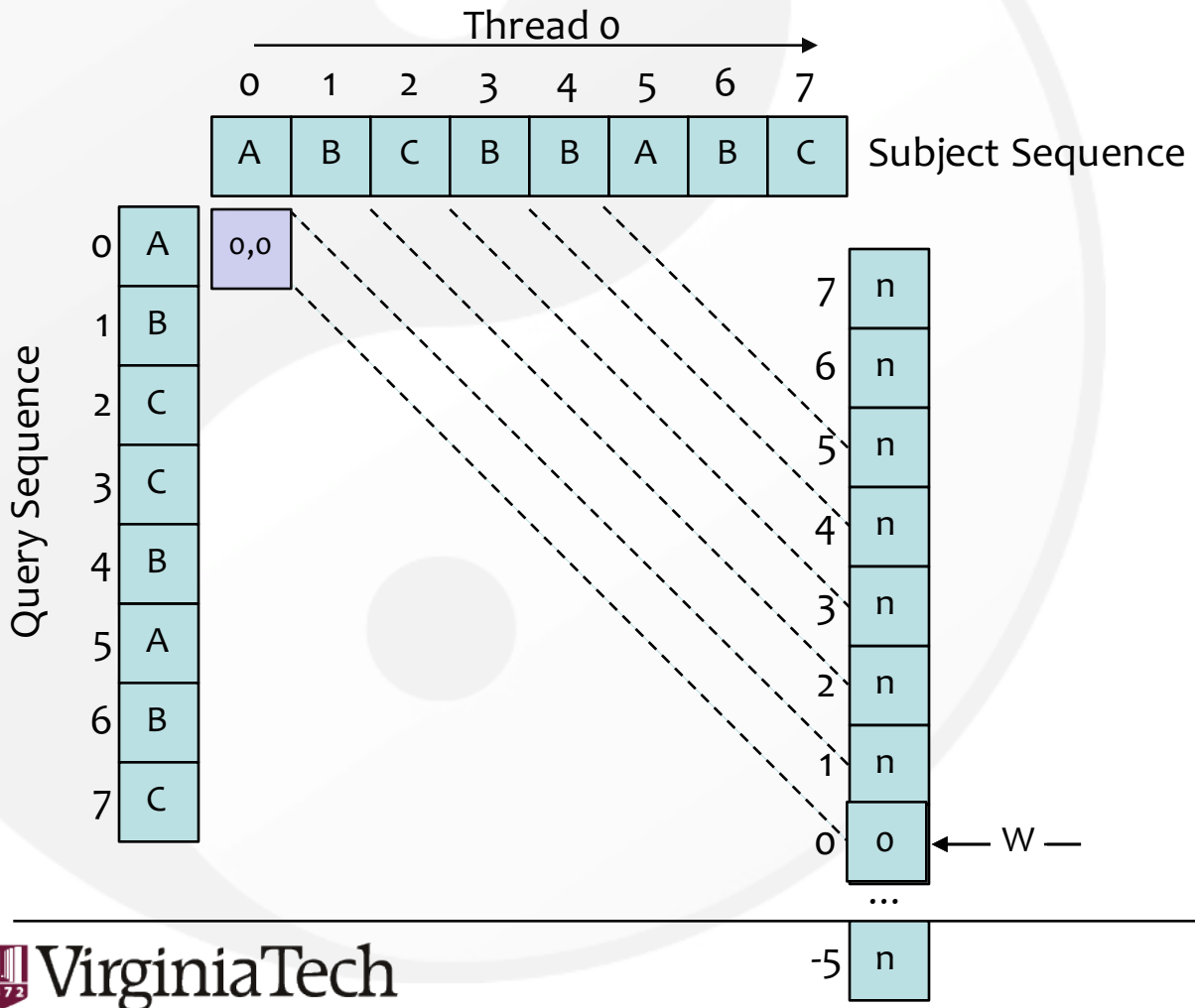
Challenge #3: Memory Access Irregularity

- Use a global array, called lastHit Array, to record the previous hit in each diagonal



Challenge #2: Memory Access Irregularity

- Read LastHit Array to get last hit position in the diagonal
- Write back current position to lastHit Array



