The SIAM Conference on Parallel Processing for Scientific Computing (SIAM PP)
February 14th, 2020 | Seattle, Washington, USA

Approximate and Exact (Multi-)Selection on GPUs

Tobias Ribizel[1], Hartwig Anzt[1,2]

[1]Karlsruhe Institute of Technology

[2]University of Tennessee

HPC-Seminar – FAU Erlangen
23.03.2021

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THE UNIVERSITY OF TENNESSEE KNOXVILLE

Selection Problem

Given an unsorted sequence of real numbers $x_0, x_1, x_2, x_3, \dots x_{n-1}$,
we want to find the element x_{i_k} such that in the sorted sequence

$$x_{i_0} \leq x_{i_1} \leq x_{i_2} \leq x_{i_3} \leq \cdots \leq \underset{\substack{\uparrow \\ k}}{x_{i_k}} \leq \dots x_{i_{n-1}}$$

the element x_{i_k} is located in position k.

We do not necessarily need to sort the complete sequence!

- Statistics (Quantiles)
- Top-k selection
- Thresholds

General Approach: Partial Sorting

```
double select(data, rank) {
    if (size(data) <= base_case_size) {
        sort(data);
        return data[rank];
    }
    // select splitters
    splitters = pick_splitters(data);
    // compute bucket sizes n_i
    counts = count_buckets(data, splitters);
    // compute bucket ranks r_i
    offsets = prefix_sum(counts);
    // determine bucket containing rank
    bucket = lower_bound(offsets, rank);
    // recursive subcall
