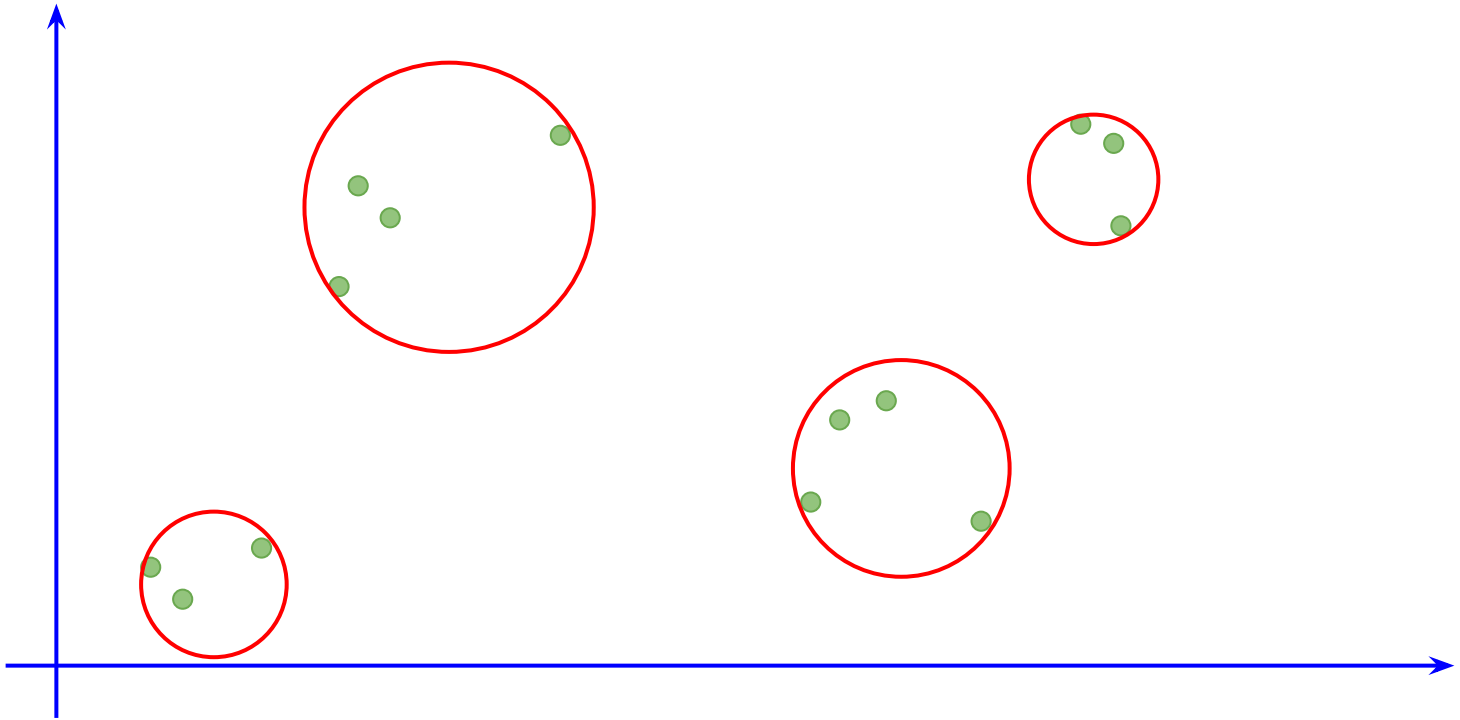
Detailed Analysis and Optimization of CUDA K-means Algorithm

Martin Kruliš, Miroslav Kratochvíl
Department of Software Engineering, Charles University, Prague Czech Republic

ICPP 2020

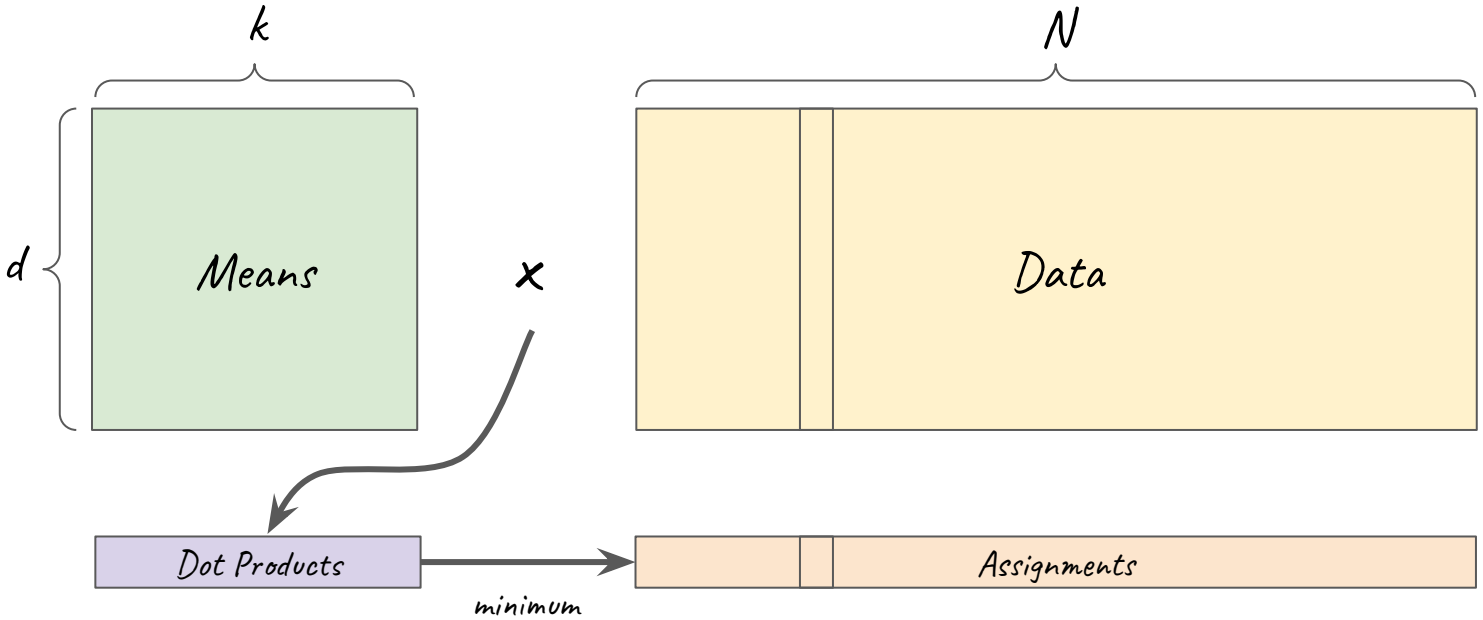
Quick Refresher: K-means Algorithm



Quick Refresher: K-means Algorithm

- Iteratively update set of centroids (means)
  - Compute point assignment
    - Compute Euclidean distance between every point and every mean
    - Find nearest mean (minimum of distances) for each point
  - Update means (per-dimension average)
    - Compute sum of coordinates (per dimension) for each assigned point
    - Divide each sum by the number of points in the corresponding cluster

Quick Refresher: K-means Algorithm



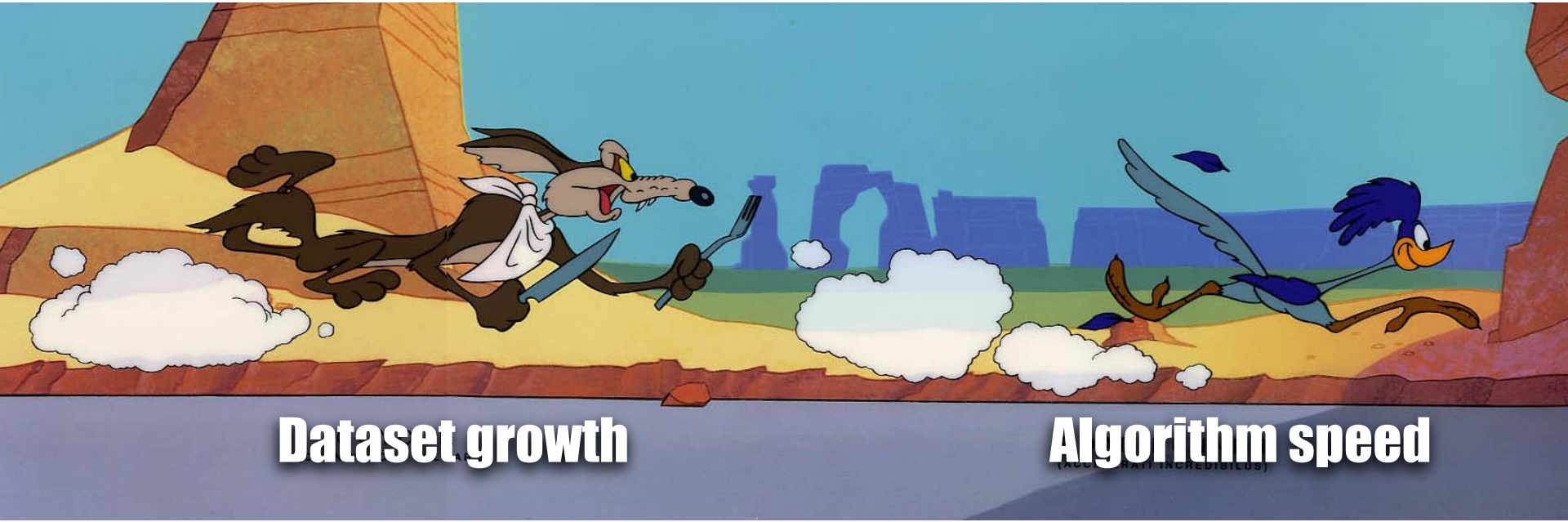
Quick Refresher: K-means Algorithm

- Iteratively update set of centroids (means)
  - Compute point assignment
    - Compute Euclidean distance and the means-wide reduction (minimum)
  - Update means (per-dimension average)
    - Compute sum of coordinates (per dimension) for each assigned point
    - Divide each sum by the number of points in the corresponding cluster