Operation	Position
Read	o
Write	o

Challenge #2: Memory Access Irregularity

- Read LastHit Array to get last hit position in the diagonal
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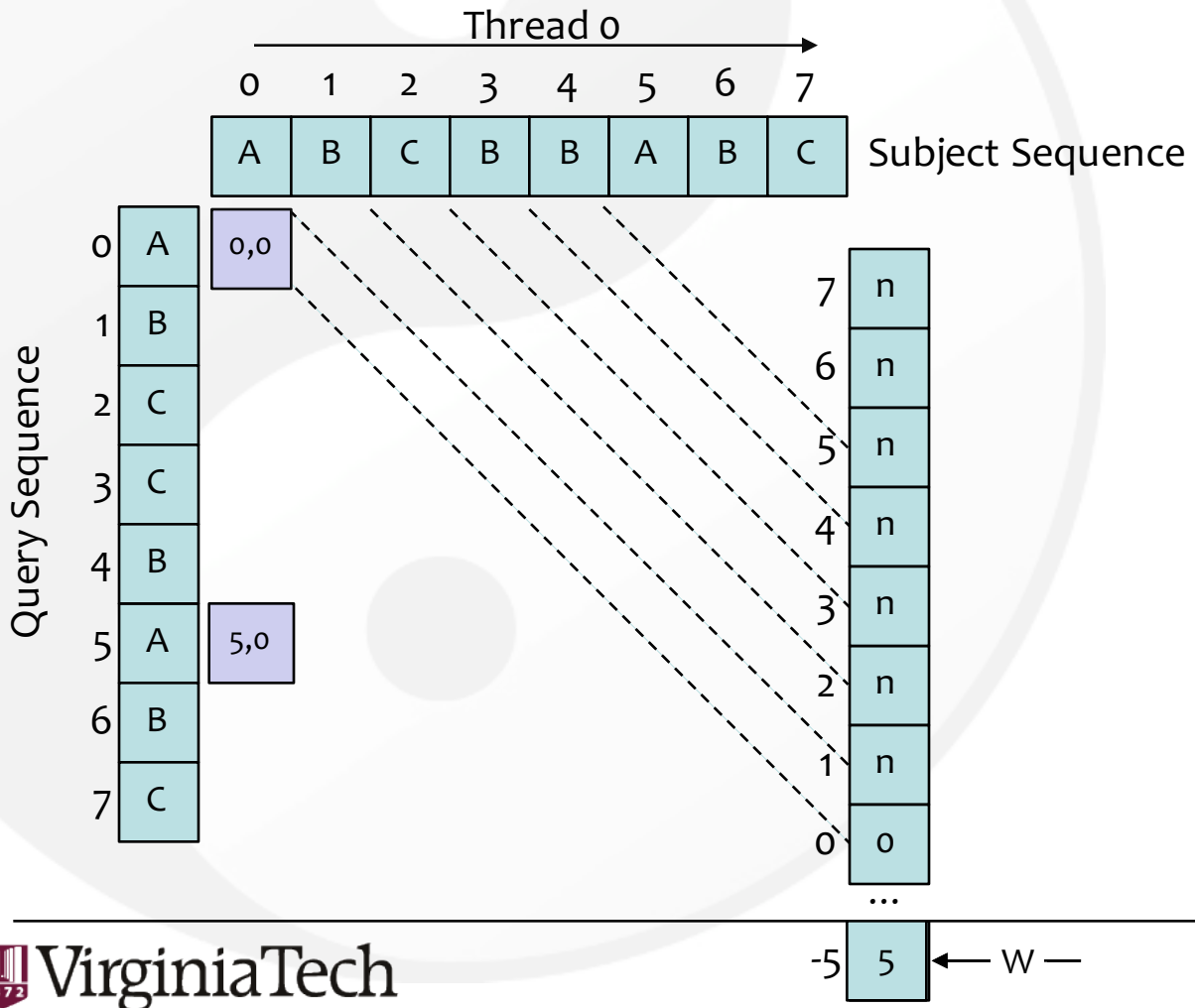
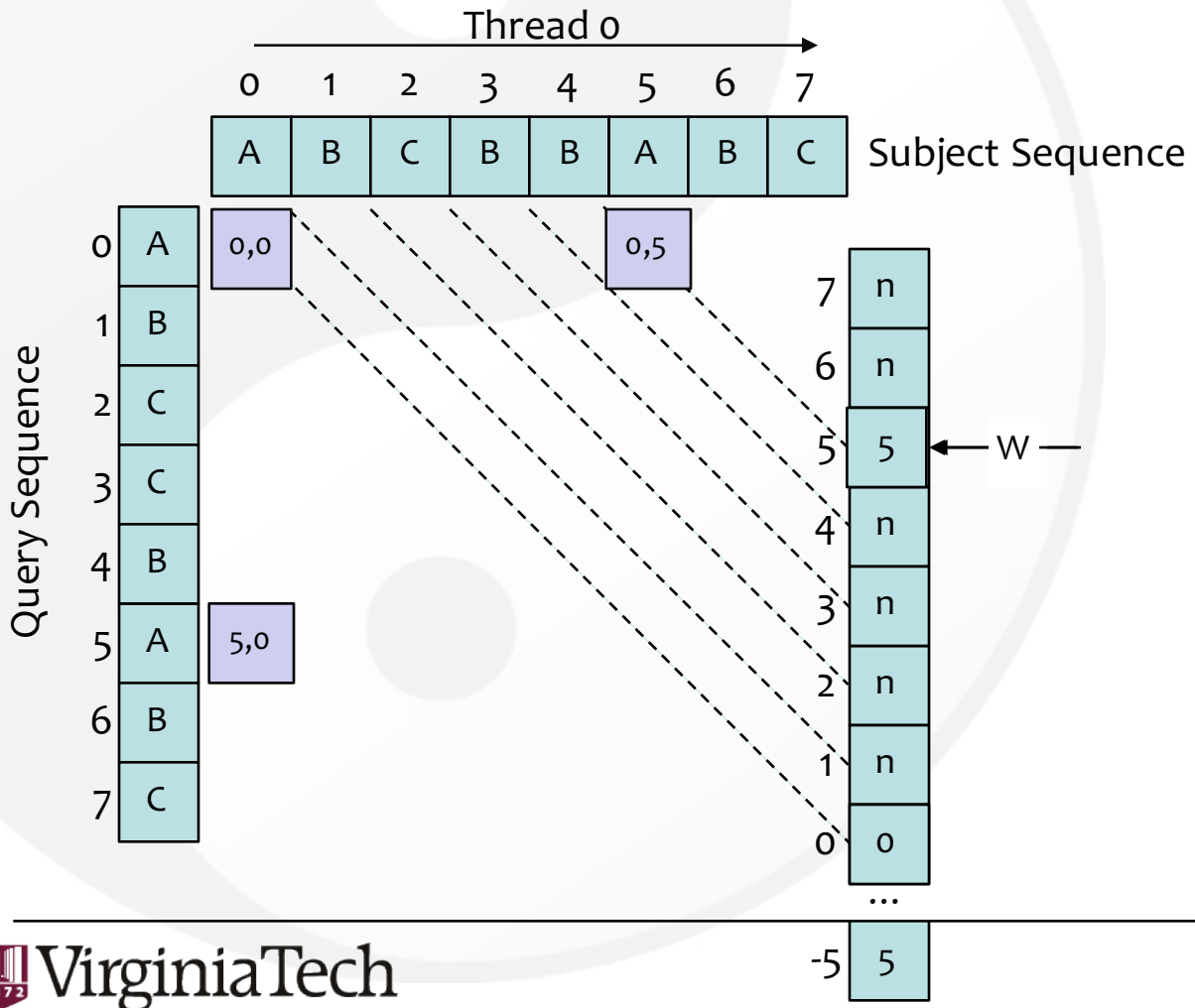


Operation	Position
Read	0
Write	0
Read	-5
Write	-5

Challenge #2: Memory Access Irregularity

- Read LastHit Array to get last hit position in the diagonal
- Write back current position to lastHit Array