    data = extract_bucket(data, bucket);
    rank -= offsets[bucket];
    return select(data, rank);
}
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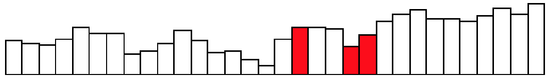
Pick splitters



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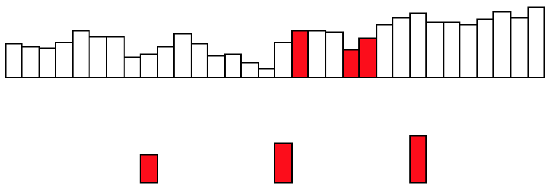

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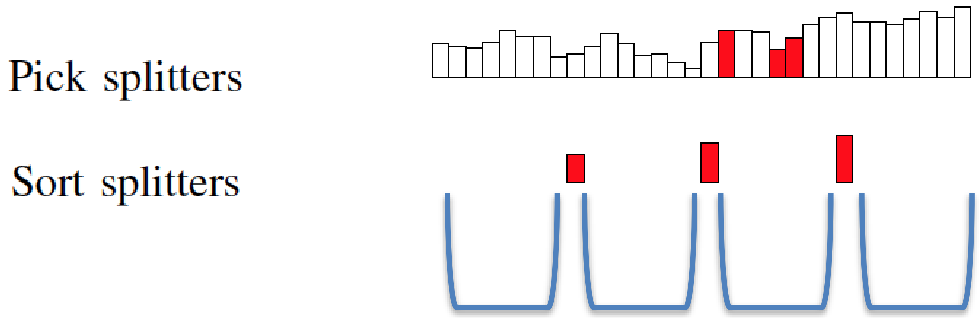

Splitters separate buckets

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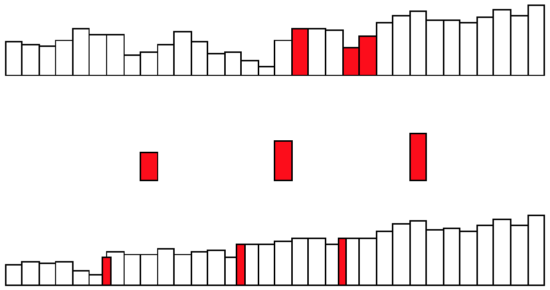
Pick splitters

Sort splitters

Group by bucket



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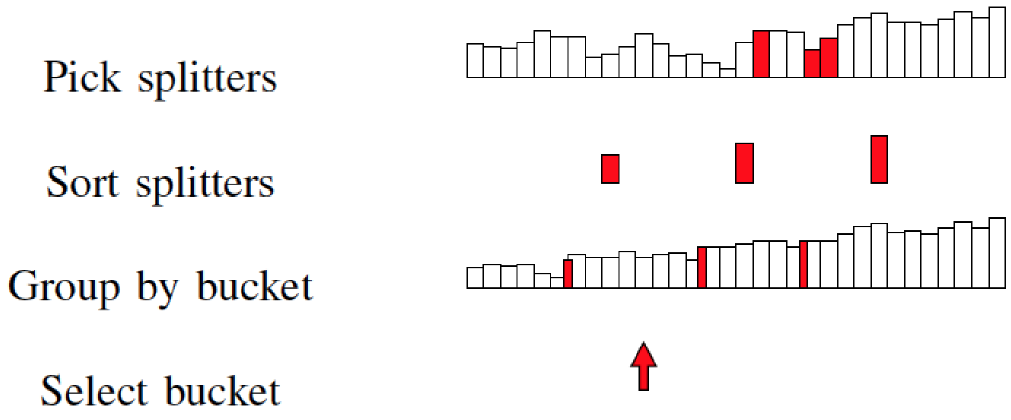

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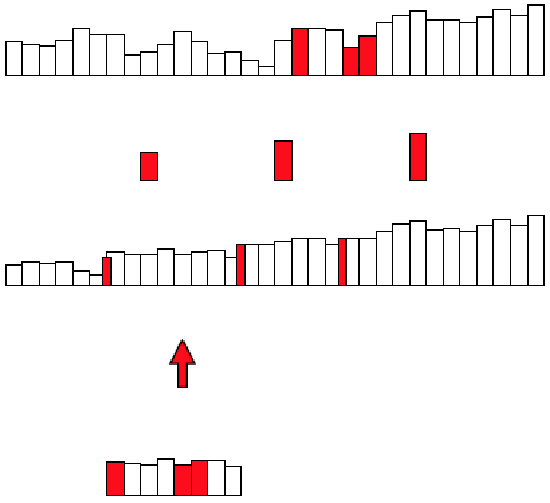
Pick splitters

Sort splitters

Group by bucket

Select bucket

Pick splitters



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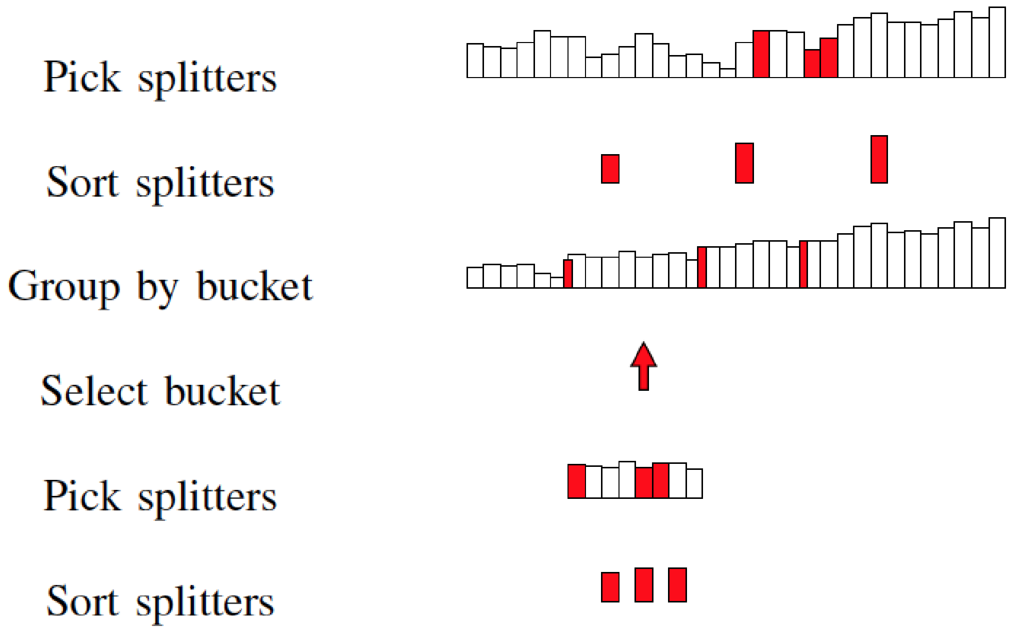

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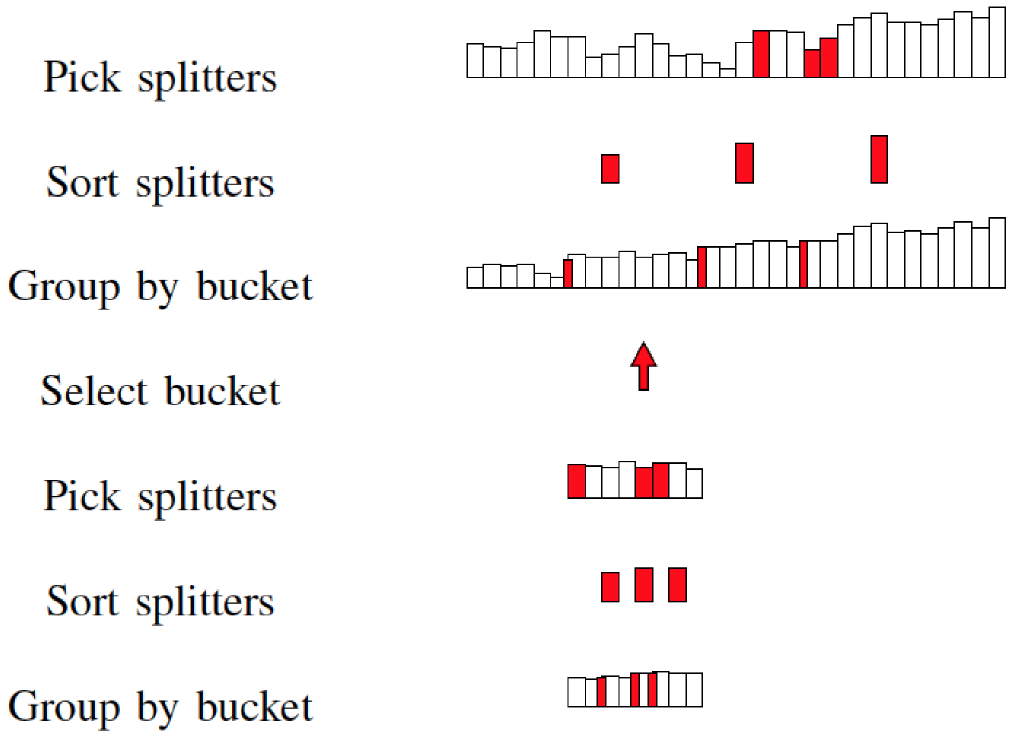

Implementation Aspects

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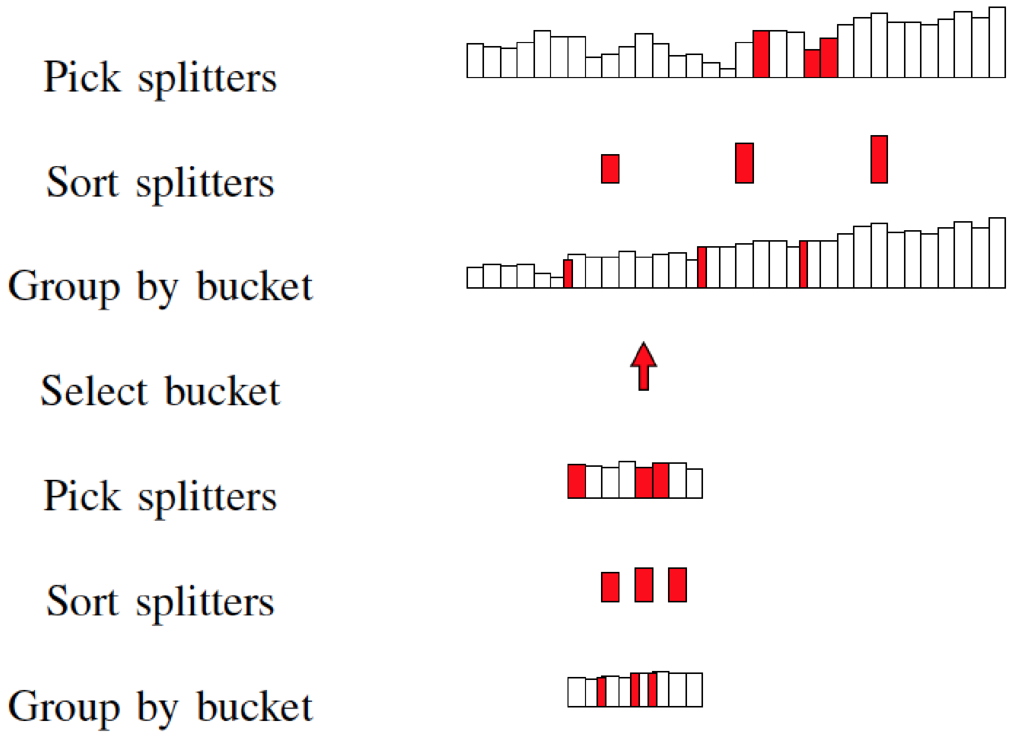
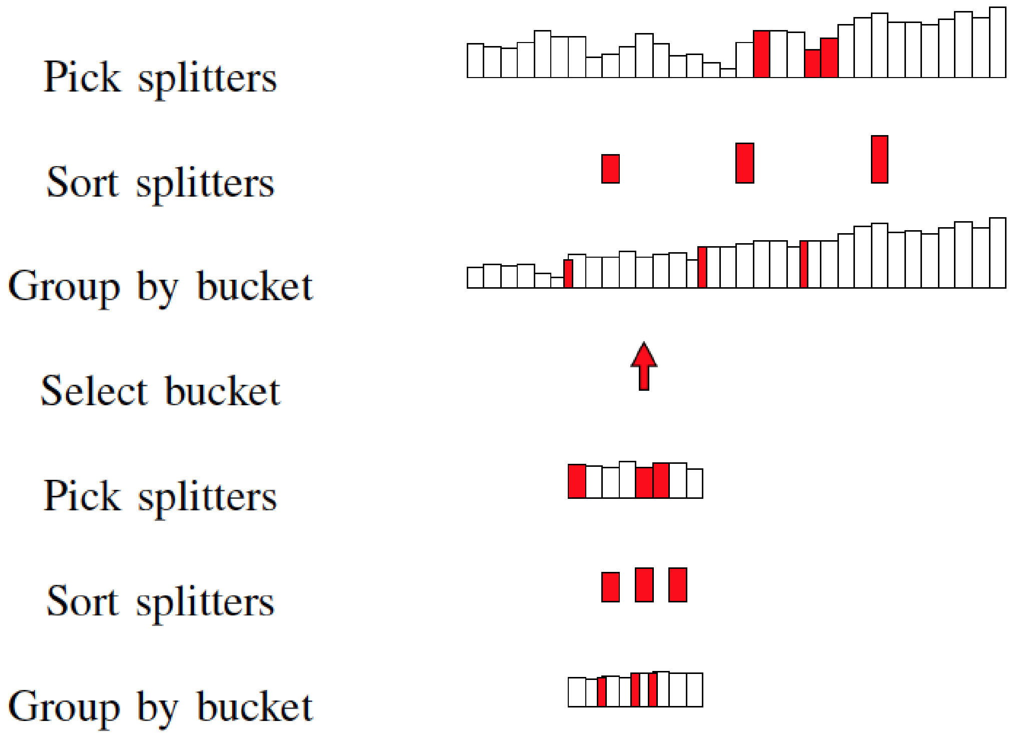


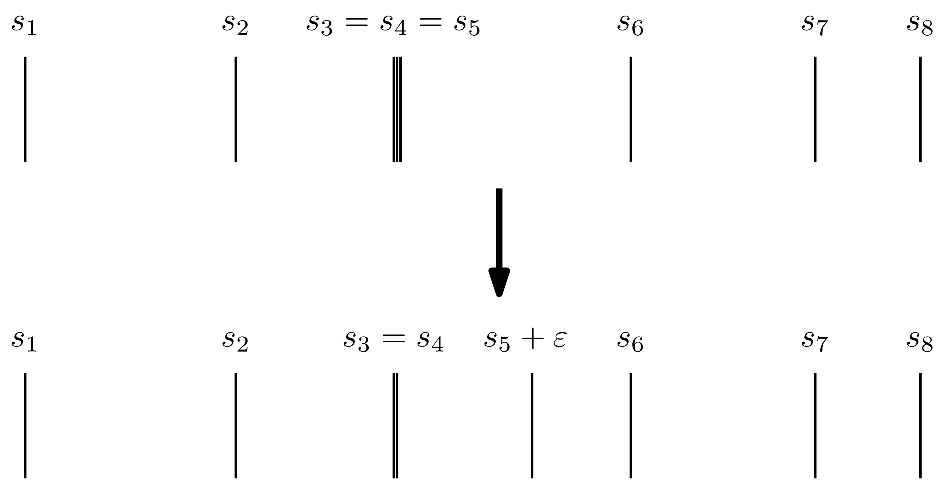
Implementation Aspects

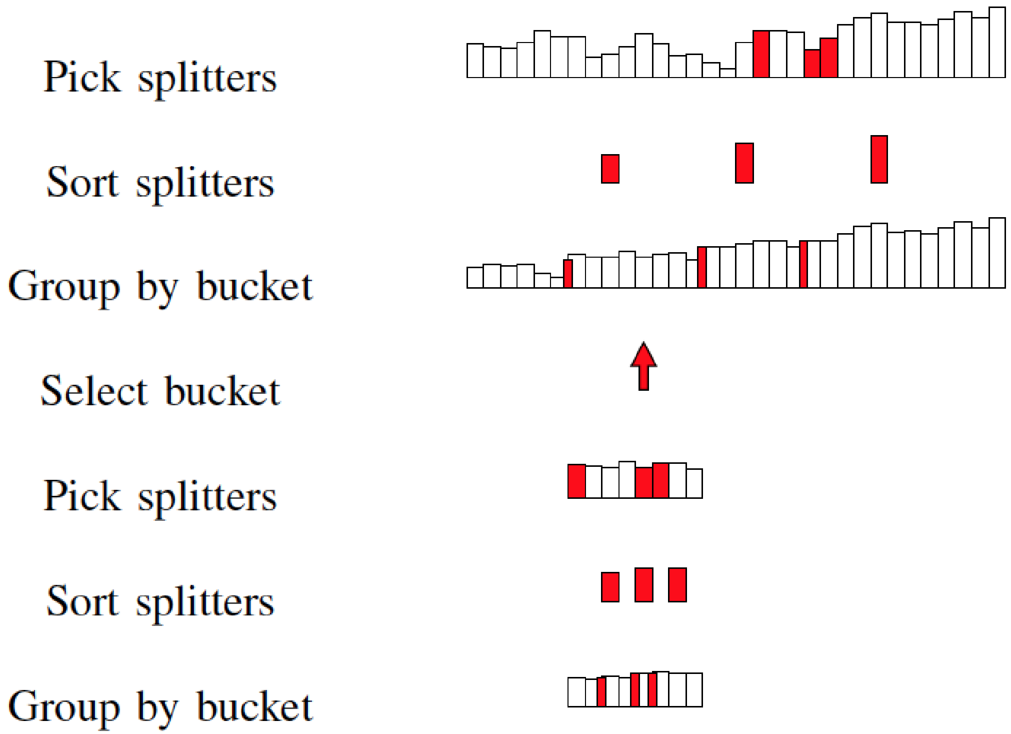
- We only copy elements of the buckets we are interested in;