Quick Refresher: K-means Algorithm

- Iteratively update set of centroids (means)
  - Compute point assignment
    - Compute Euclidean distance and the means-wide reduction (minimum)
    - Add point coordinates (per dimension) to its nearest cluster
  - Update means (per-dimension average)
    - Divide each sum by the number of points in the corresponding cluster

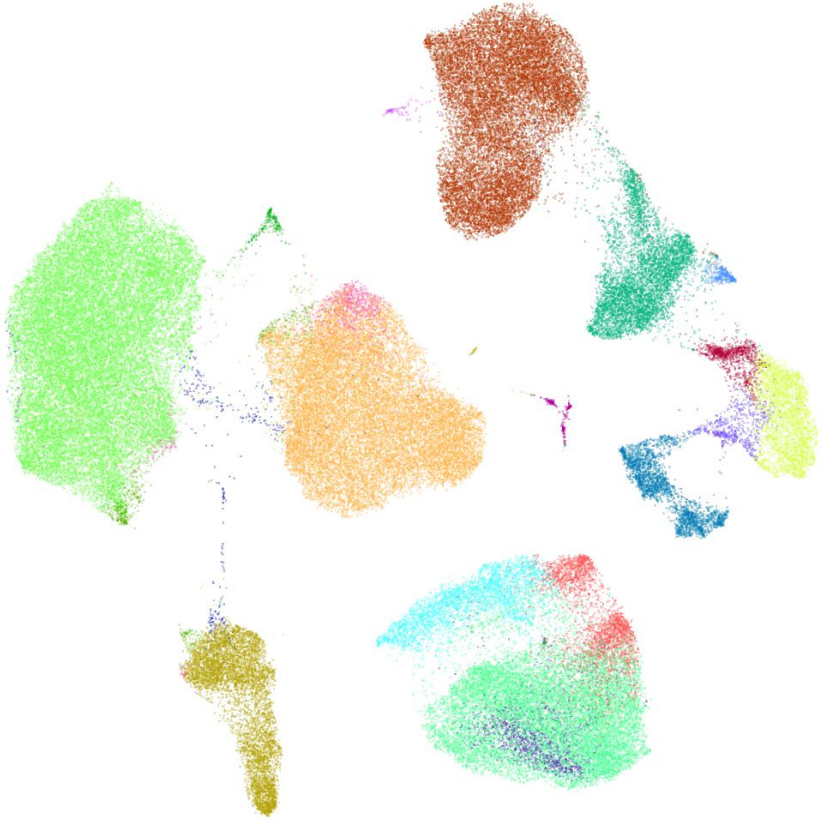
Why k-means again?



High-performance use cases

Meta-clustering single-cell data

- <50 dimensions
- Millions of data points
- Time available: a few seconds
  (the analysis is interactive)



UMAP projection of 32-dim data to 2D

High-performance use cases

Video browsing & retrieval

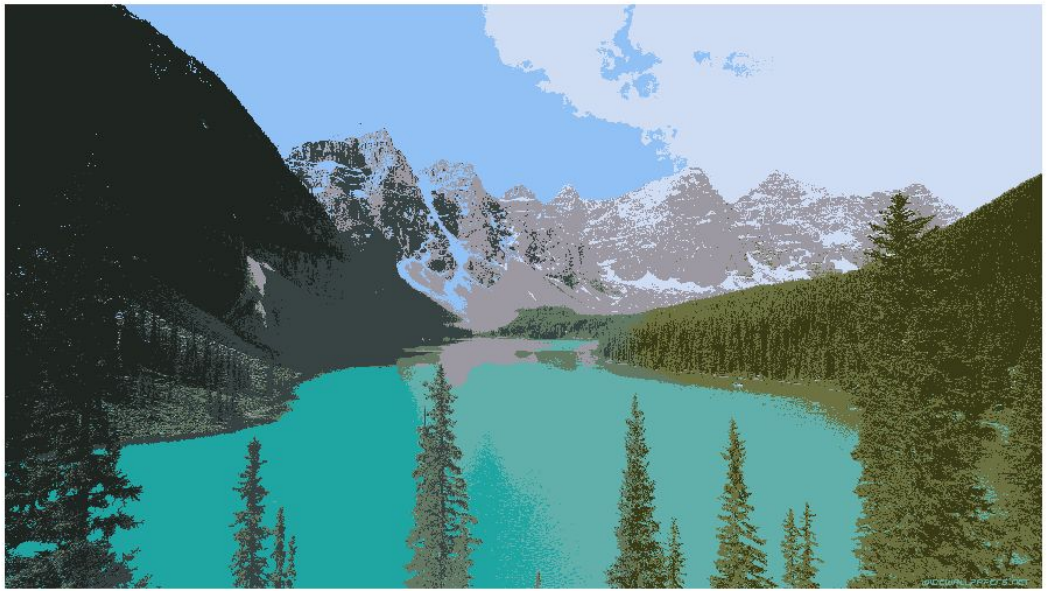
- ~1000 dimensions from a neural net
- Millions of data points
- Time available: <1s

SOMHunter, interactive video retrieval system
(VBS competition winner at MMM2020)

High-performance use cases

Real-time video super-pixel segmentation in Full HD

- <10 dimensions
- ~2 million data points
- Time available: ~50ms



News in CUDA-kmeans:
Raw performance

2 million data points, 32 dimensions, time per iteration:

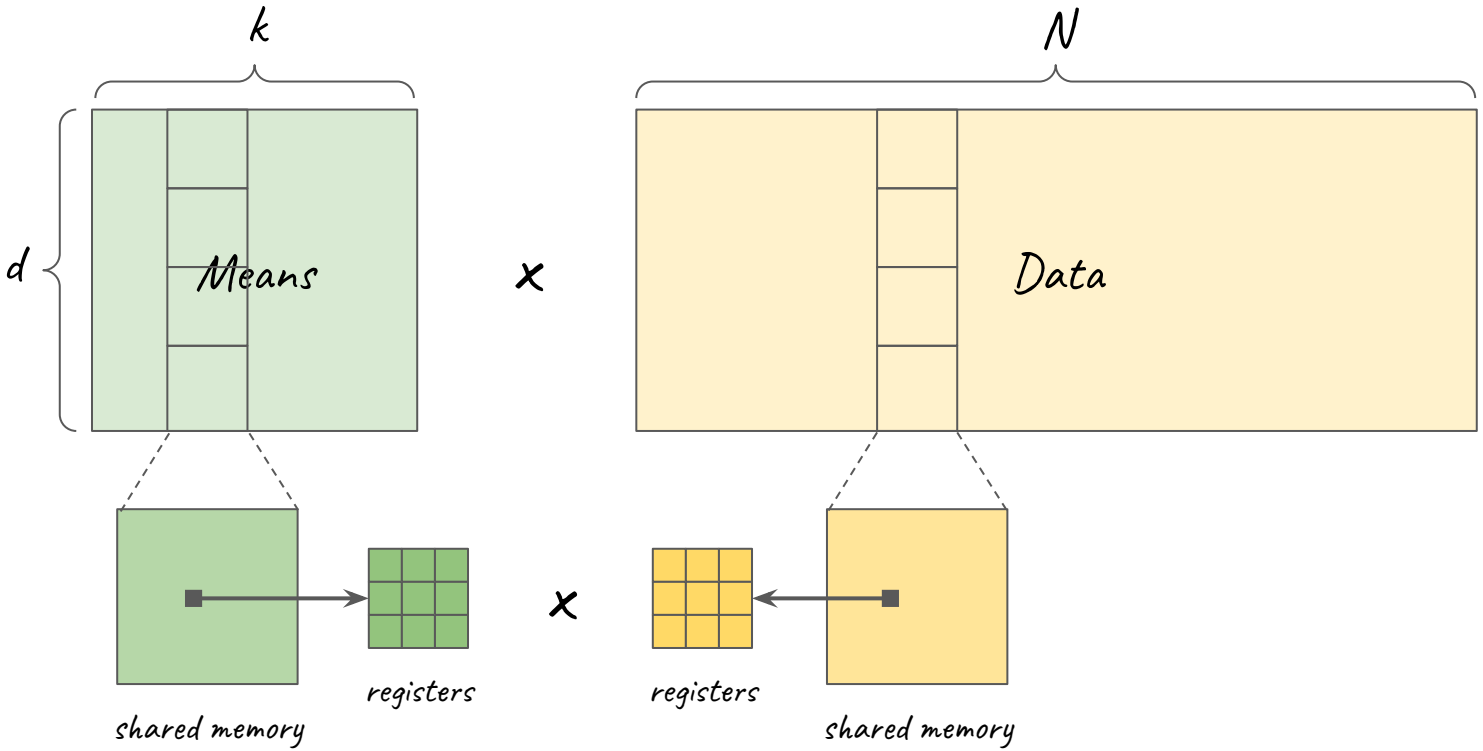
	16 clusters	1024 clusters
nVidia GTX 980	**7.31 ms** = 136 ips	**104.84 ms** = 9 ips
nVidia V100 SXM2	**1.58 ms** = 632 ips	**25.45 ms** = 39 ips