Operation	Position
Read	0
Write	0
Read	-5
Write	-5
Read	5
Write	5

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- Read LastHit Array to get last hit position in the diagonal
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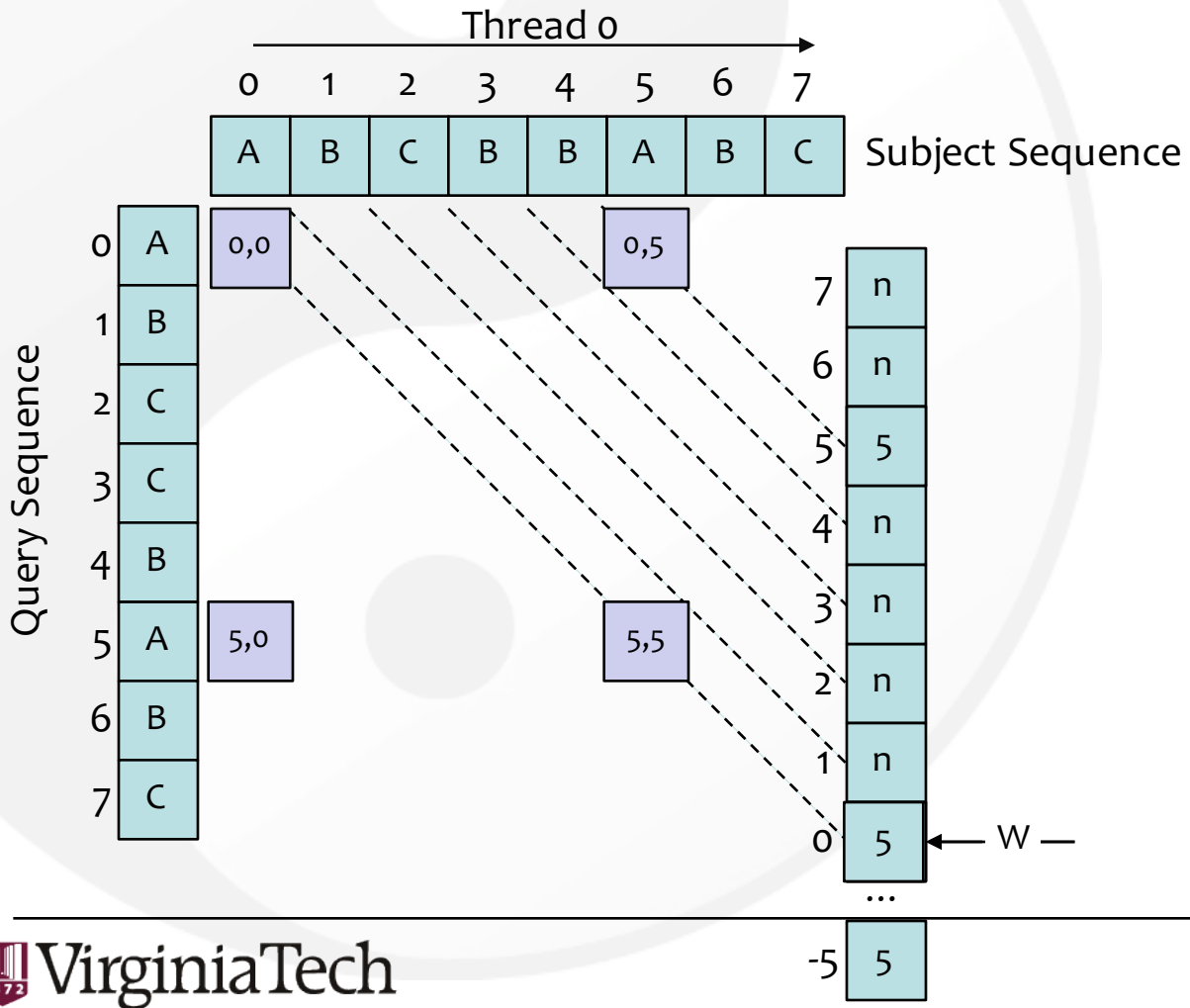
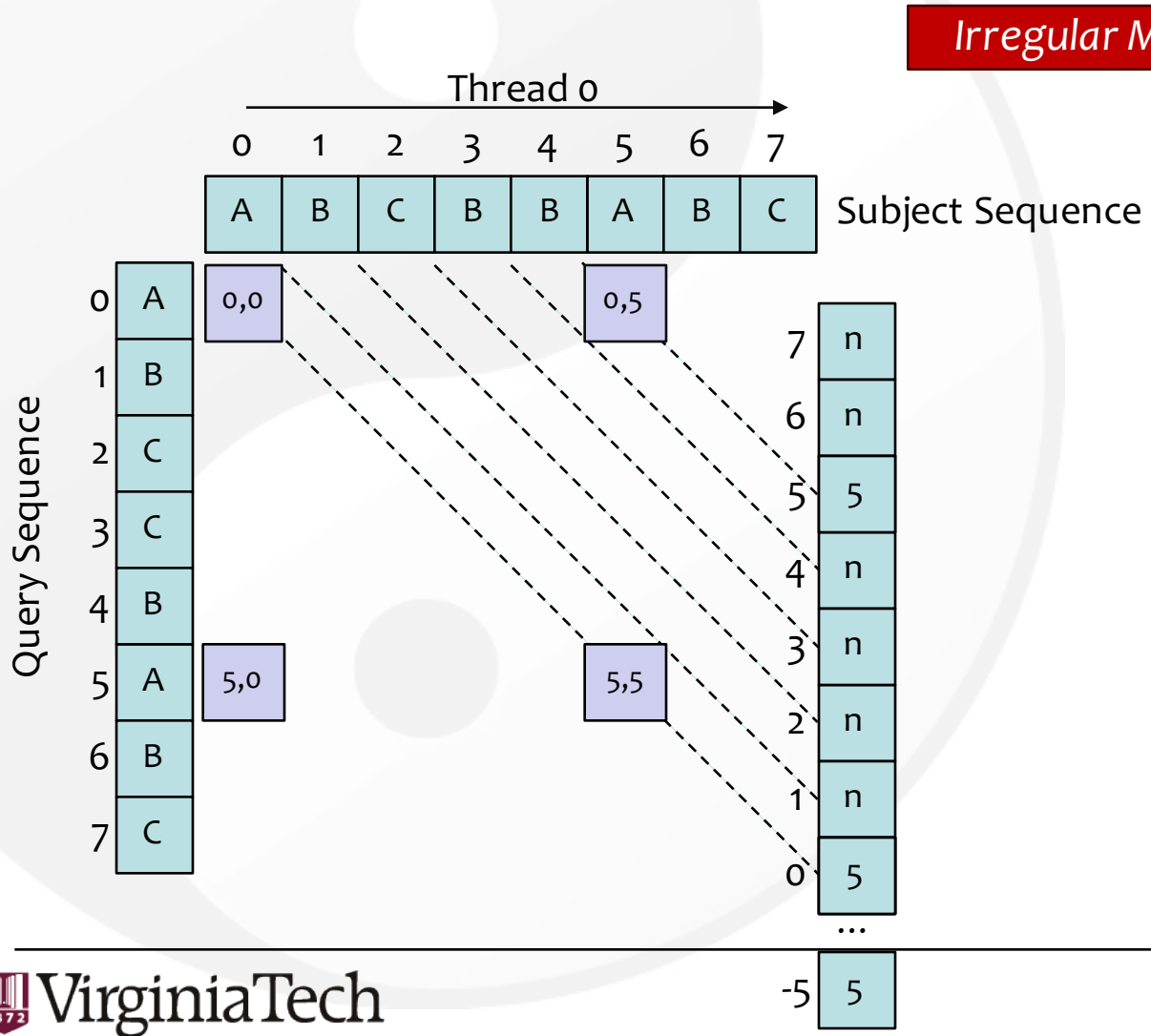


