GWAS ON GPUS:

Streaming Data from HDD for Sustained Performance

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Thanks to the AICES HPAC group and DFG grant GSC111

OUTLINE

- Intoduction and motivation
- Problem description
- CPU-only algorithm
- Leveraging the GPU
- Results and conclusion

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SINGLE NUCLEOTIDE POLYMORPHISM

nucleotide differs between two individuals of a species

link to traits, diseases?

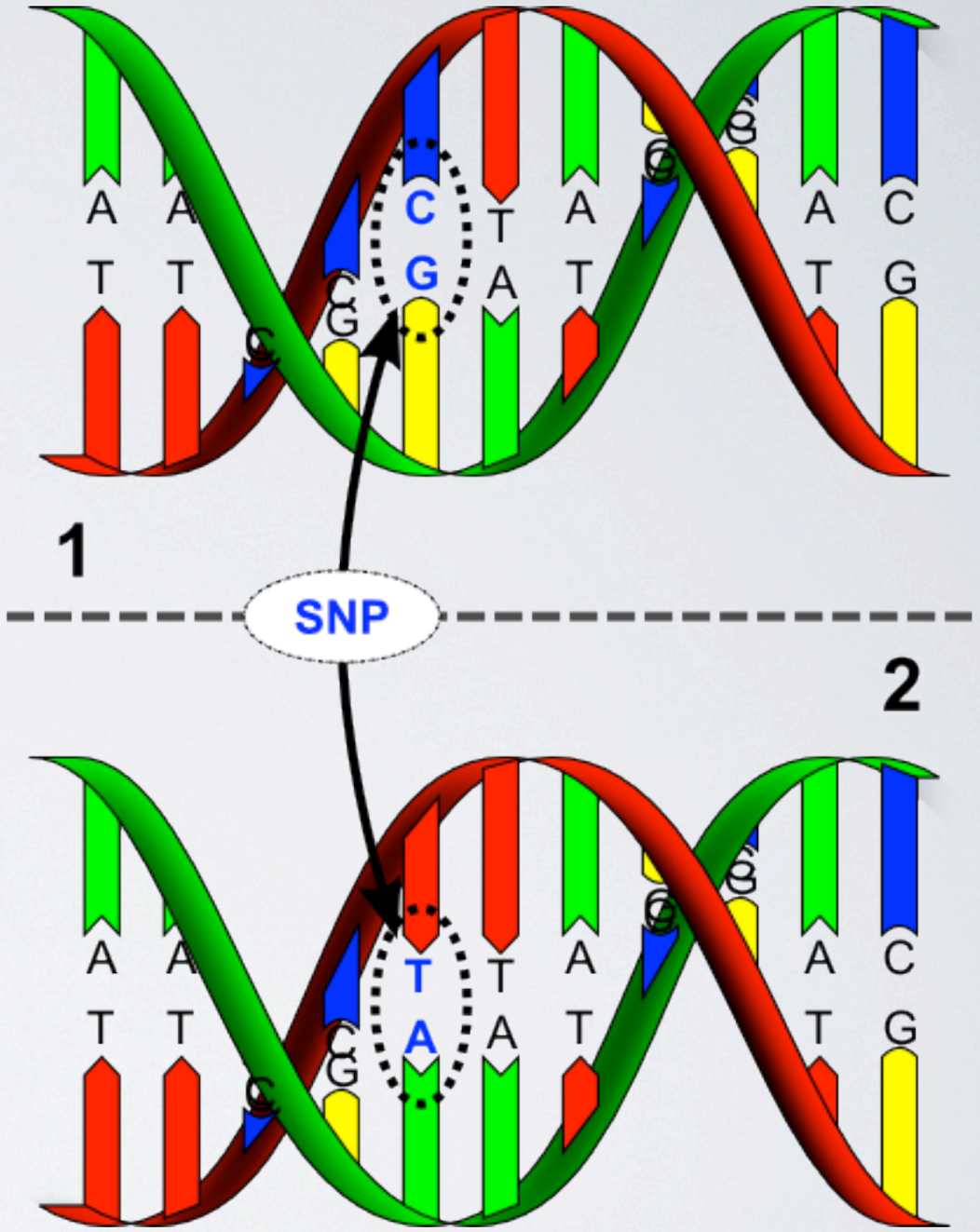


Image credit: David Hall

GWAS

- Human Genome project HUGO (2004)
- Genome-wide association studies (GWAS)
  - Find correlations between SNPs and traits (diseases)