Our Contribution

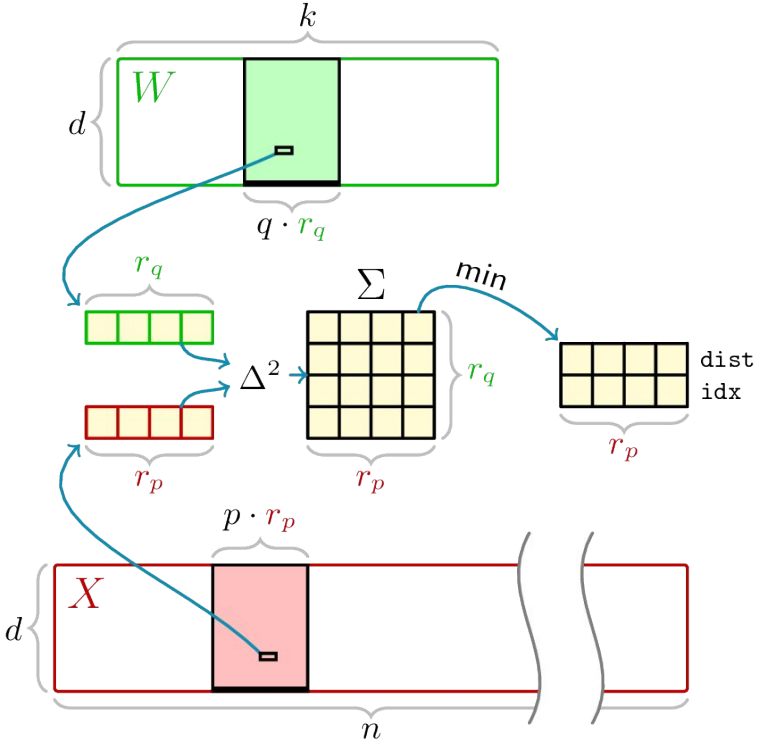
Cores/memory bandwidth ratio

Lockstep (SIMT) execution

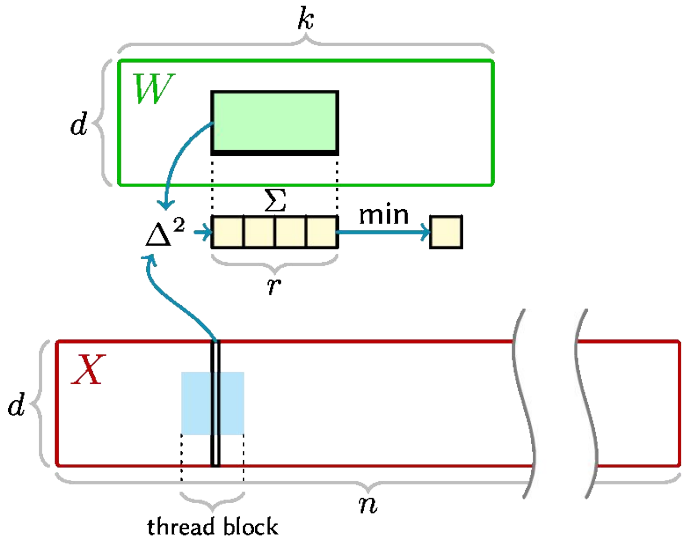
Assignment Step - Clever Caching



Assignment Step - Clever Caching

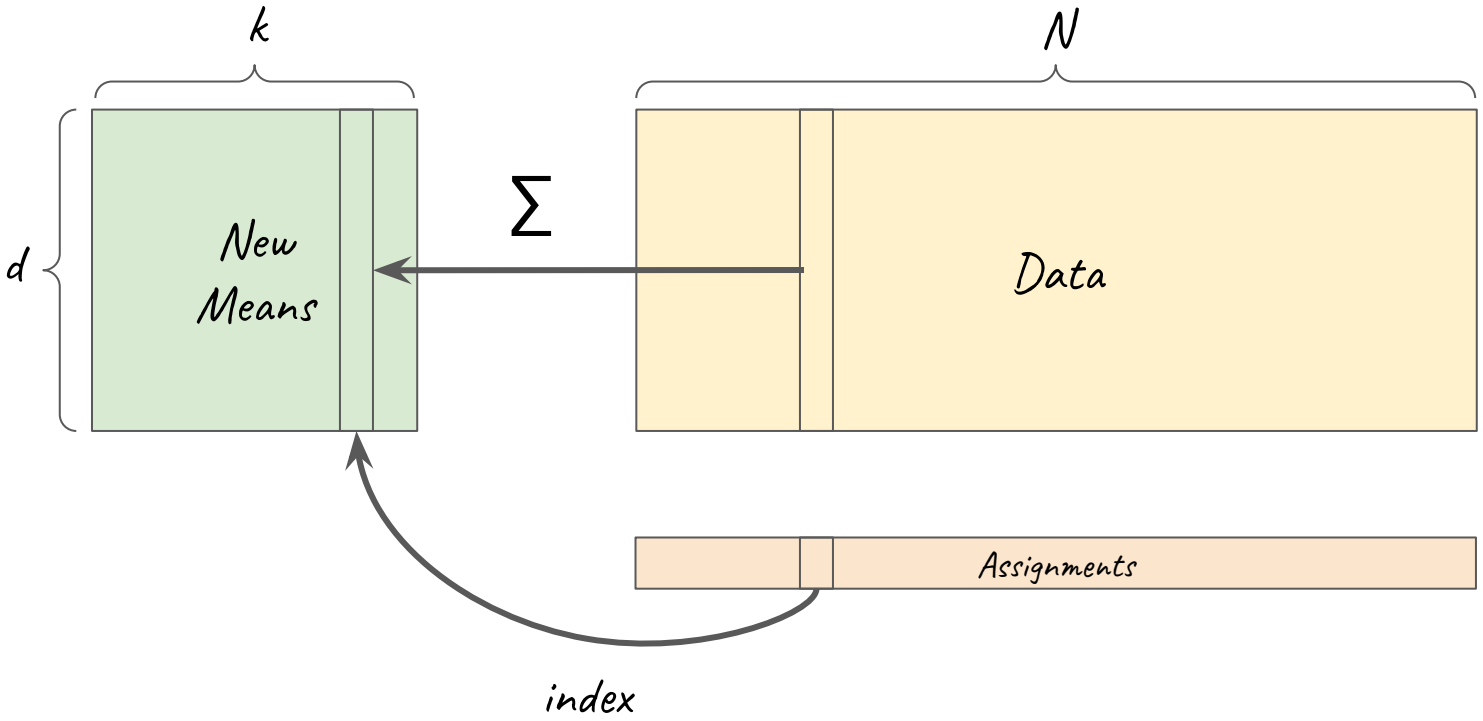


Regs caching strategy

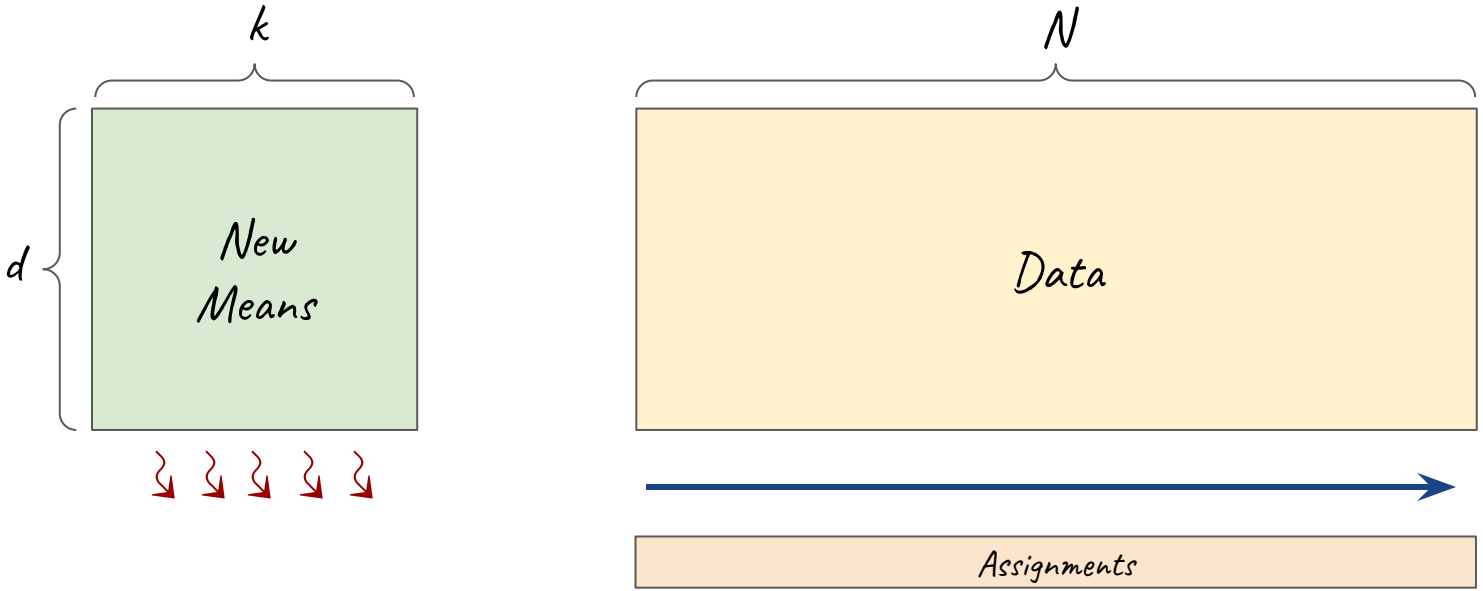


Fixed caching strategy

Update Step



Update Step - Thread Allocation



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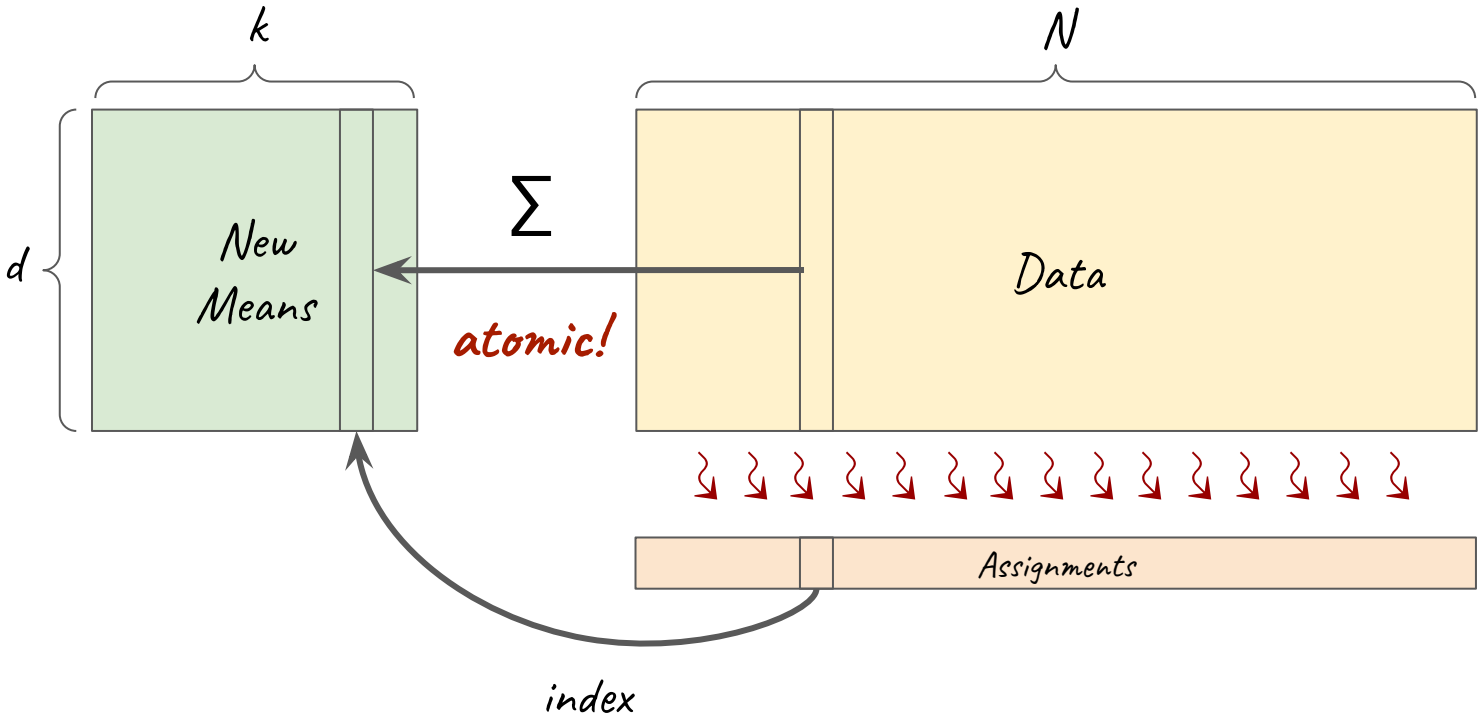