Operation	Position
Read	0
Write	0
Read	-5
Write	-5
Read	5
Write	5
Read	0
Write	0

Challenge #2: Memory Access Irregularity

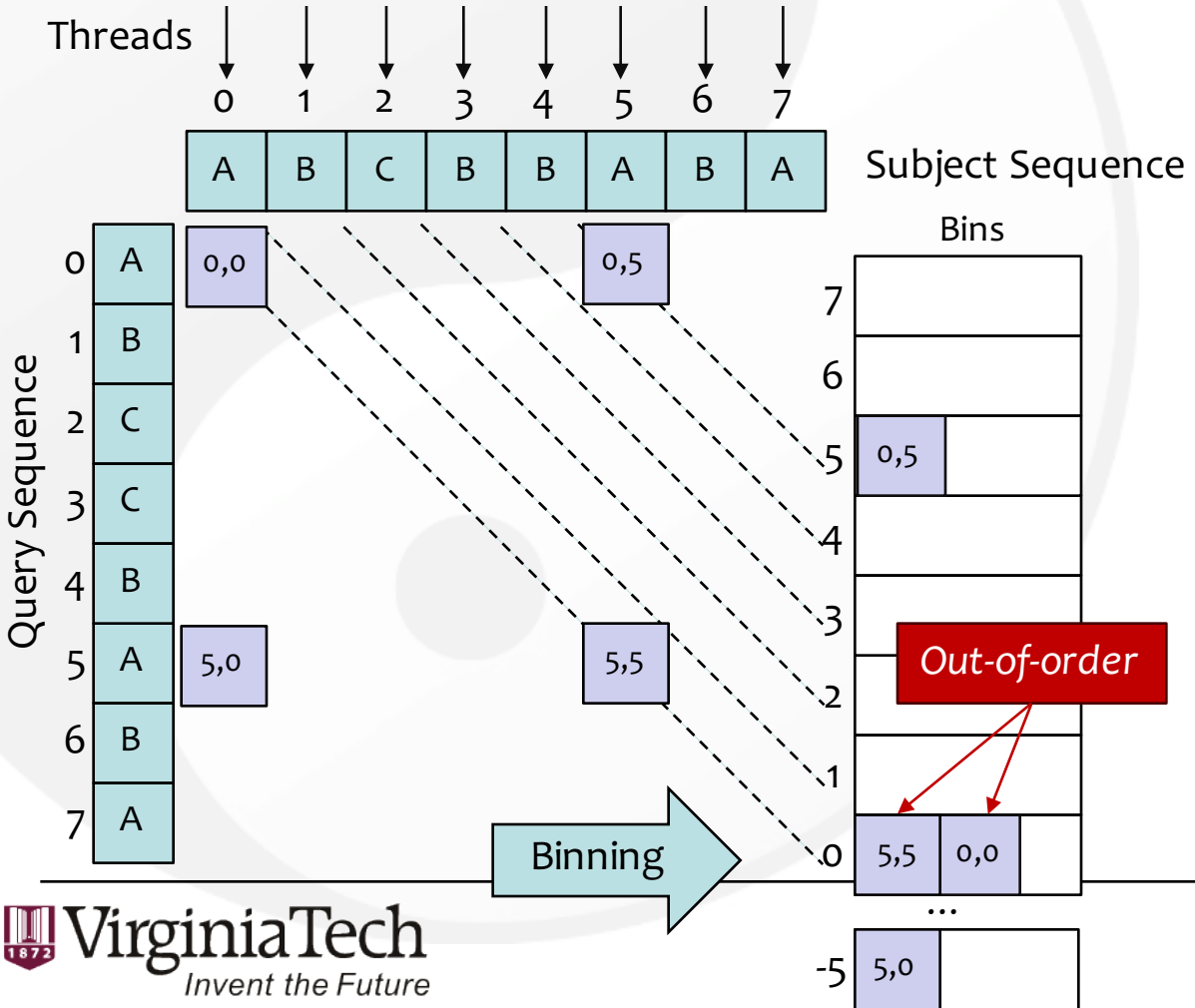
- Irregular Read/Write Ops on LastHit array