Implementation Aspects

- We only copy elements of the buckets we are interested in;
- In case of identical splitter elements, they are placed in an *equality bucket*;
- If target rank is in an *equality bucket*, the algorithm can terminate early by returning lower bound;





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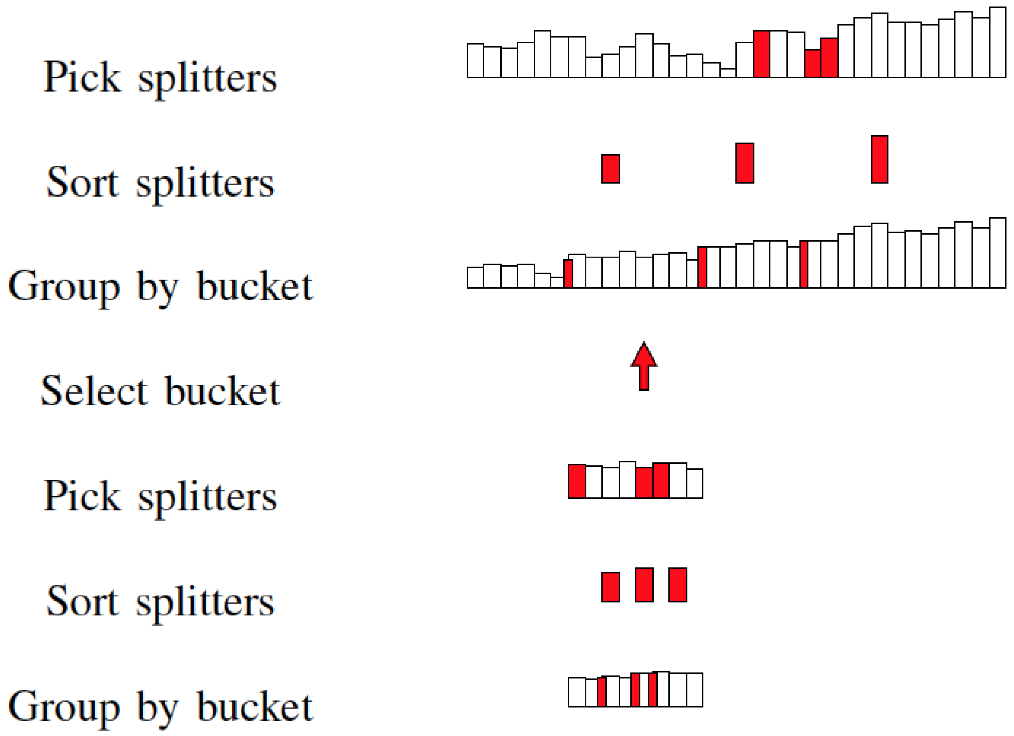
- For sorting the splitters, small input datasets, and the lowest recursion level a *bitonic sort* in registers + shared memory is used;



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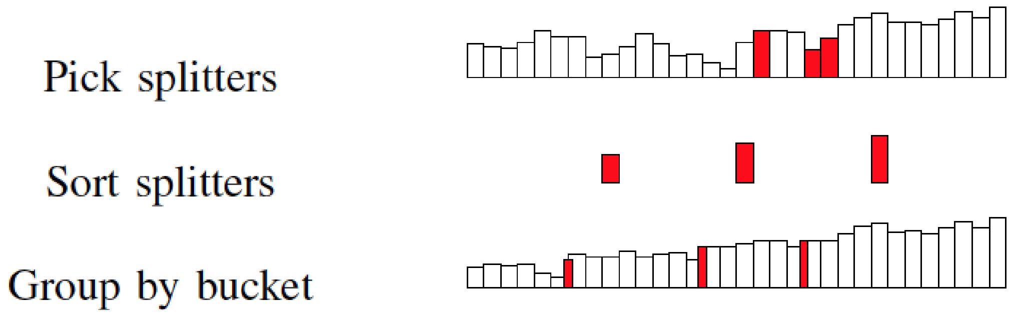
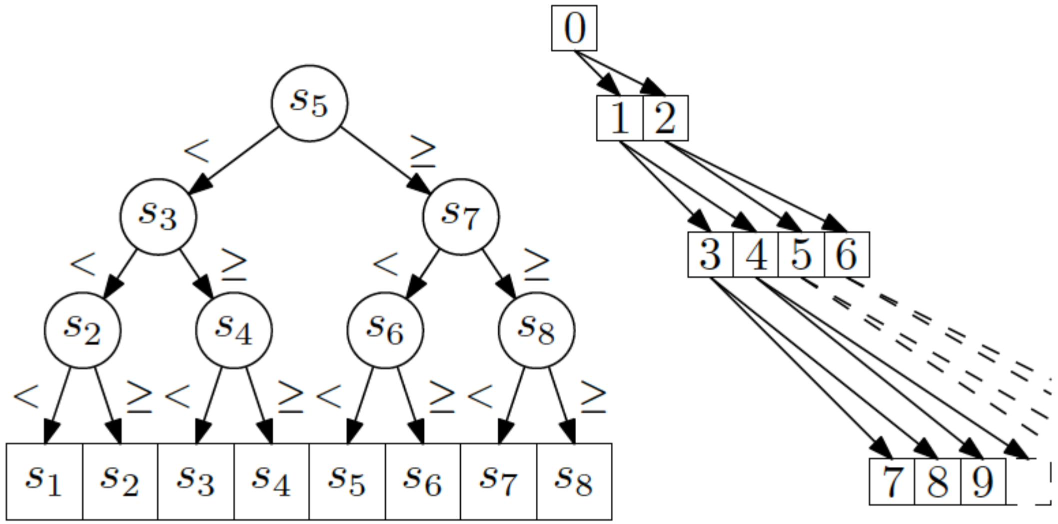
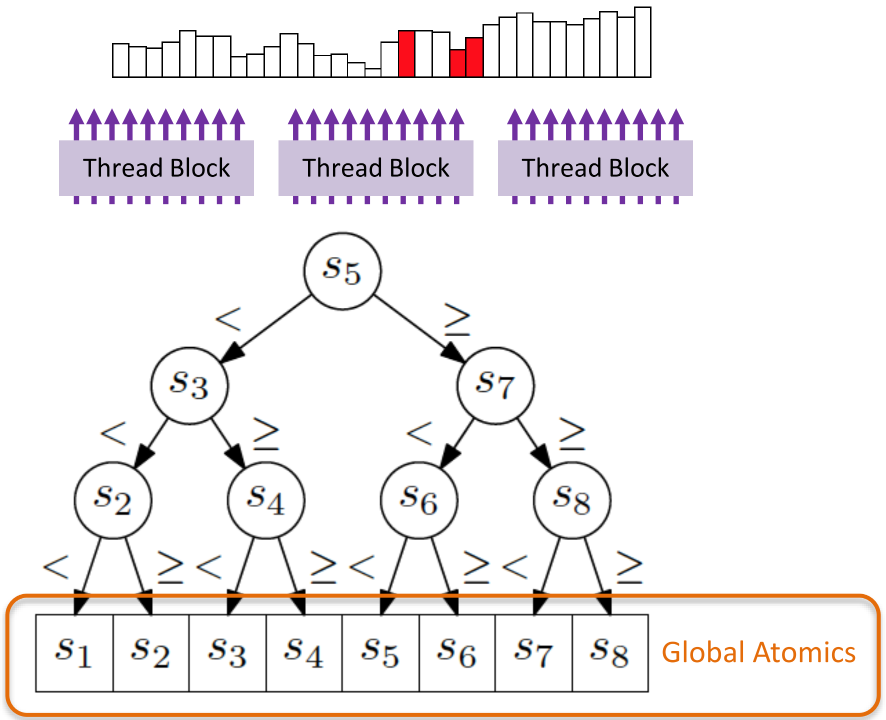
- We only copy elements of the buckets we are interested in;
- In case of identical splitter elements, they are placed in an *equality bucket*;
- If target rank is in an *equality bucket*, the algorithm can terminate early by returning lower bound;
- For sorting the splitters, small input datasets, and the lowest recursion level a *bitonic sort* in registers + shared memory is used;
- Use a *binary search tree* to sort elements into the buckets;
- Store the bucket indices to avoid recomputation (also helpful for kernel fusion)





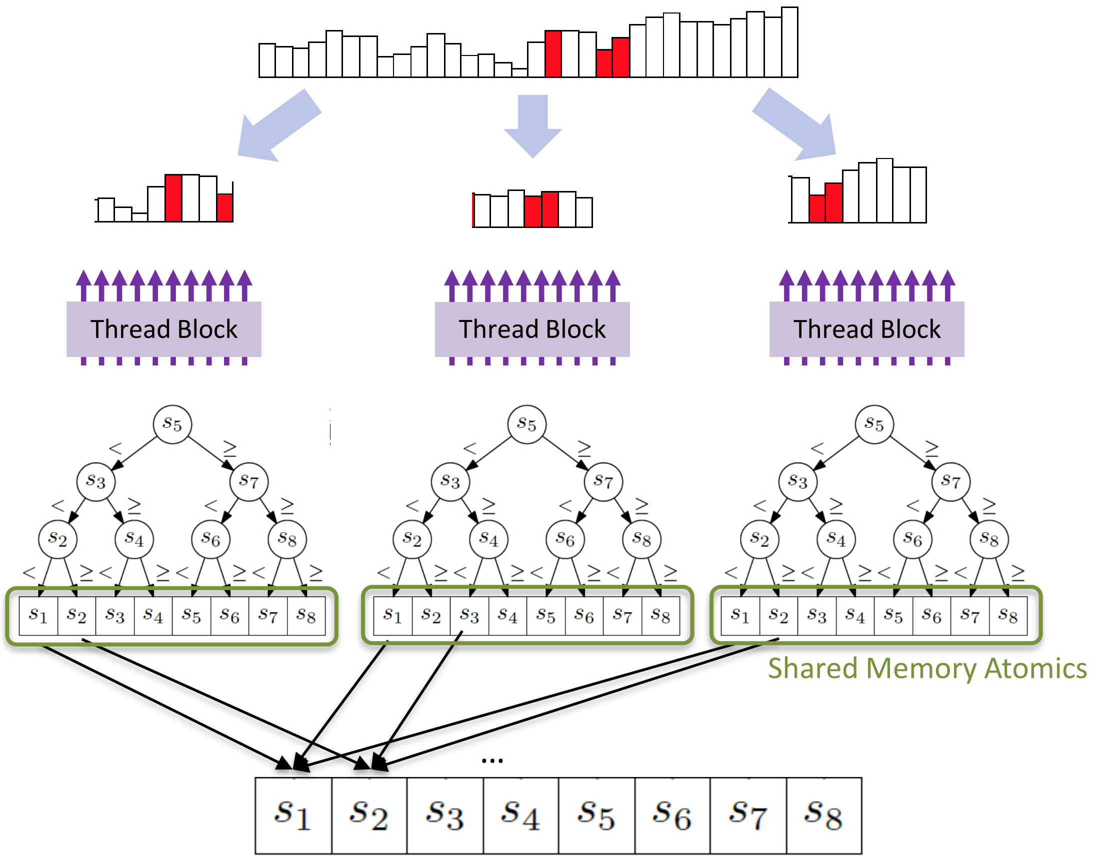
Parallelization & Communication

Global Memory Atomics



- Run SampleSelect using all resources on complete data set;