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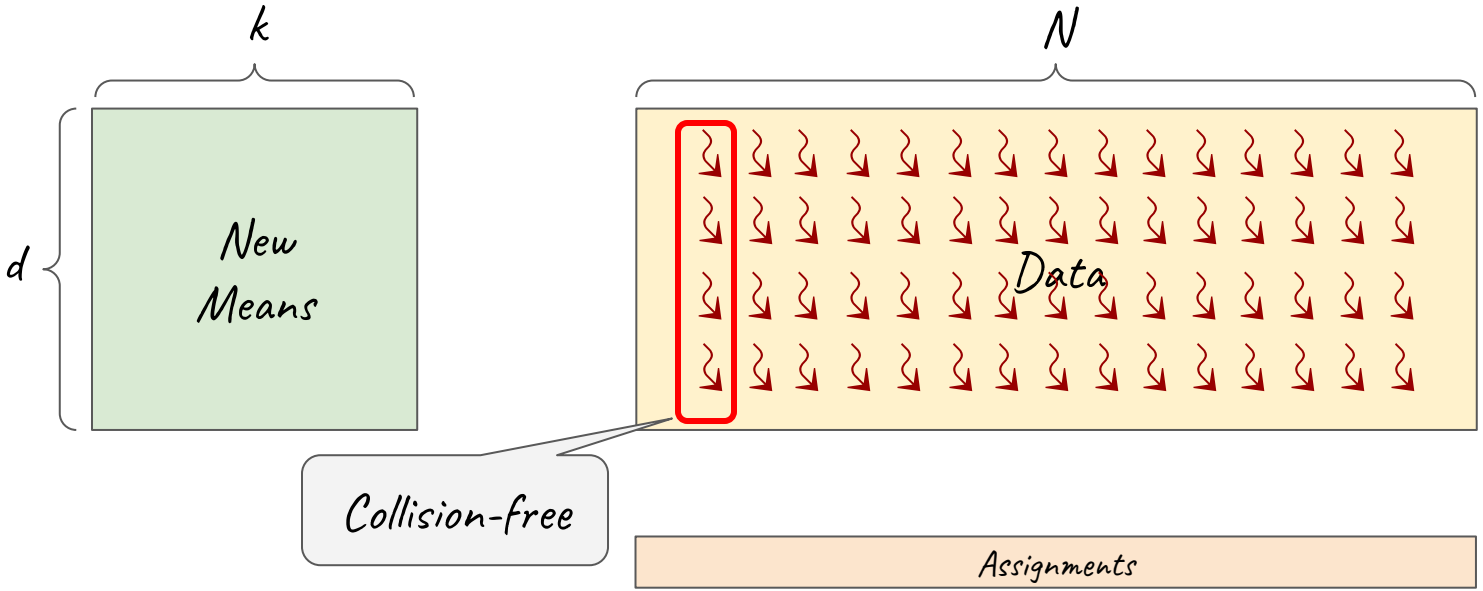
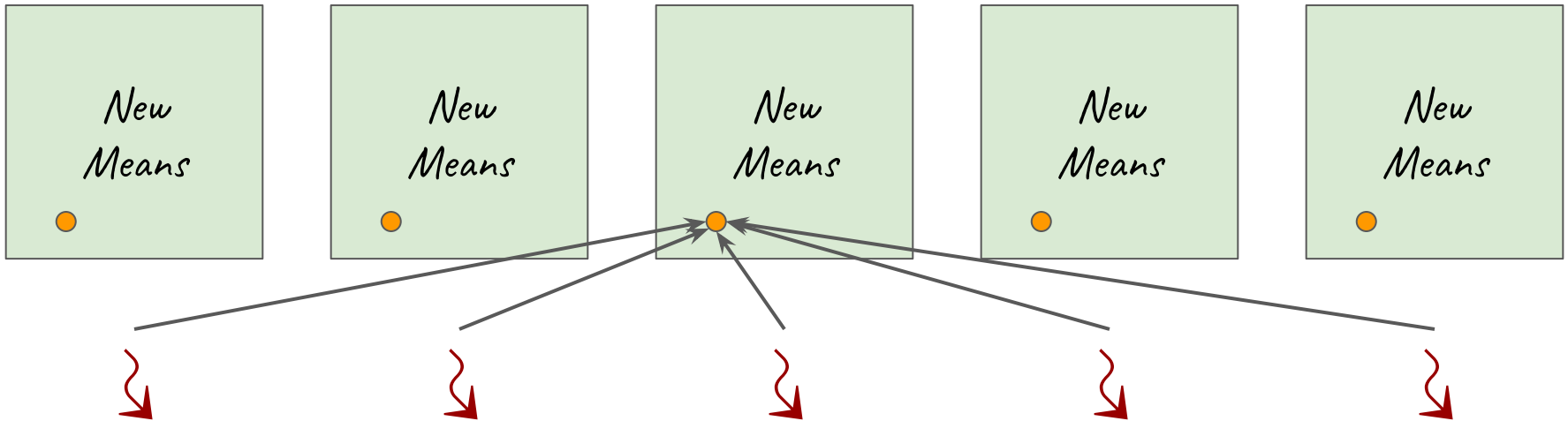
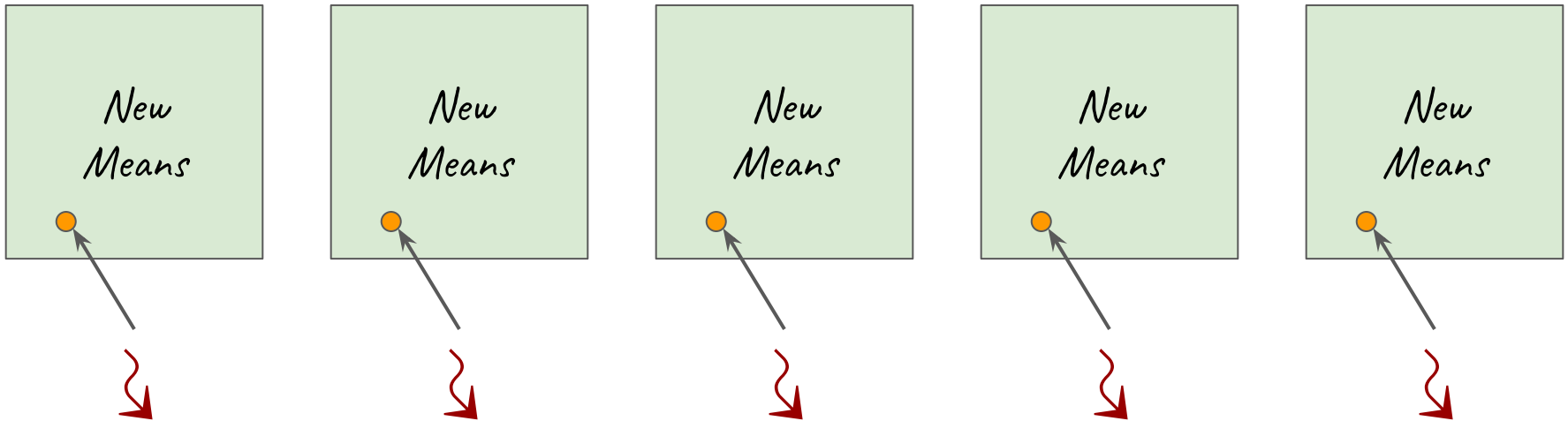


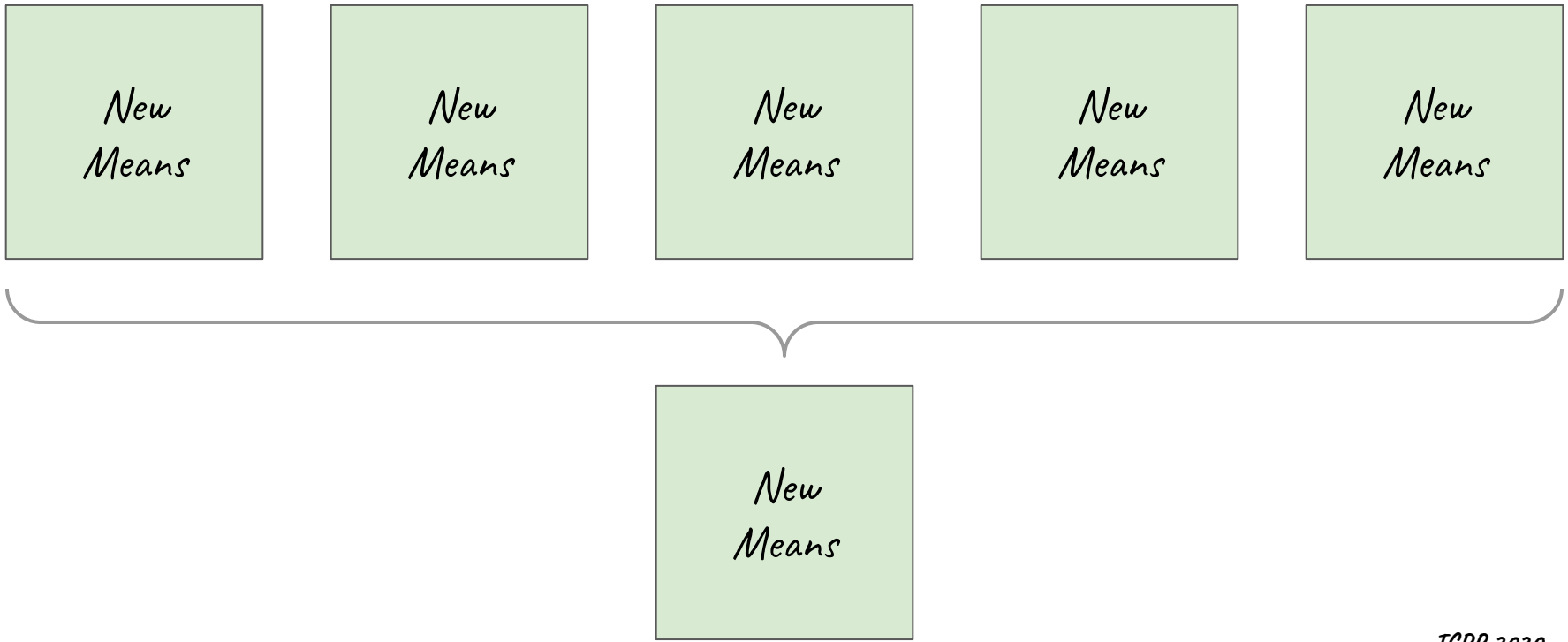
Increasing Atomic Throughput: Privatization



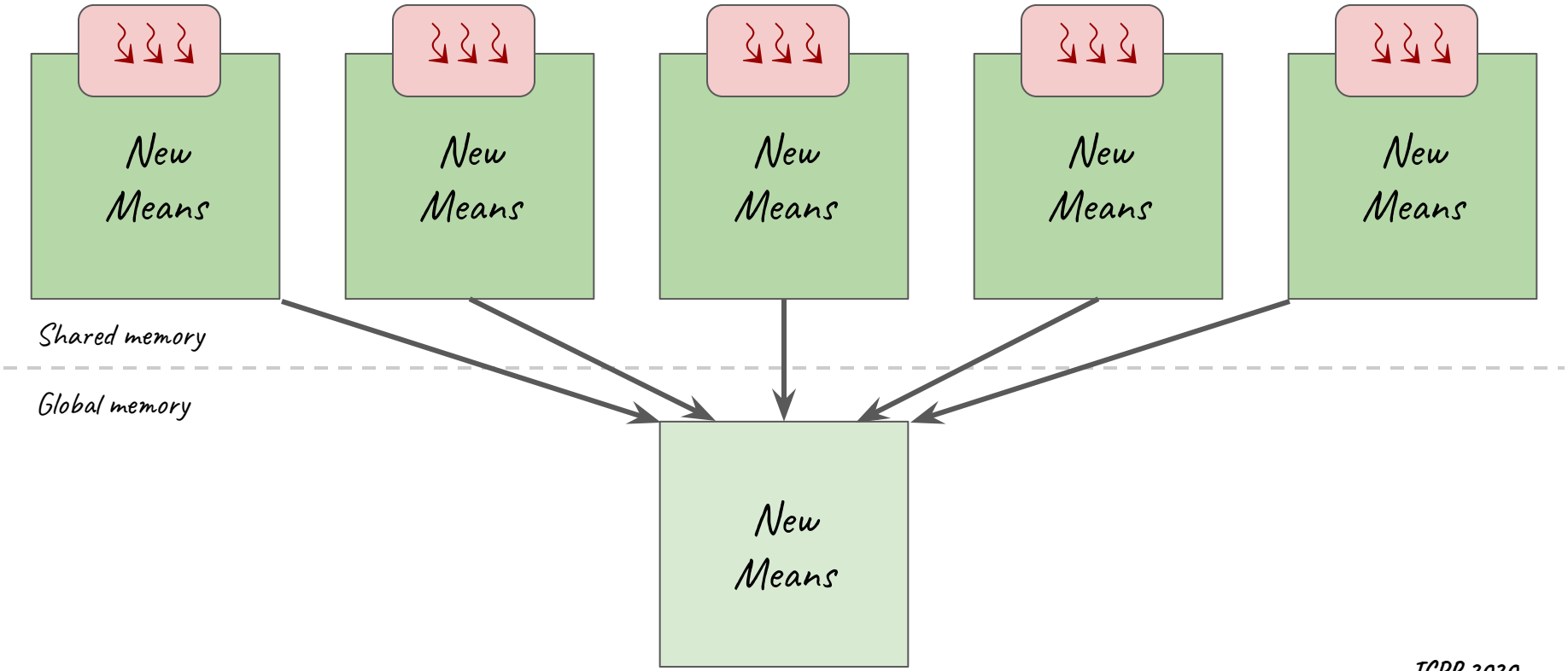
Increasing Atomic Throughput: Privatization