Operation	Position
Read	0
Write	0
Read	-5
Write	-5
Read	5
Write	5
Read	0
Write	0

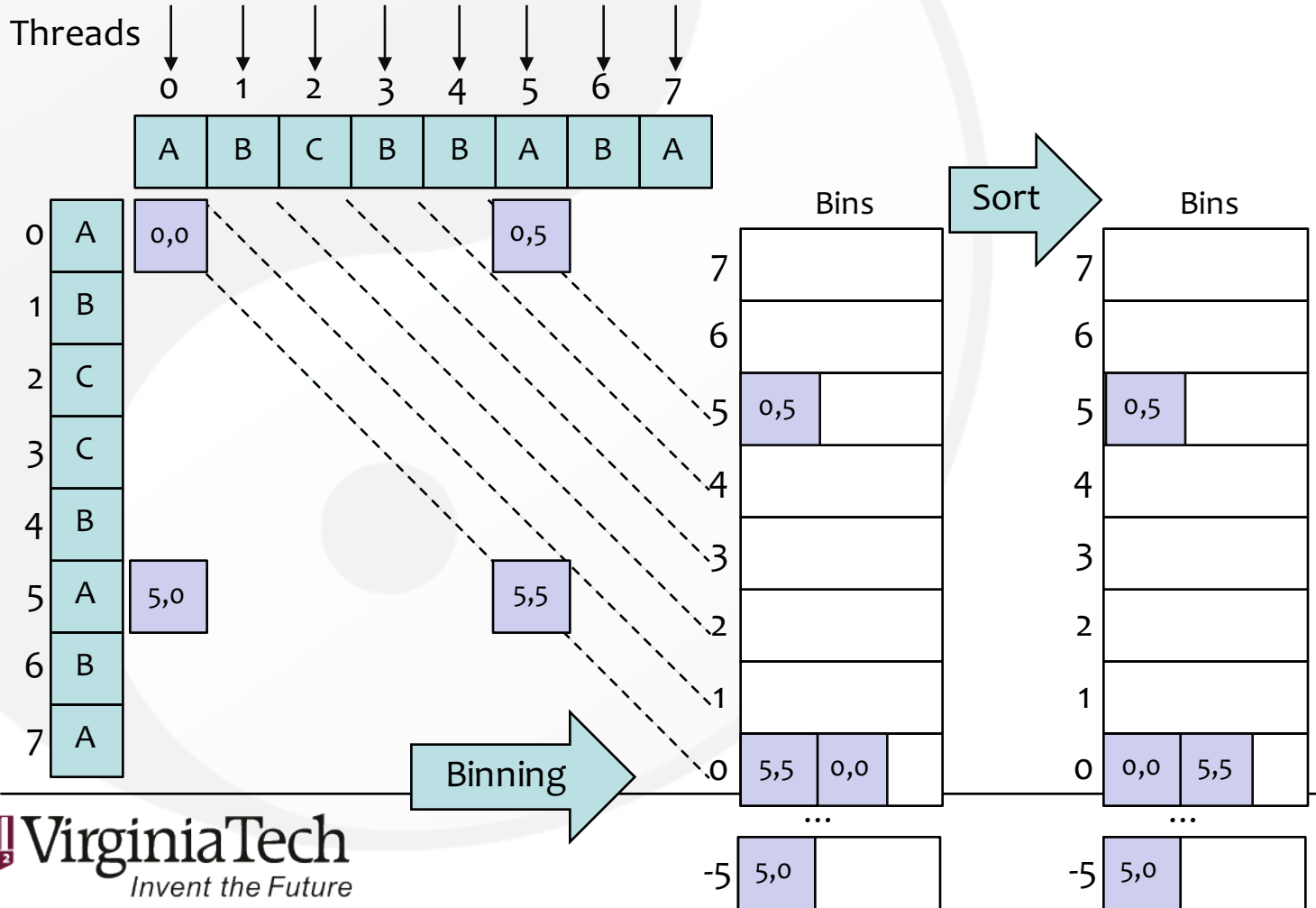
Solution: Memory Access Reordering

- Collect and group hits by diagonal numbers via binning



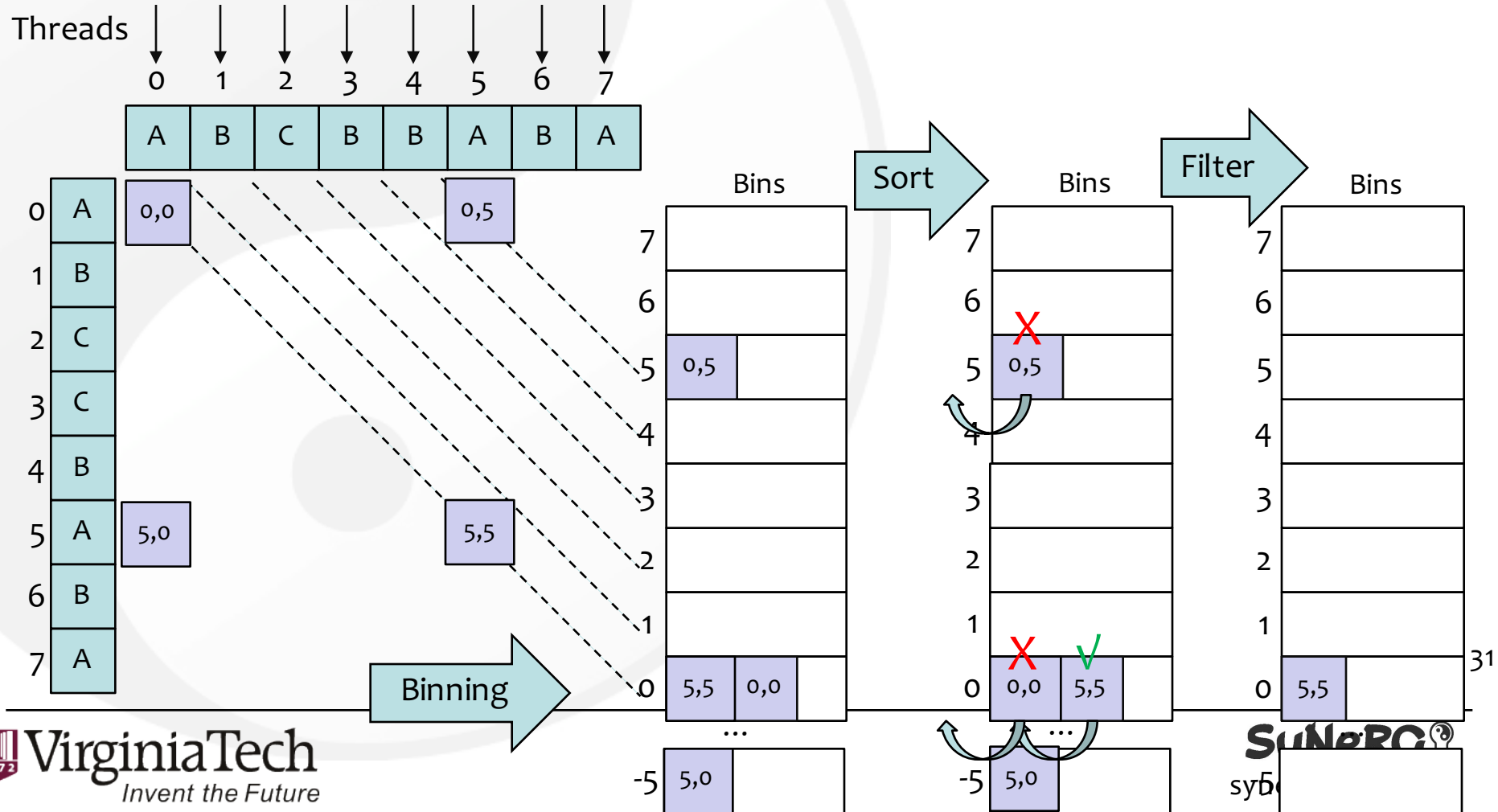
Solution: Memory Access Reordering