- Use global atomics to generate bucket counts;

Shared Memory Atomics



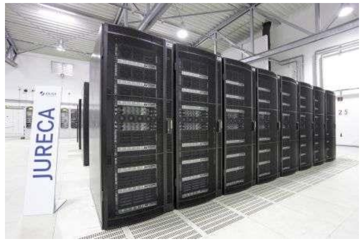
- Split data set into chunks, assign to thread blocks;
- Each thread block runs bucket count on its data;
- Use a global reduction to get global bucket counts;

Experiment Setup

- 2 distinct GPU architectures
- Input datasets with 2^{16} to 2^{28} elements
- *d= 1, 16, 128, 1024, n* distinct values
- All results averaged over 10 runs
- Single precision input data

- Comparison against QuickSelect kernel
- QuickSelect and SampleSelect have same performance optimization level
- Correctness check using C++ std::nth_element

	NVIDIA K40	NVIDIA V100
Architecture	Kepler	Volta
DP Performance	1.2 TFLOPs	7 TFLOPs
SP Performance	3.5 TFLOPs	14 TFLOPs
HP Performance	–	112 TFLOPs
SMs	13	80
Operating Freq.	0.75 GHz	1.53 GHz
Mem. Capacity	5 GB	16 GB
Mem. Bandwidth	208 GB/s	900 GB/s
Sustained BW	146 GB/s	742 GB/s
L2 Cache Size	1.5 MB	6 MB
L1 Cache Size	64 KB	128 KB
	2013	*2017*



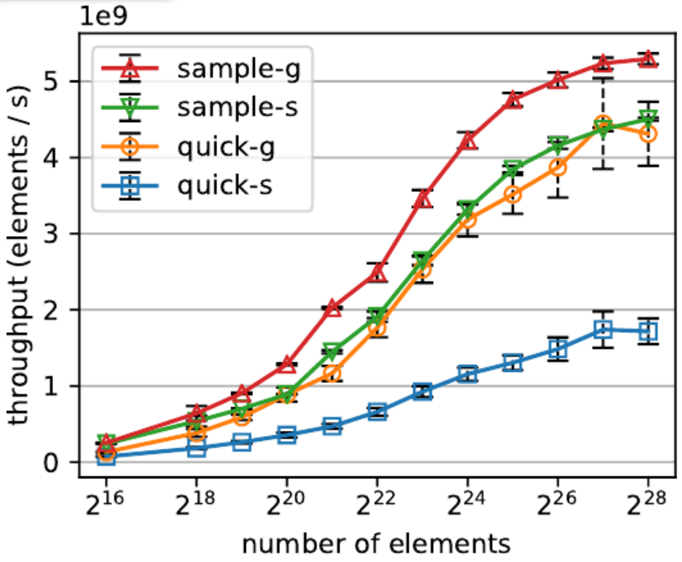
#44@TOP500

#1@TOP500

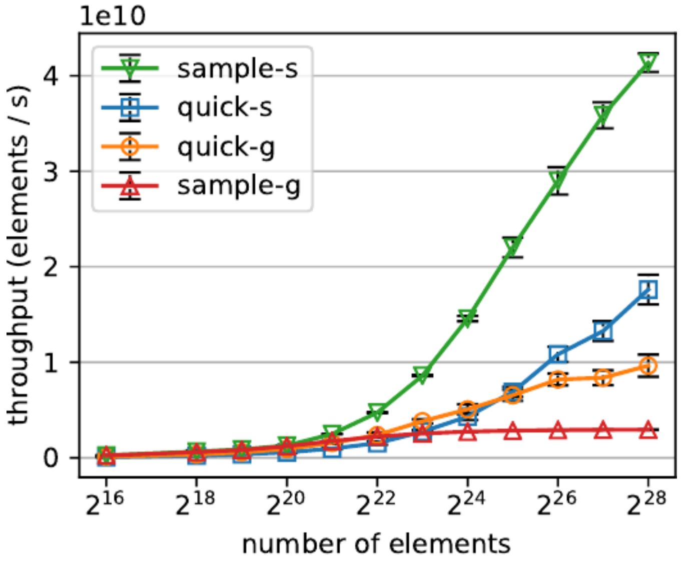
Kernel Performance: **Global vs. Shared Atomics**

-g : global memory atomics
-s: shared memory atomics

NVIDIA K40



NVIDIA V100



Larger performance variation for QuickSelect as we are more likely to run into the "*Worst-Case*" performance.