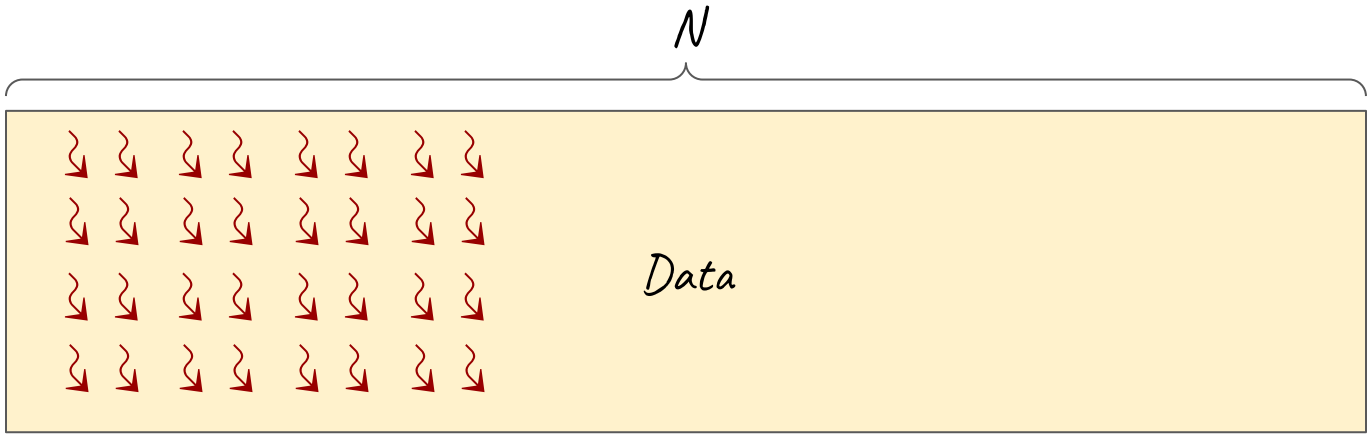
Increasing Atomic Throughput: Privatization