- Sort hits by positions in each bin



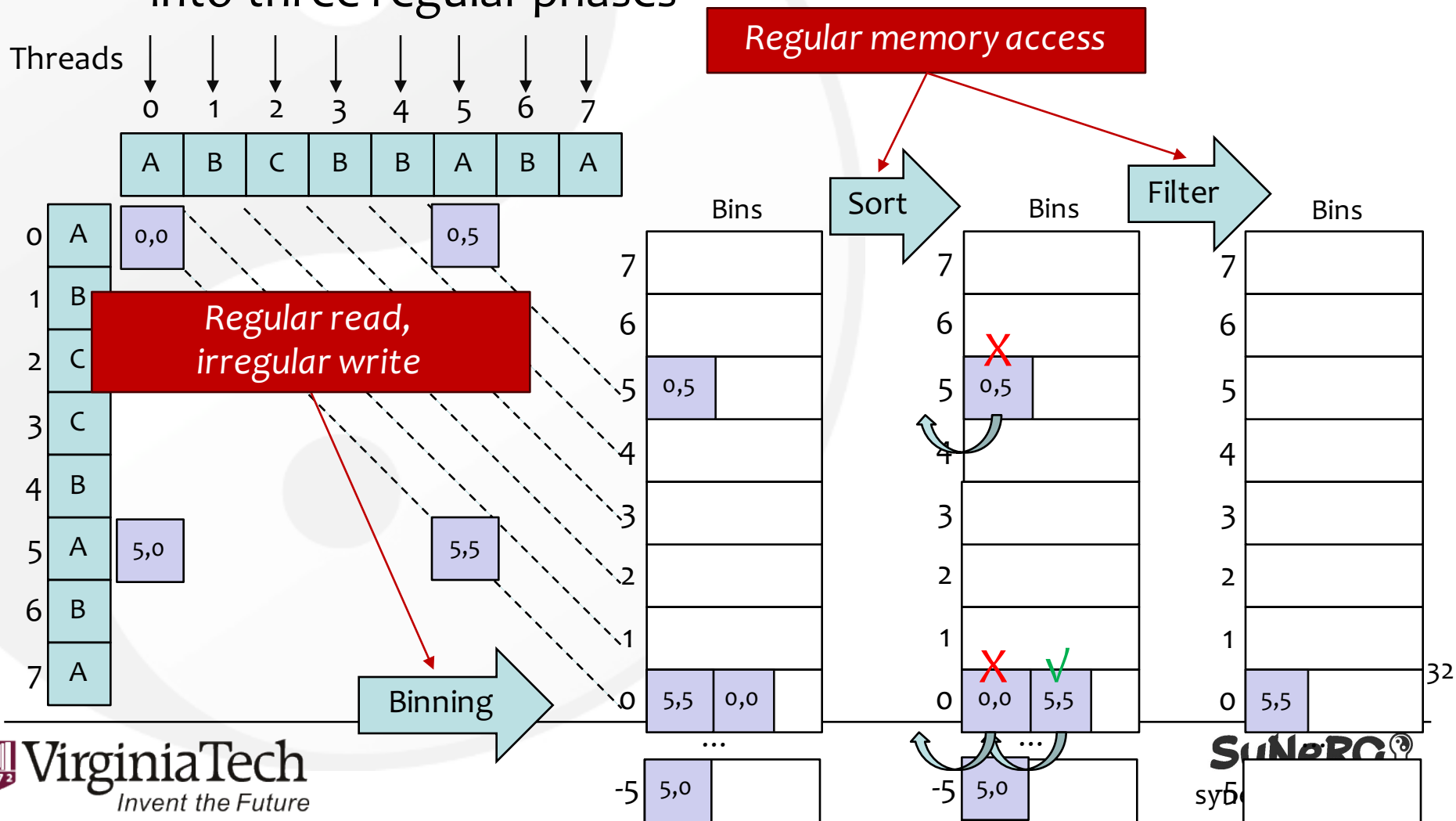
Solution: Memory Access Reordering

- Filter out non-extenable hits by distance of adjacent hits



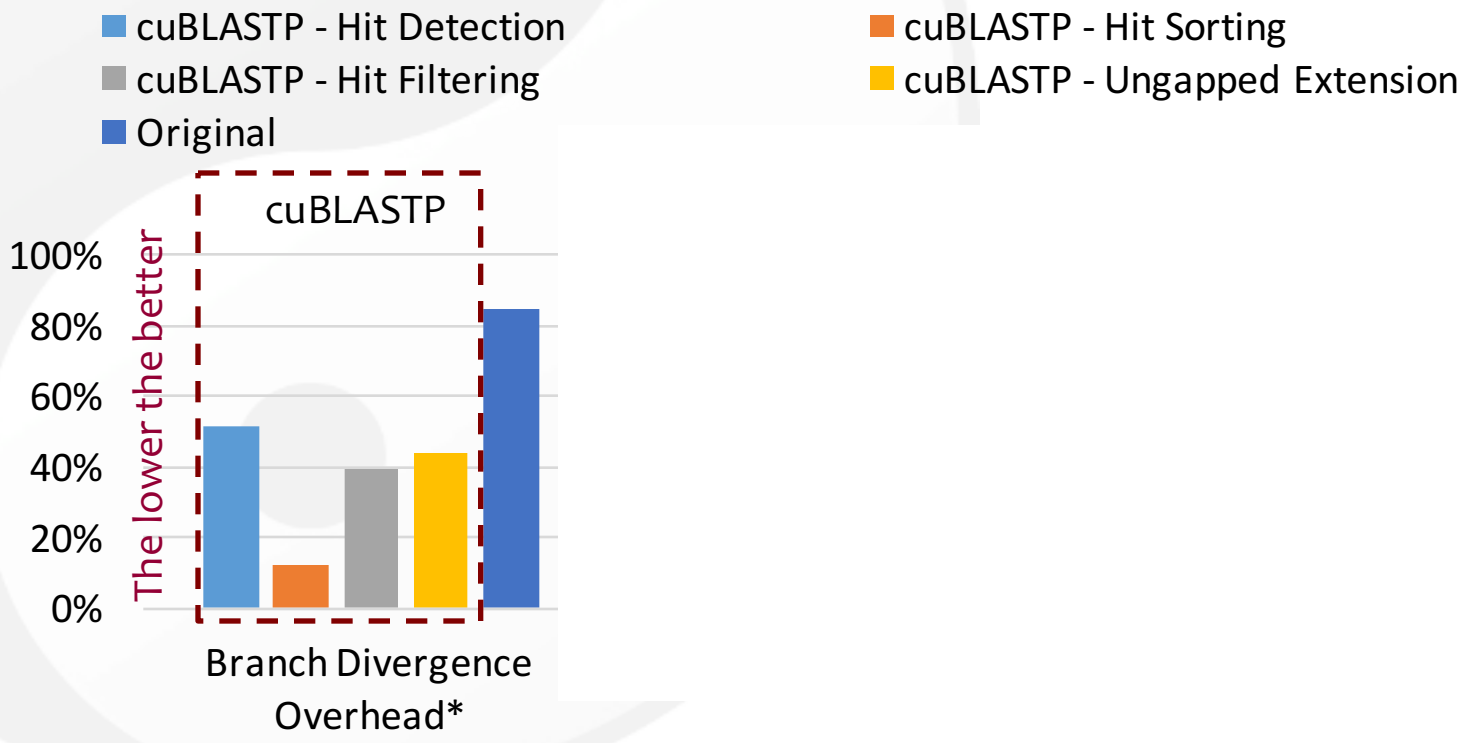
Solution: Memory Access Reordering