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-g : global memory atomics
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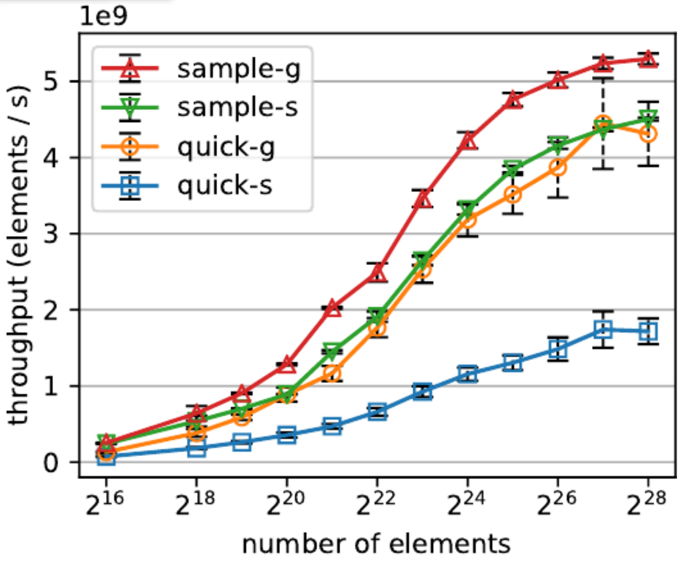
NVIDIA K40



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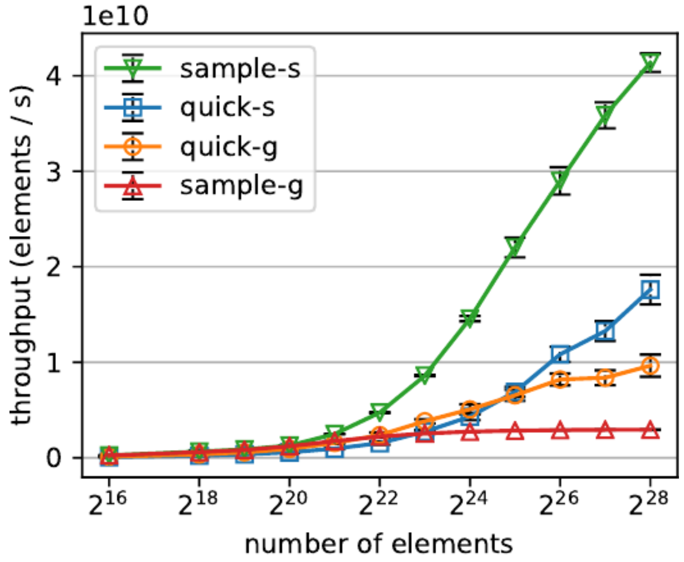
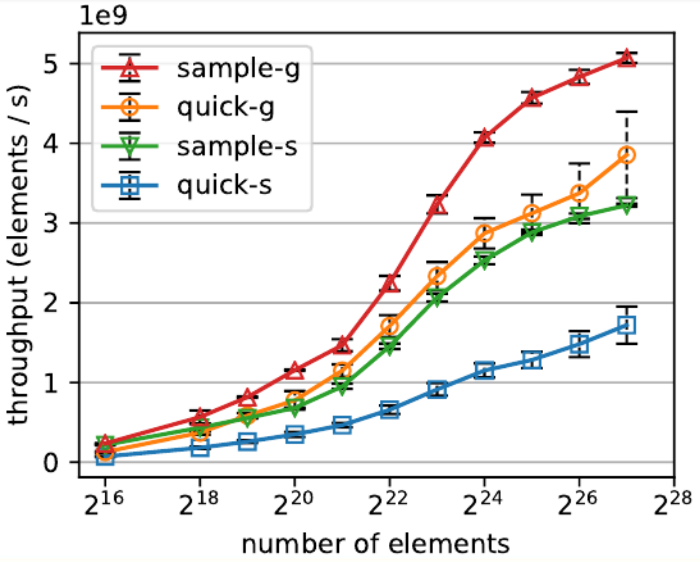
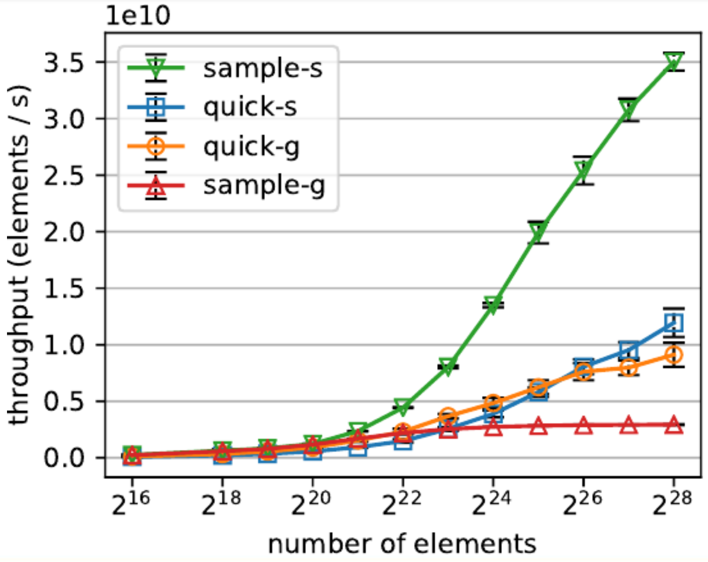


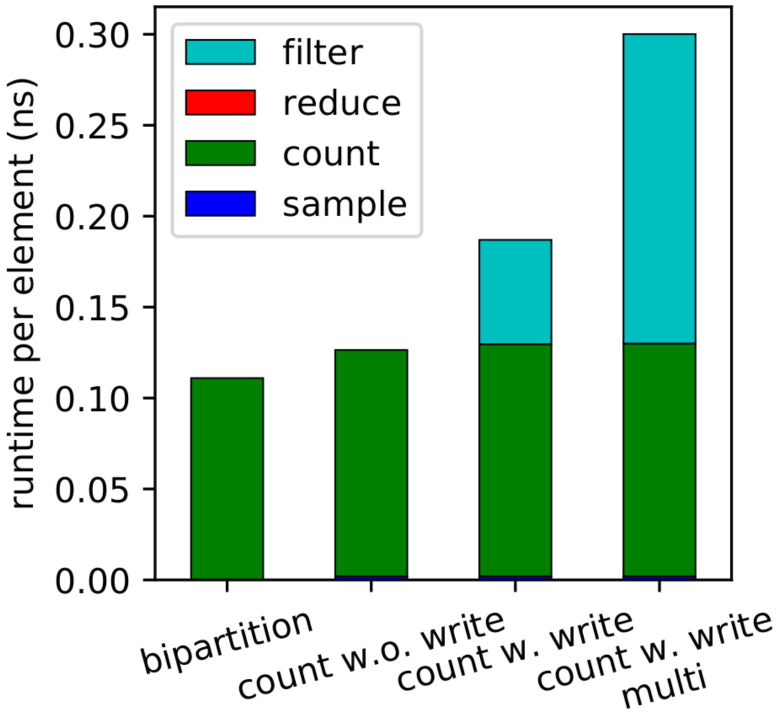


double precision

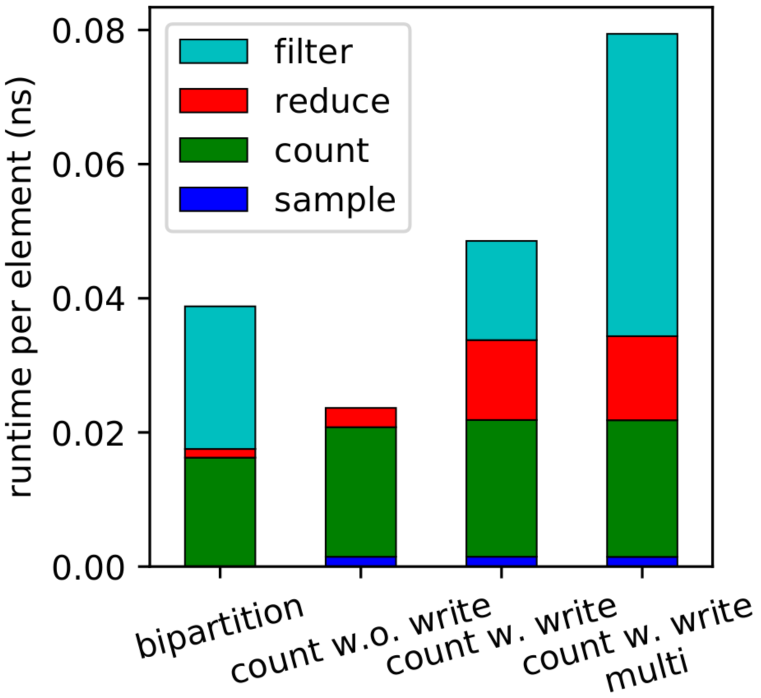


Runtime breakdown

NVIDIA K40
(global atomics)



NVIDIA V100
(shared atomics)

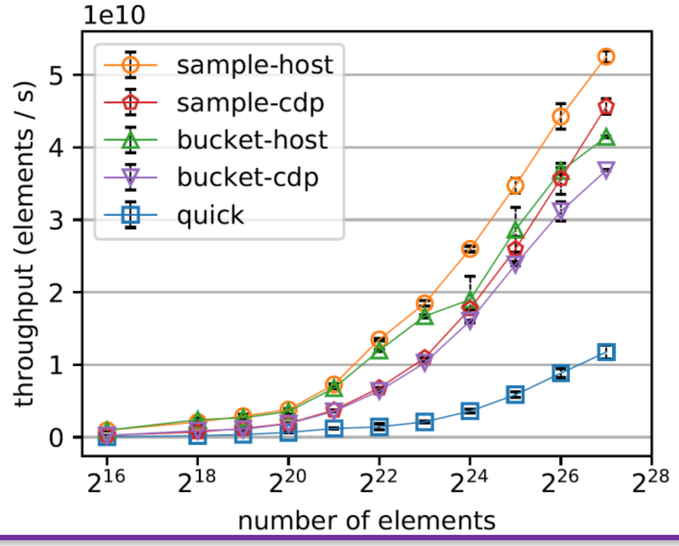