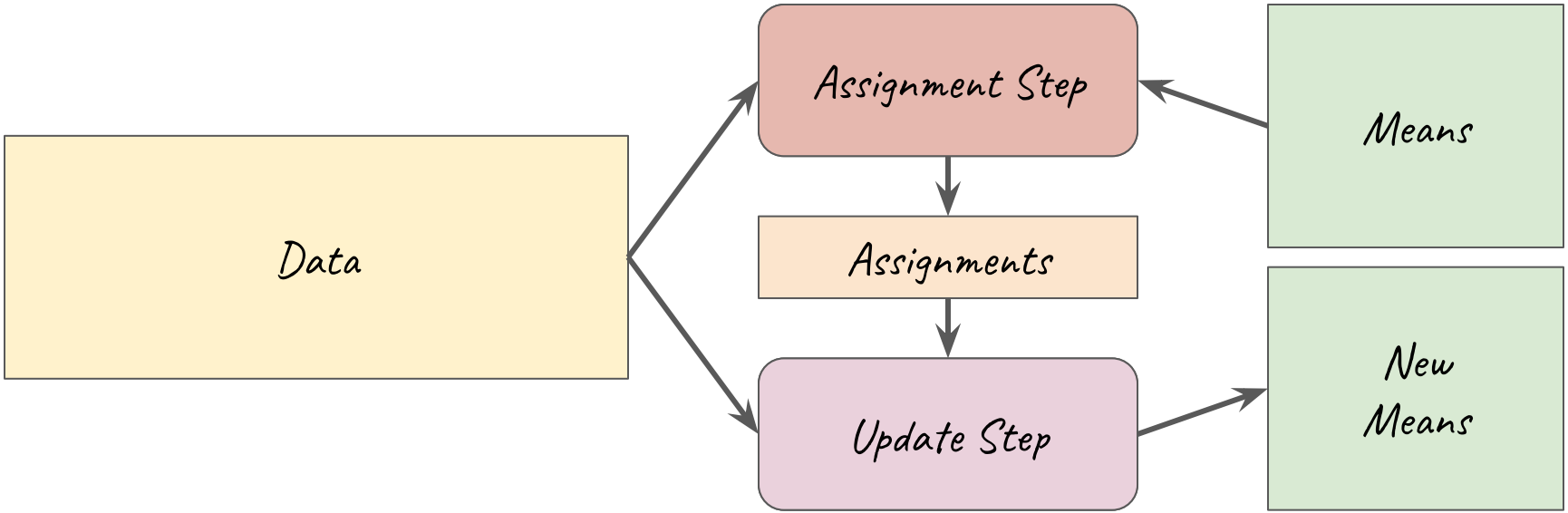
Privatization in Shared Memory



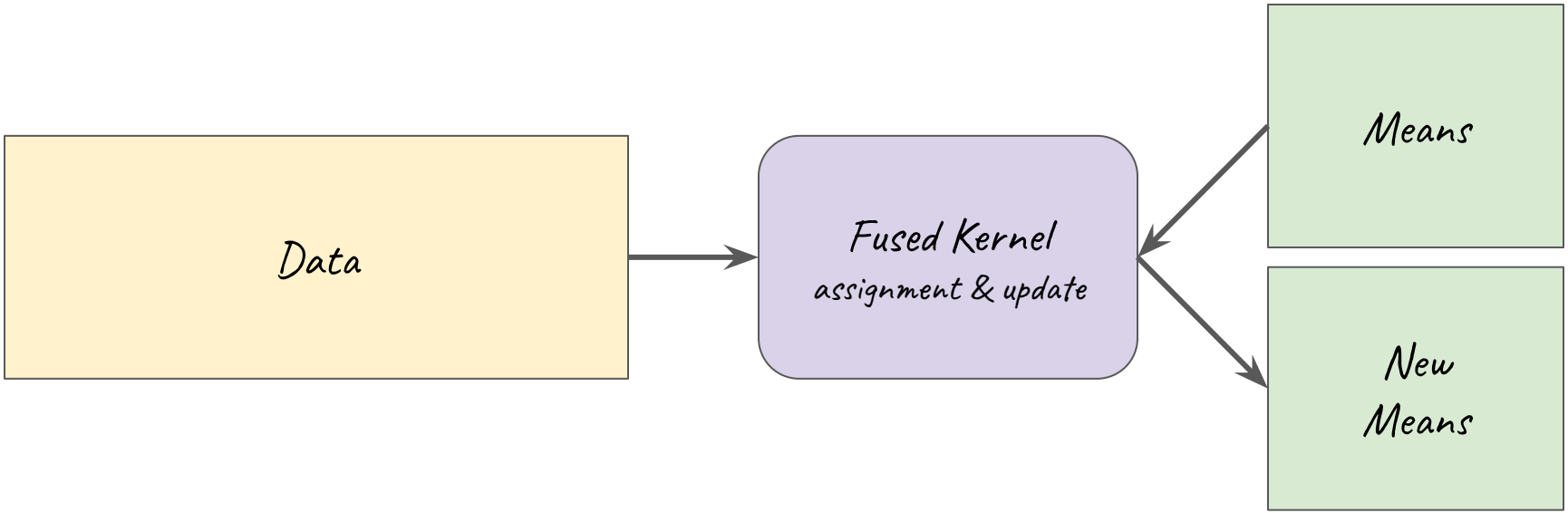
Privatization in Shared Memory



Complete Solution



Complete Solution - Fused Kernels

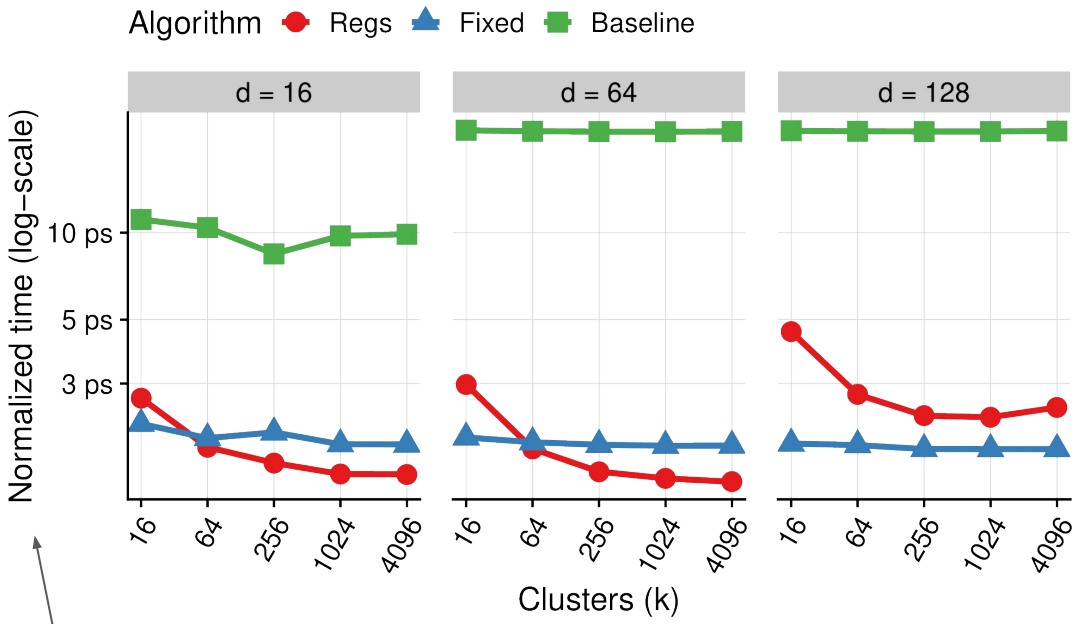


Technical Details

- Best data layout
- Atomic addition implementation
- Update step actually comprise two kernels - sum and division
- Code templating and loop unrolling