- Transform an irregular algorithm (lastHit array method) into three regular phases



Performance Numbers

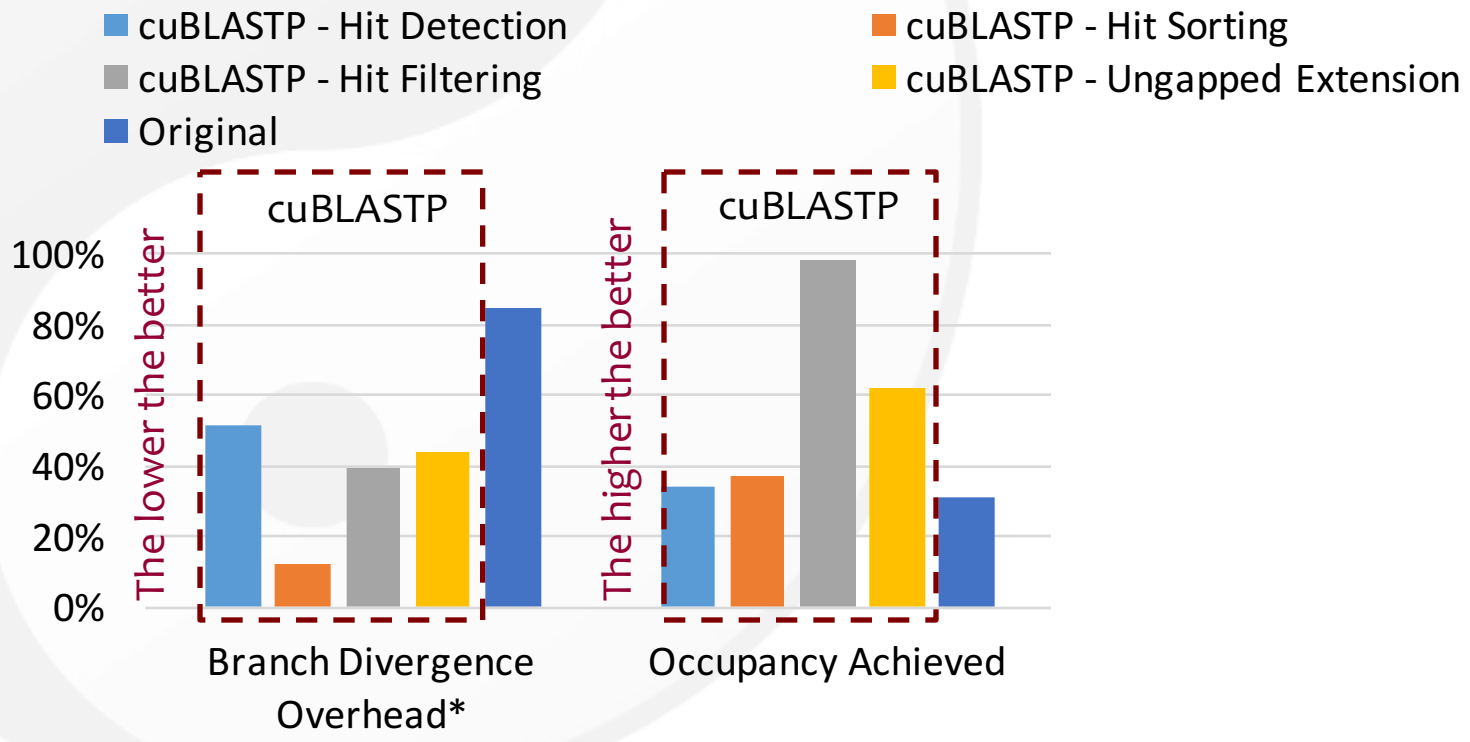
- Compared to original version, cuBLASTP has …
  - Less branch divergence overhead



*: Branch Divergence Overhead: the ratio of divergent execution to total execution