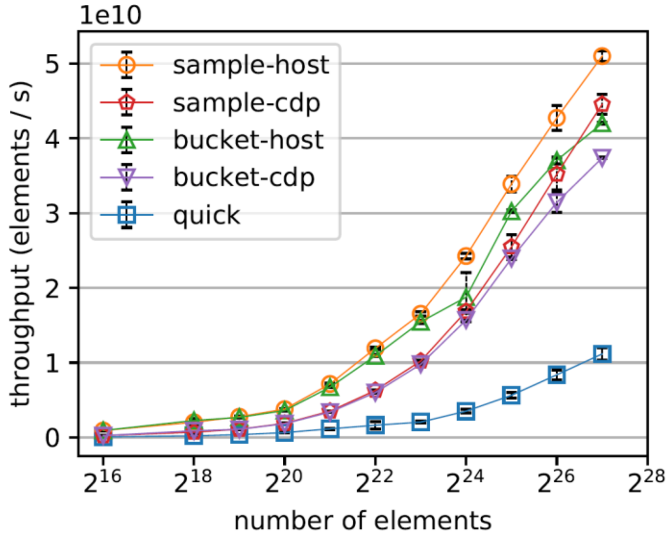
$n = 2^{24}$, single precision

Kernel Performance: **Host vs. Device recursion**

-host: Host launches recursive kernels
-cdp: CUDA dynamic parallelism

NVIDIA A100





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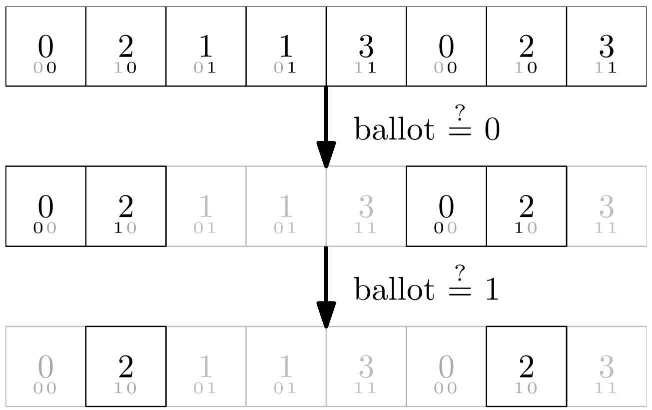
Kernel Optimization: **Element Repetition**

Idea: use warp aggregations to mitigate the performance impact from atomic collisions.



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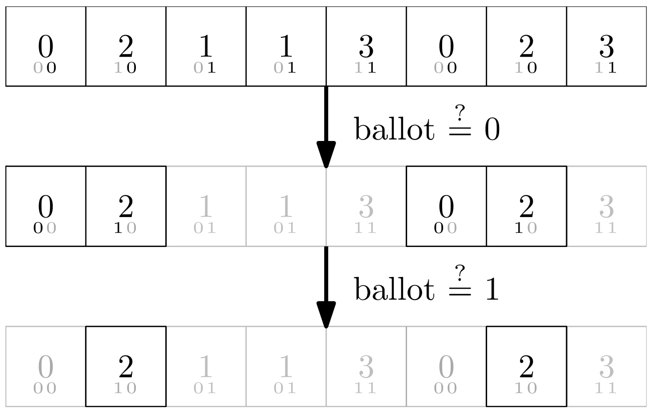
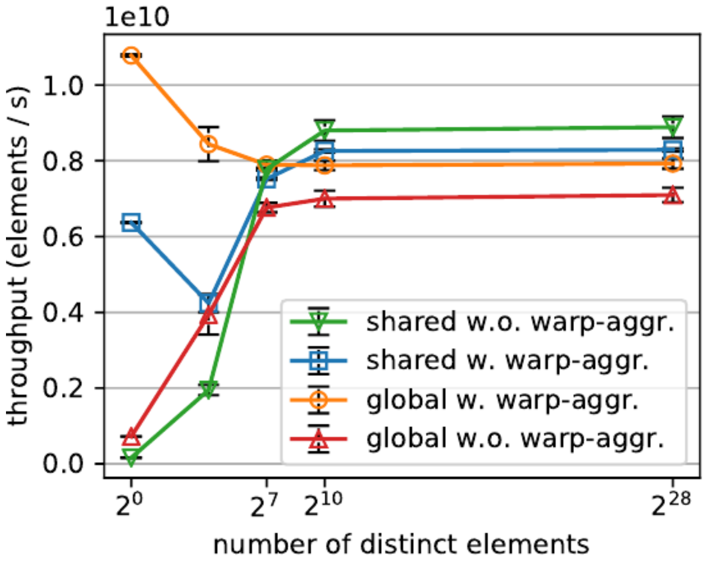
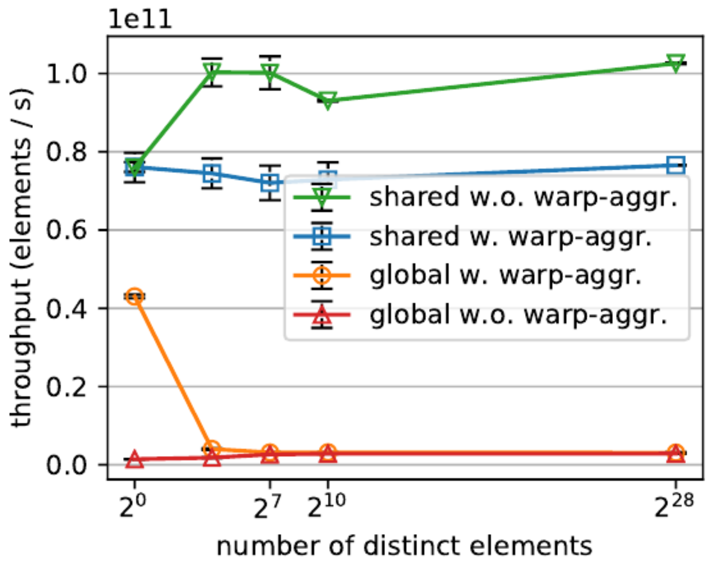