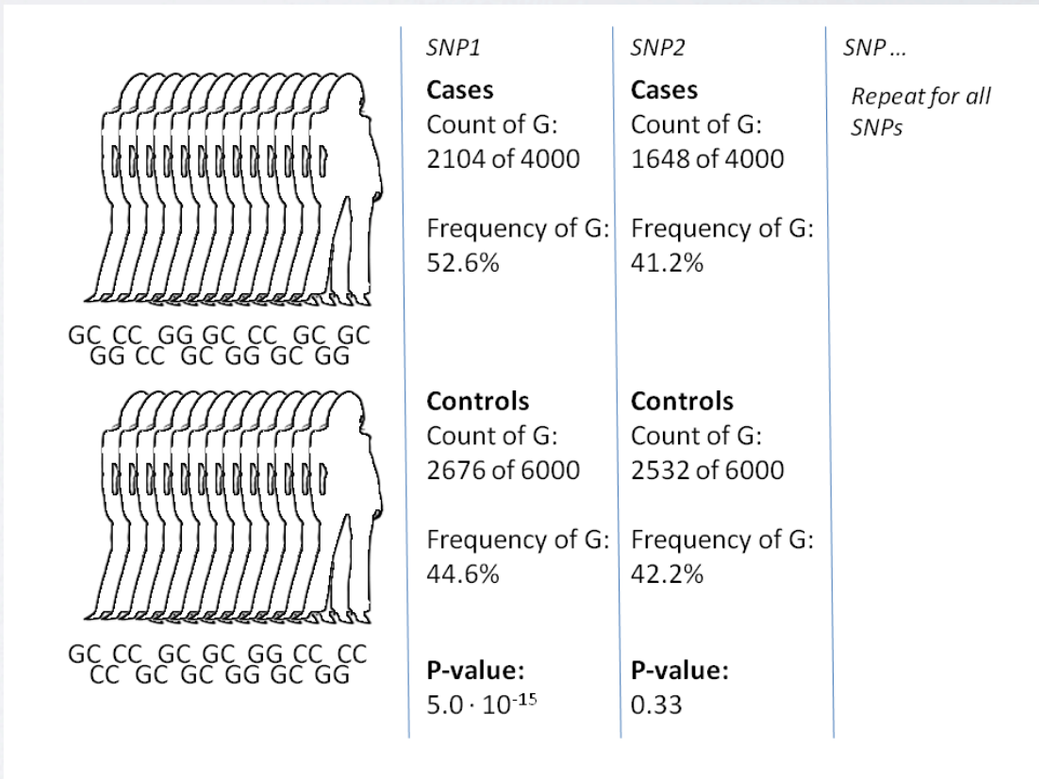
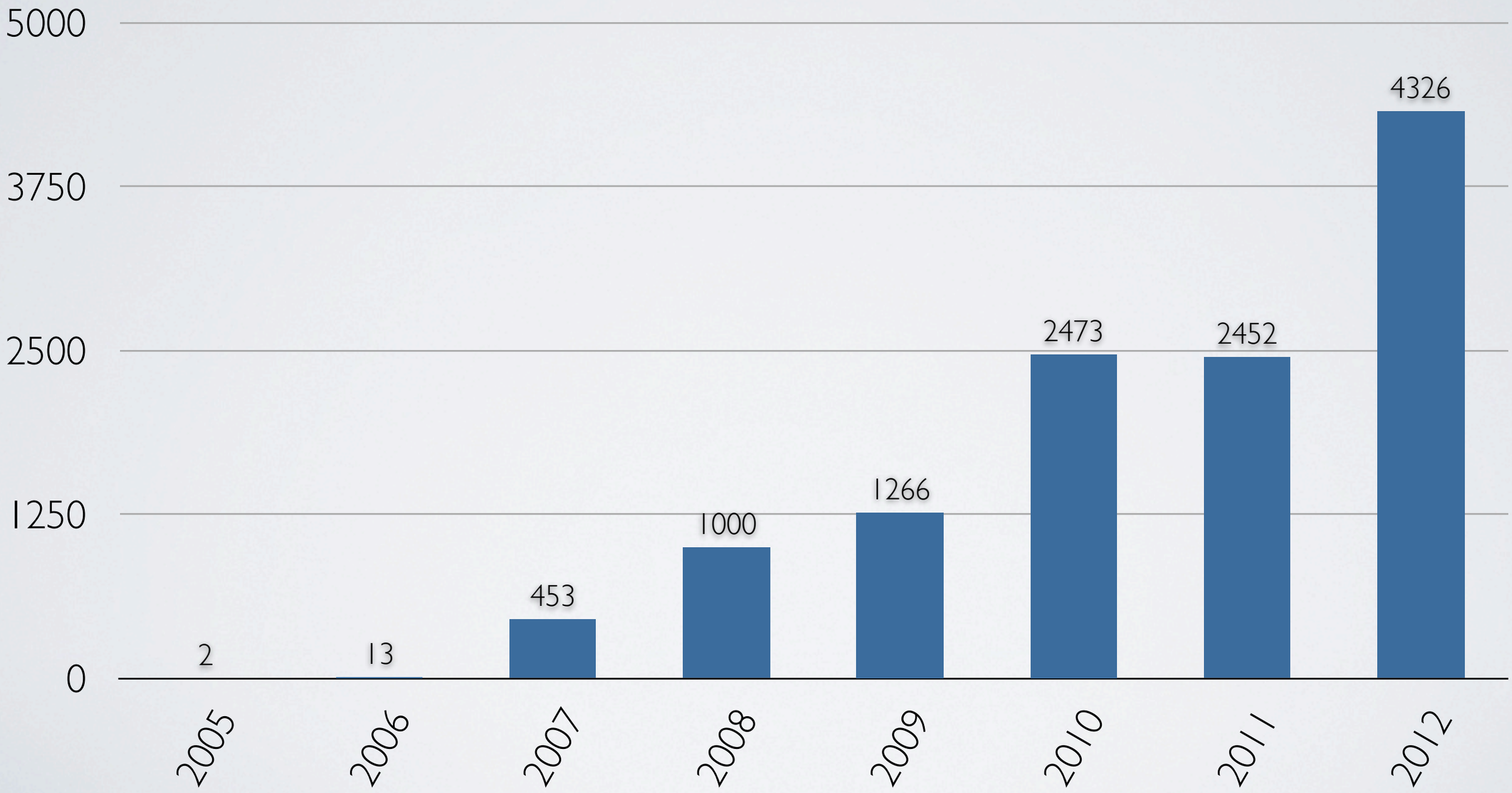