- Thread block shape and size
- ...

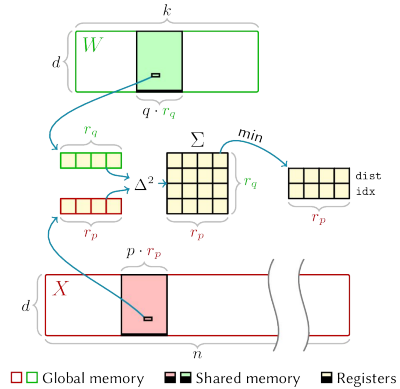
Experimental Results

Assignment step

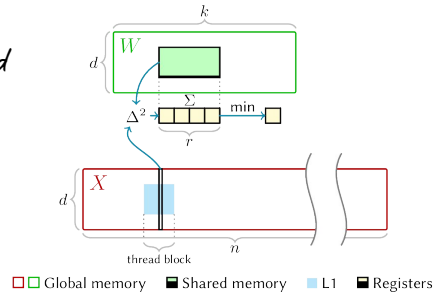


Actual time divided by N*D*k

Regs



Fixed



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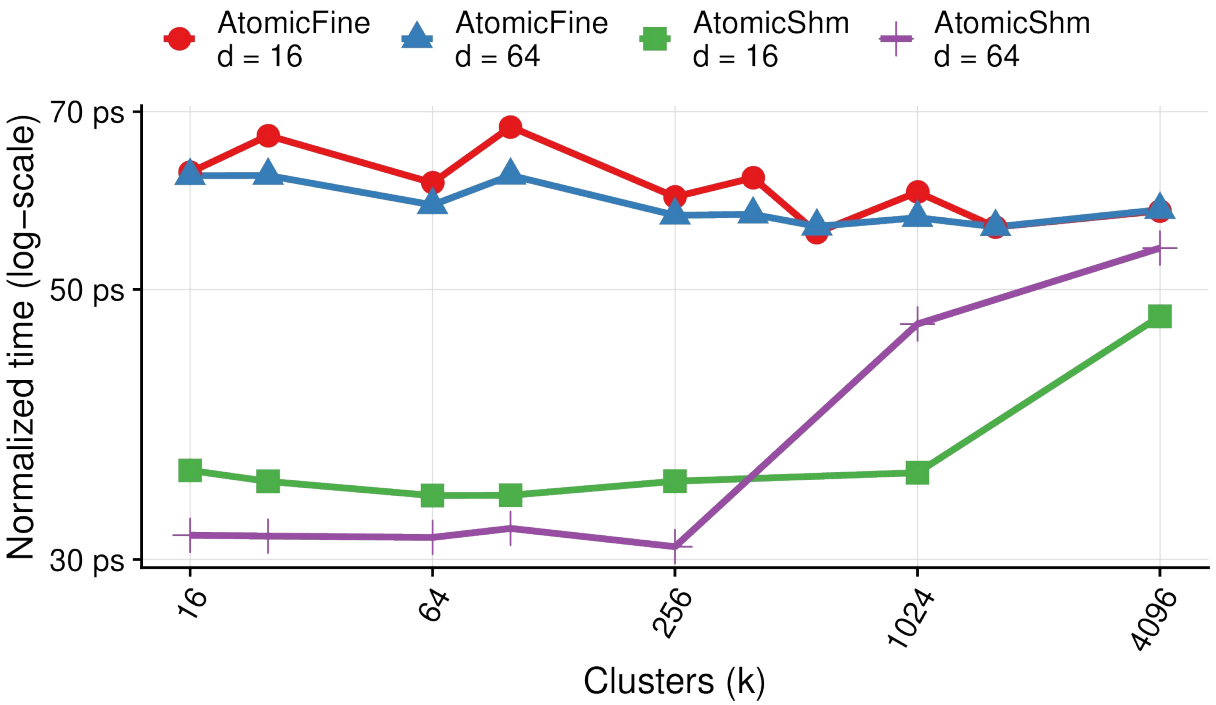
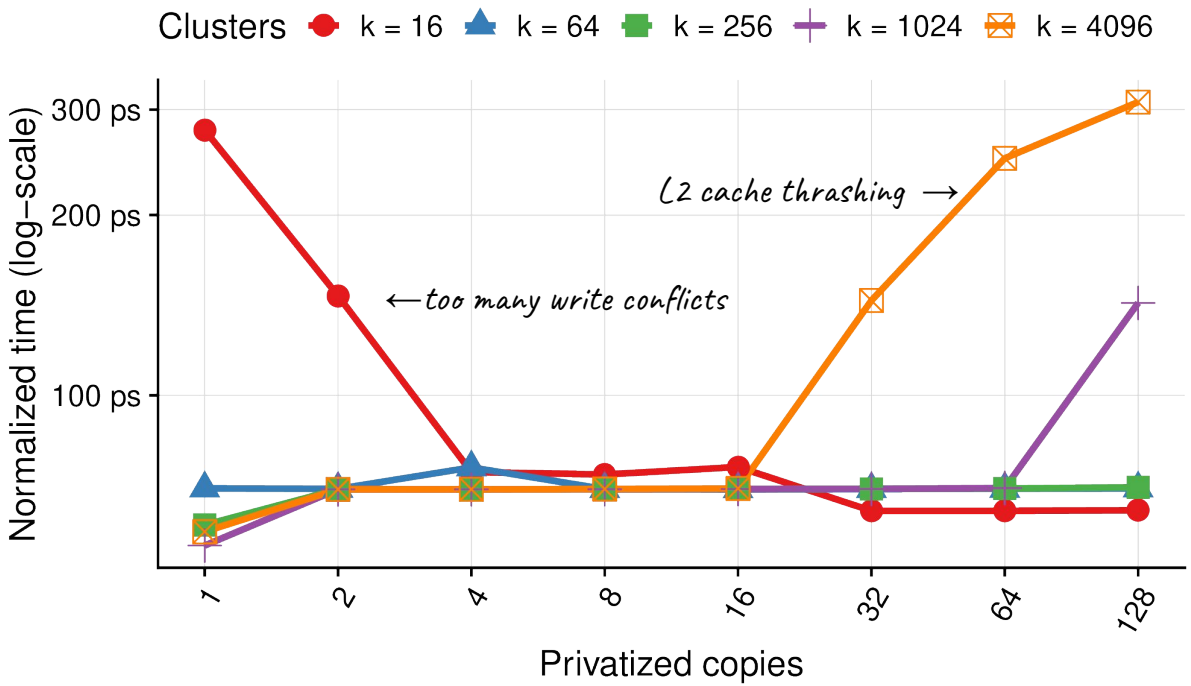
Update step - avoiding write conflicts