NVIDIA K40



more collisions

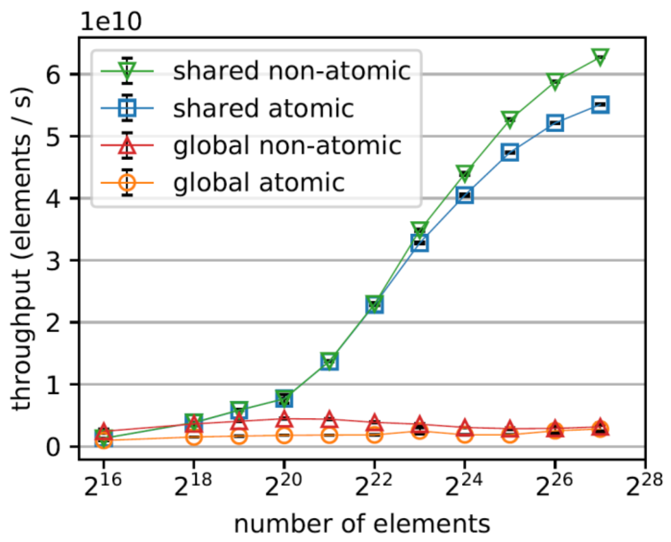
NVIDIA V100



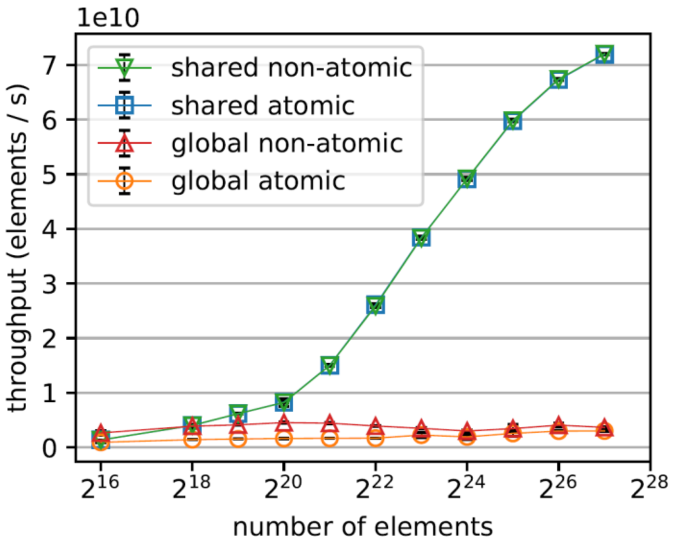
more collisions

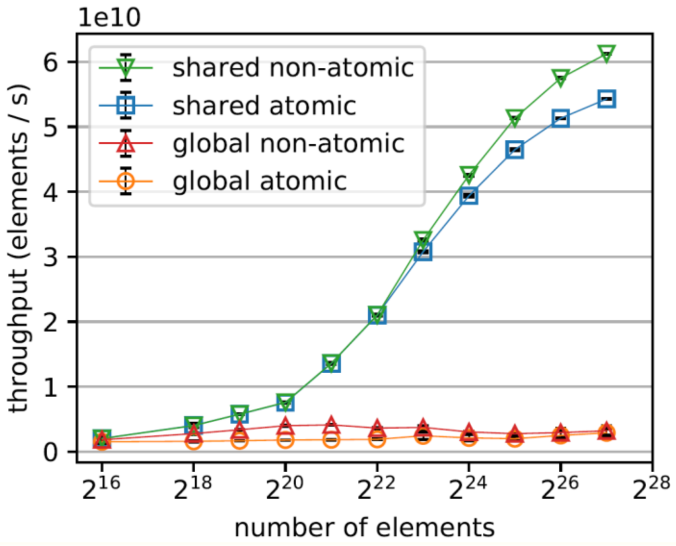
Kernel Performance: **What if we needed no atomics?**

NVIDIA A100 with warp-aggregation



NVIDIA A100 without warp-aggregation





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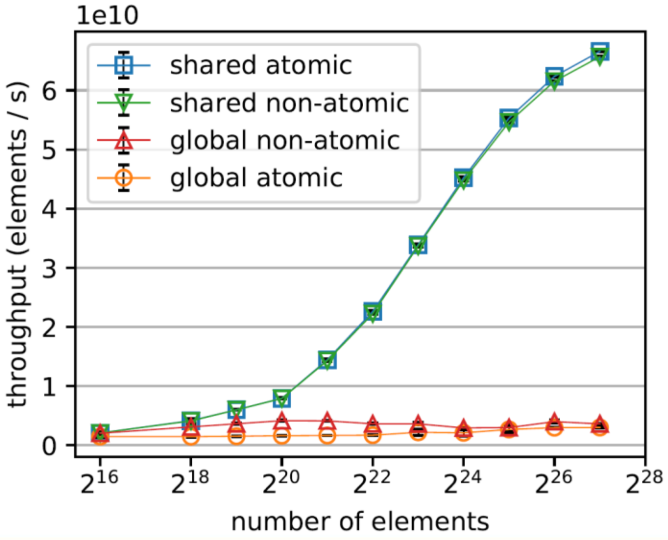
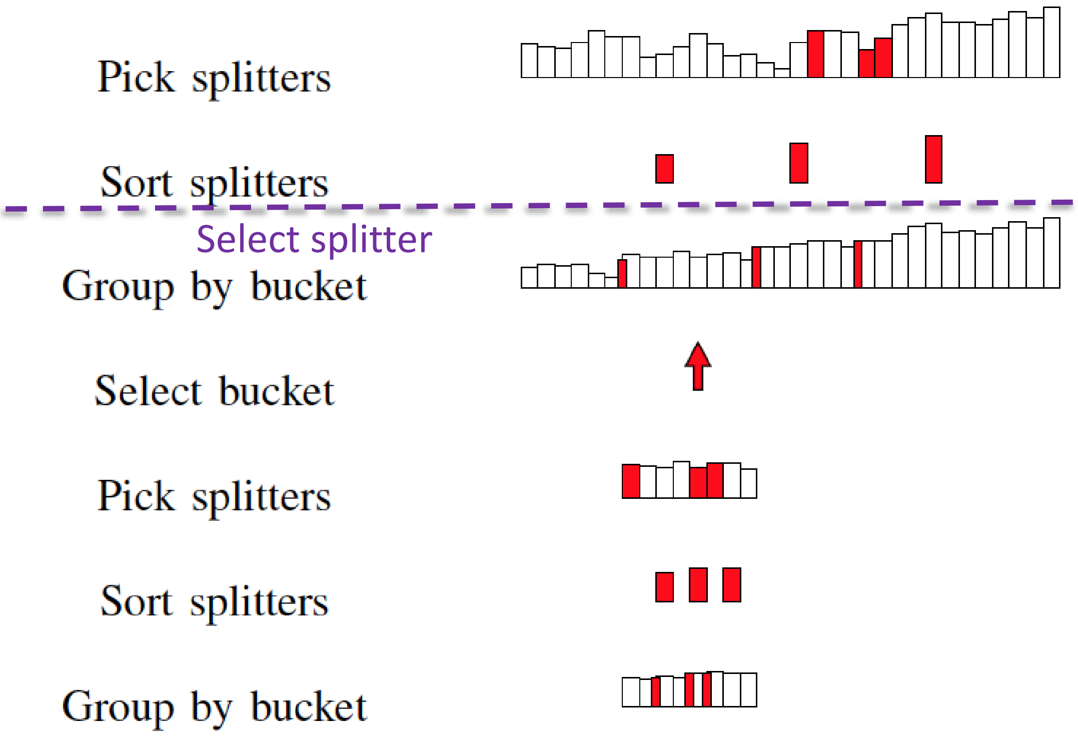


Approximate Selection

We do not descend to the lowest level of the recursion tree, but limit to one single bucket selection.