Performance Numbers

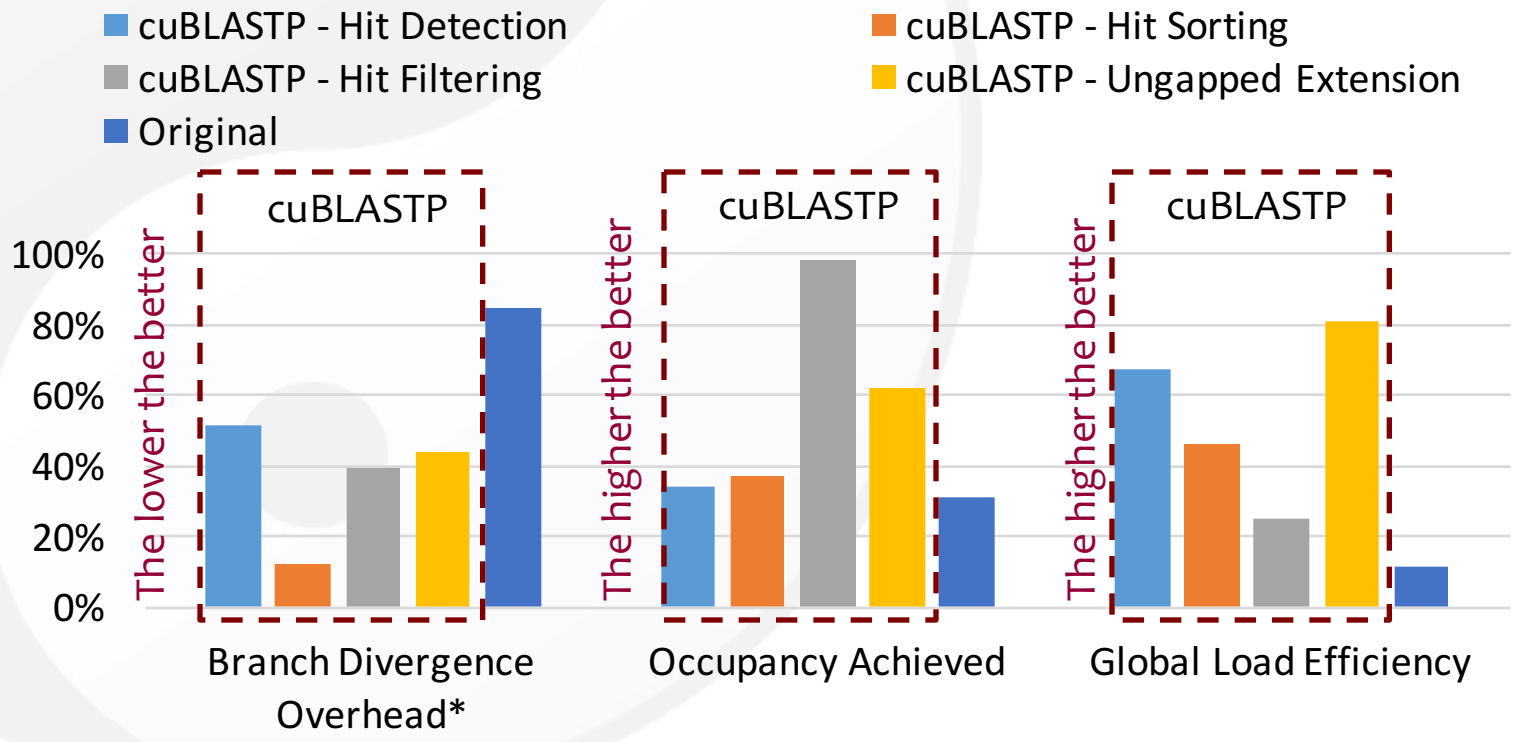
- Compared to original version, cuBLASTP has …
  - Less branch divergence overhead
  - Better occupancy



*: Branch Divergence Overhead: the ratio of divergent execution to total execution

Performance Numbers

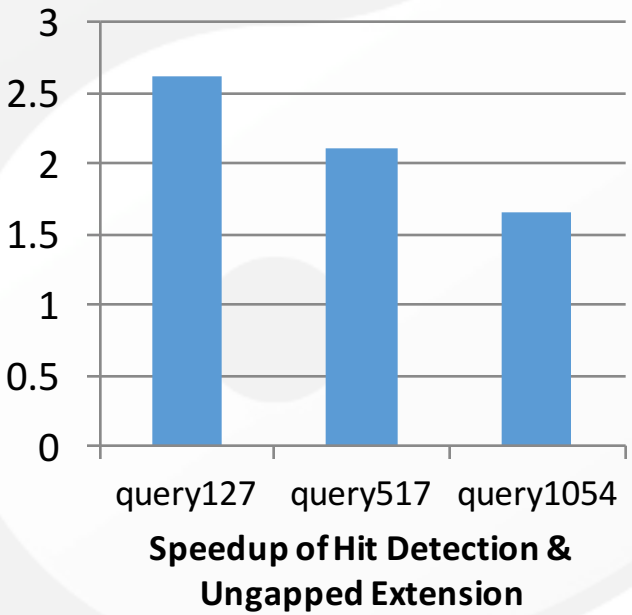
- Compared to original version, cuBLASTP has …
  - Less branch divergence overhead
  - Better occupancy
  - Better load efficiency

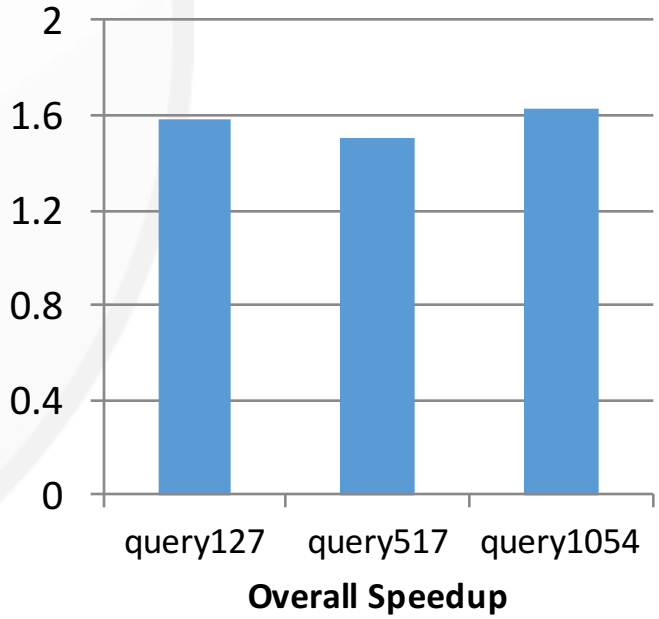


*: Branch Divergence Overhead: the ratio of divergent execution to total execution

Speedup

- With swissprot database, cuBLASTP achieves …
  - Up to 2.6-fold speedup of hit detection and ungapped extension over GPU-BLASTP, which is the fastest GPU-based BLAST
  - Up to 1.6-fold overall speedup over GPU-BLASTP (cuBLASTP has parallelization of the rest of stages)





Conclusion and Future Work

Conclusion

- Mapping irregular algorithms to heterogeneous system is non-trivial, need couples of transformation and adaption on algorithms and data structures
- But these concepts of transformations are propagable
  - Kernel fission, memory access reordering, warp-centric execution, …

Future Work

- Generalize optimizations from cuBLASTP for different algorithms and other heterogeneous systems
- Design a library for irregular algorithms with optimized irregular data structure and operations

Other Research Topics

- Optimizing BWA (Burrows Wheeler Alignment) on multicore CPU and Intel Xeon Phi
- dbblast: database index based BLAST on multicore CPU and Intel Xeon Phi
- Dynamic parallelism on AMD APU (New)
- Optimizing irregular applications for GPU/Xeon Phi clusters (Future)

- Other Research Interests
  - Cloud computing
  - MapReduce with accelerators