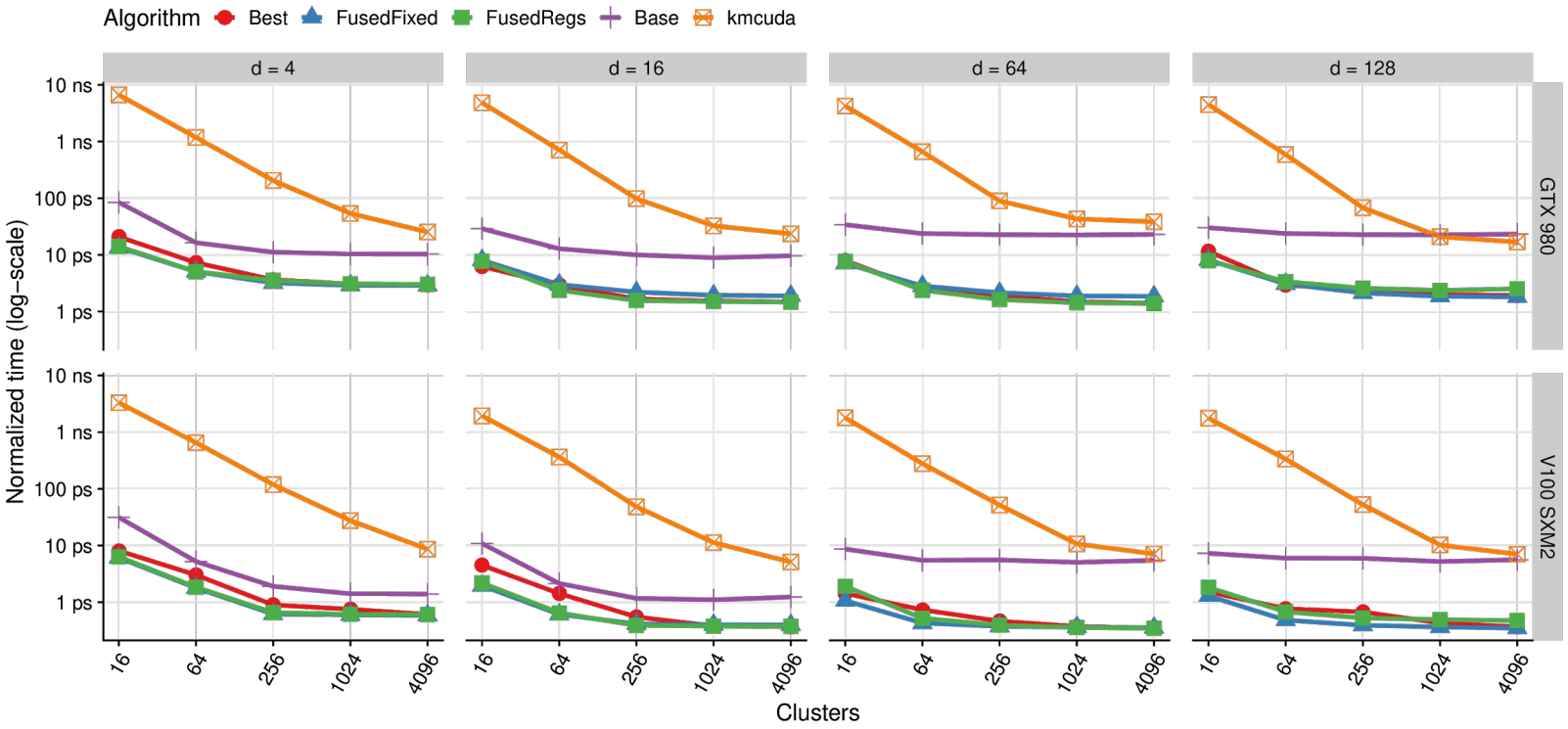
← N*D parallel threads

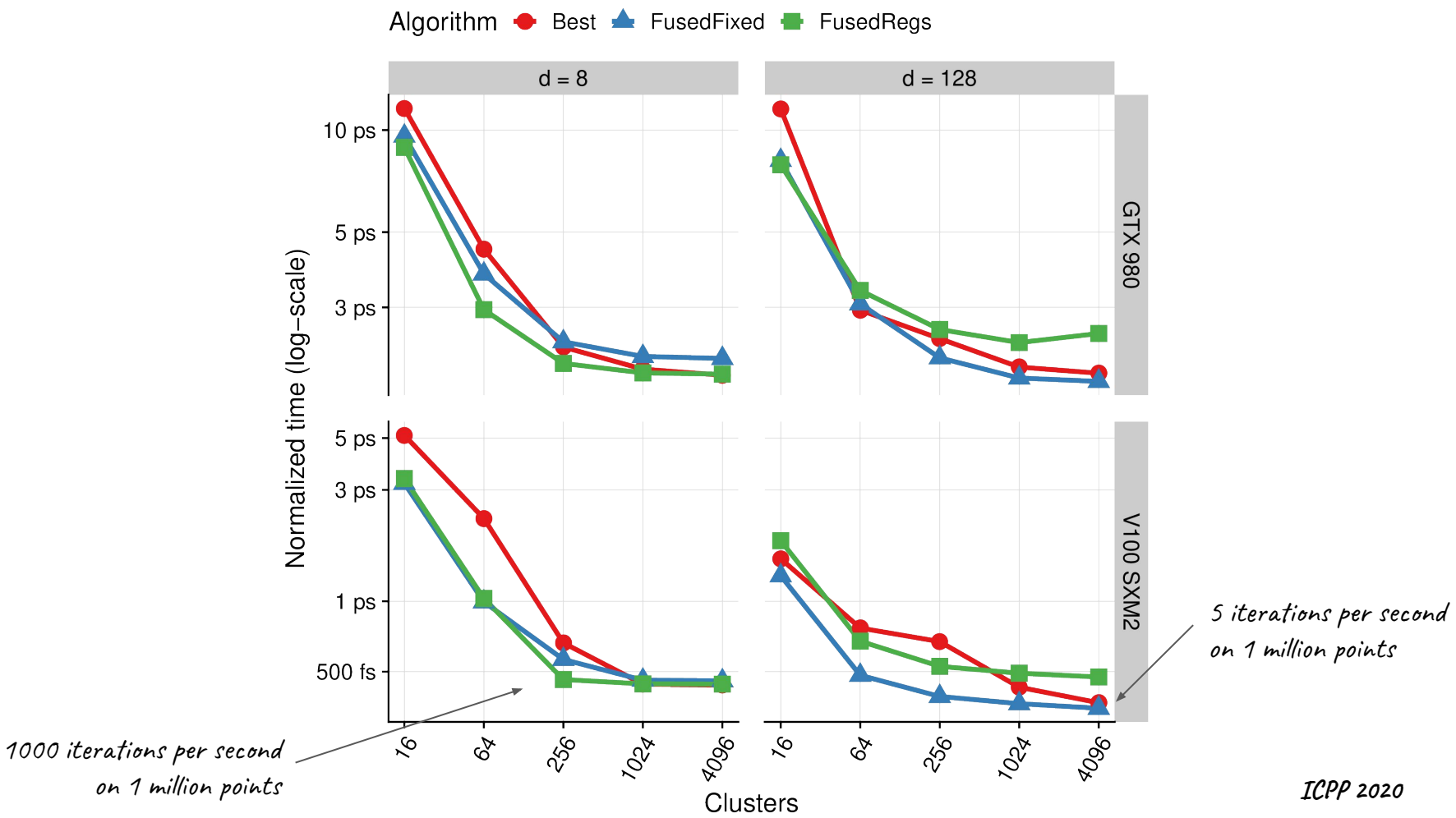
← aggregate some writes in SHM

Update step - write conflicts of N*D threads



Combined results




Algorithm
Best
FusedFixed
FusedRegs
d = 8
d = 128
GTX 980
V100 SXM2
Normalized time (log−scale)
10 ps
5 ps
3 ps
1 ps
500 fs
16
64
256
1024
4096
Clusters
1000 iterations per second
on 1 million points
5 iterations per second
on 1 million points
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https://github.com/krulis-martin/cuda-kmeans

Thank you for watching!

Martin Kruliš, Ph.D.

Department of software engineering, Charles University

Prague, Czech Republic

krulis@ksi.mff.cuni.cz

http://www.ksi.mff.cuni.cz/~krulis

ORCID: 0000-0002-0985-8949

Miroslav Kratochvíl, M.Sc.

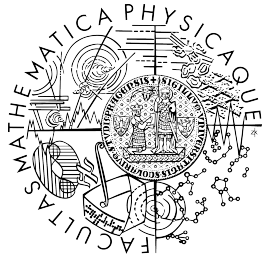
Department of software engineering, Charles University

Prague, Czech Republic

kratochvil@ksi.mff.cuni.cz

https://www.ksi.mff.cuni.cz/~kratochvil

ORCID: 0000-0001-7356-4075



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