- Accuracy depends on the number of splitters vs. dataset size
- Accuracy independent of value distribution (works on ranks, only)



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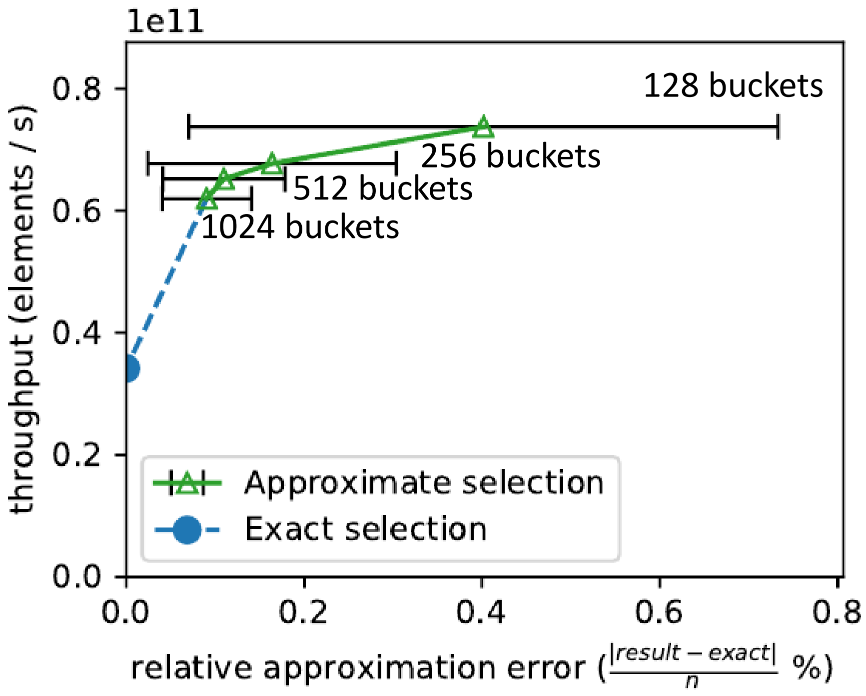
Test problem:

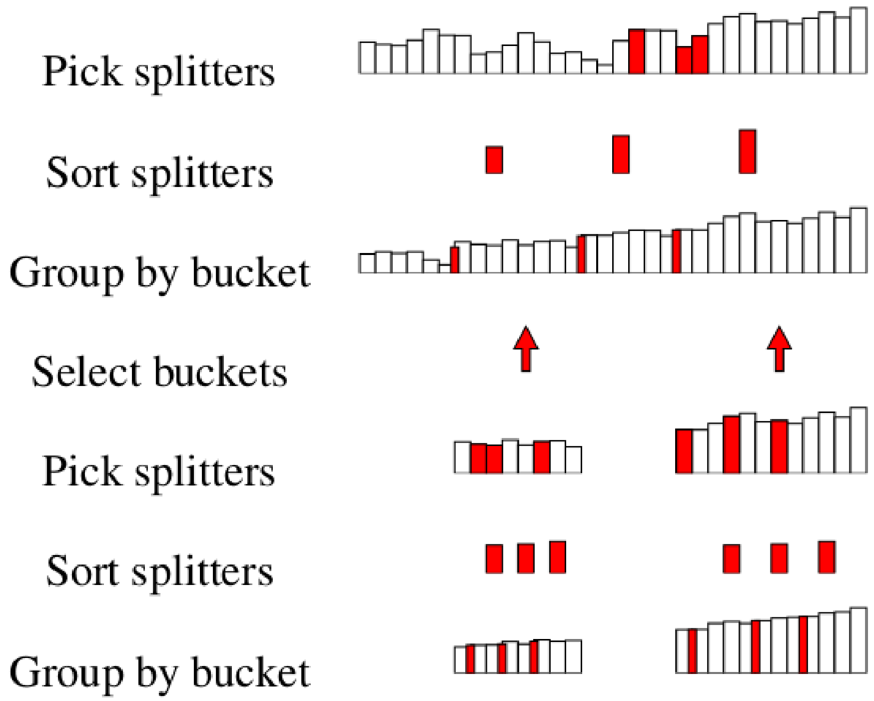
- 2^{28} uniformly distributed single precision values
- Approximate selection uses 1 level only
- We report statistics over 10 runs



Multiple Selection

Generalization: Select elements at *multiple ranks* $k_1, \dots, k_m$ simultaneously

- Determine which buckets contain k_i using binary search
- Extract elements from all these buckets simultaneously
- Launch multiple subcalls using CUDA *dynamic parallelism*



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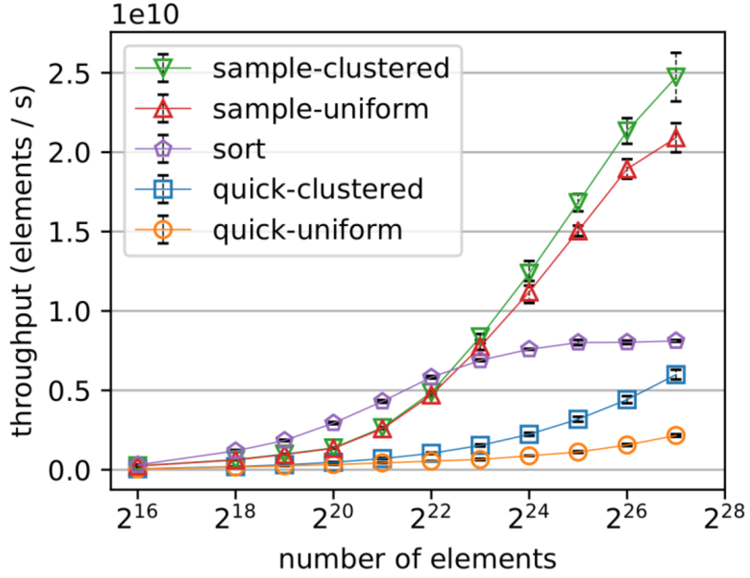
- Launch multiple subcalls using CUDA *dynamic parallelism*
- Comparison with *QuickSelect* and CUB *RadixSort*
- Input ranks: *clustered* with $k_i = 2^i$ (best case)
  uniform with $k_i = \frac{i}{32} \cdot n$ (worst case)

NVIDIA V100



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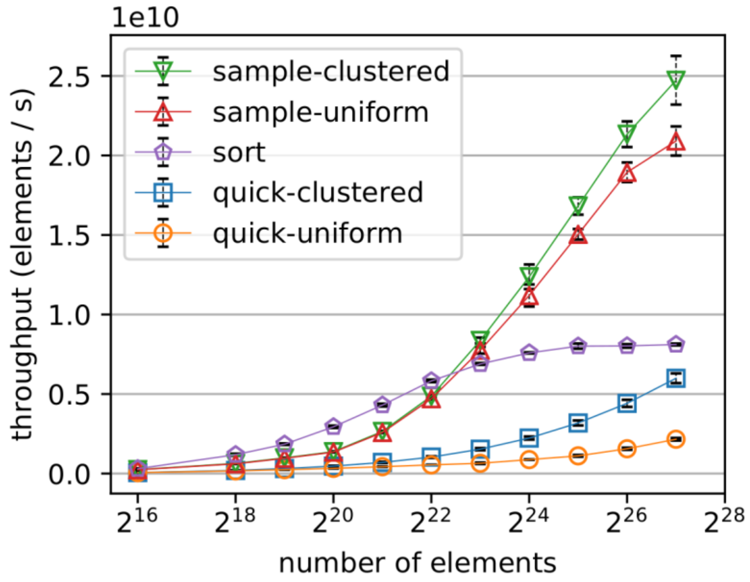
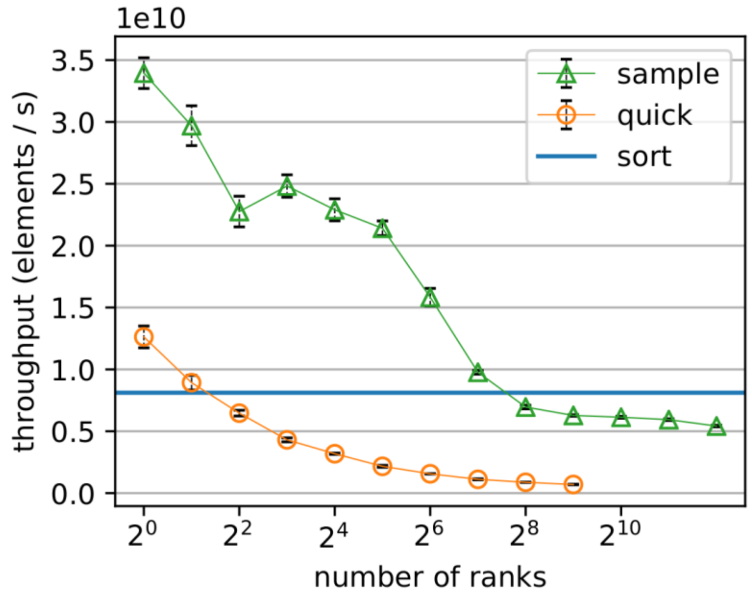
- Comparison with *QuickSelect* and CUB *RadixSort*
- Input ranks: *uniform* with $k_i = \frac{i}{\#ranks} \cdot n$ for $n = 2^{27}$

NVIDIA V100





Summary and Outlook

- SampleSelect kernel much faster than QuickSelect
- 36% (single) 48% (double) of experimental
  peak memory bandwidth on NVIDIA V100
- Approximate selection >2x faster than exact selection
- Multiple selection faster than sorting for up to 128 ranks

From a performance engineering standpoint (overgeneralized take-aways ☺):

- Hardware support beats warp-aggregation for atomics
- Shared-memory atomics are blazingly fast
- Host-side kernel launches outperform dynamic parallelism for tail recursion
- Pruning your recursion tree can be worthwile (if you still have enough parallelism left)

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