Image credit: Lasse Folkersen

GWAS STATS

of GWAS carried out each year



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$$r_i \leftarrow (X_i^T M^{-1} X_i)^{-1} X_i^T M^{-1} y$$

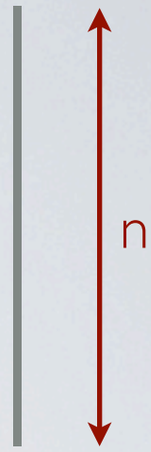
GENOME-WIDE ASSOCIATION STUDIES

lots of GLS because i = 0 ... millions

input

output

$$r_i \leftarrow (X_i^T M^{-1} X_i)^{-1} X_i^T M^{-1} y$$



GENOME-WIDE ASSOCIATION STUDIES

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$y \in \mathbb{R}^n$ observations (phenotype)

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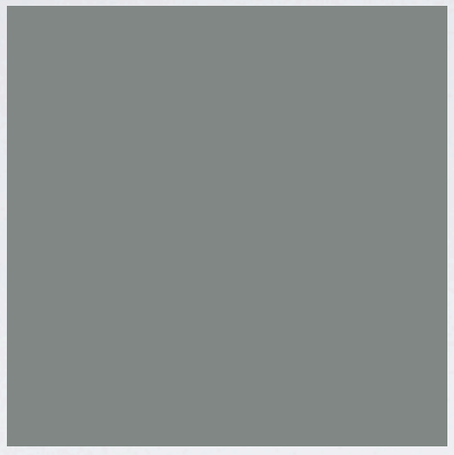

GENOME-WIDE ASSOCIATION STUDIES

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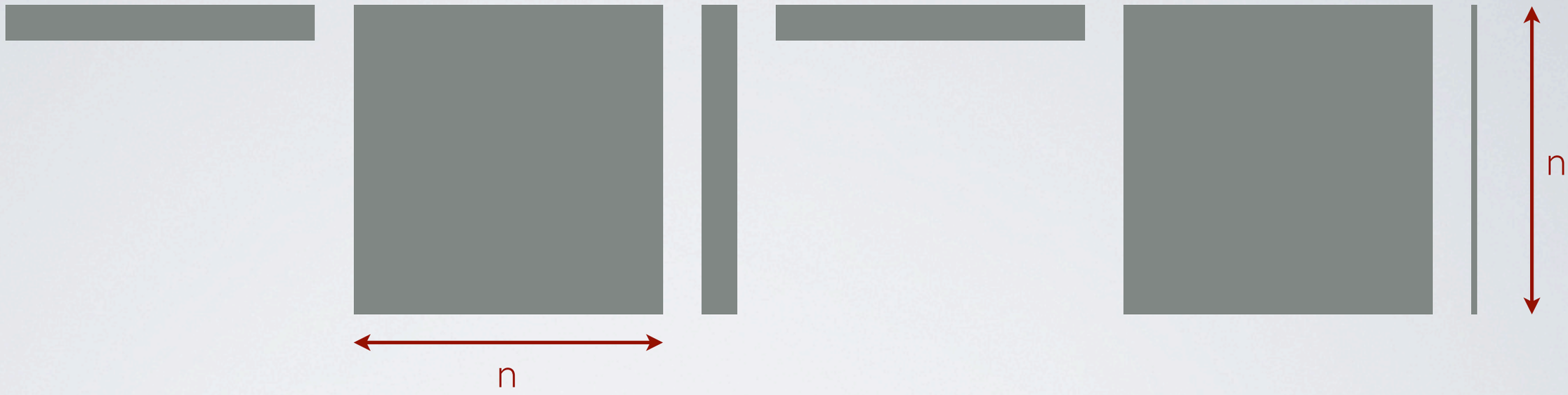
input	$y \in \mathbb{R}^n$	observations (phenotype)
	$M \in \mathbb{R}^{n \times n}$	observation dependencies
output		

$$r_i \leftarrow (X_i^T M^{-1} X_i)^{-1} X_i^T M^{-1} y$$



GENOME-WIDE ASSOCIATION STUDIES

lots of GLS because i = 0 ... millions

input	$y \in \mathbb{R}^n$	observations (phenotype)
	$M \in \mathbb{R}^{n \times n}$	observation dependencies
	$X_i \in \mathbb{R}^{n \times p}$	genome measurements/covariates
output		

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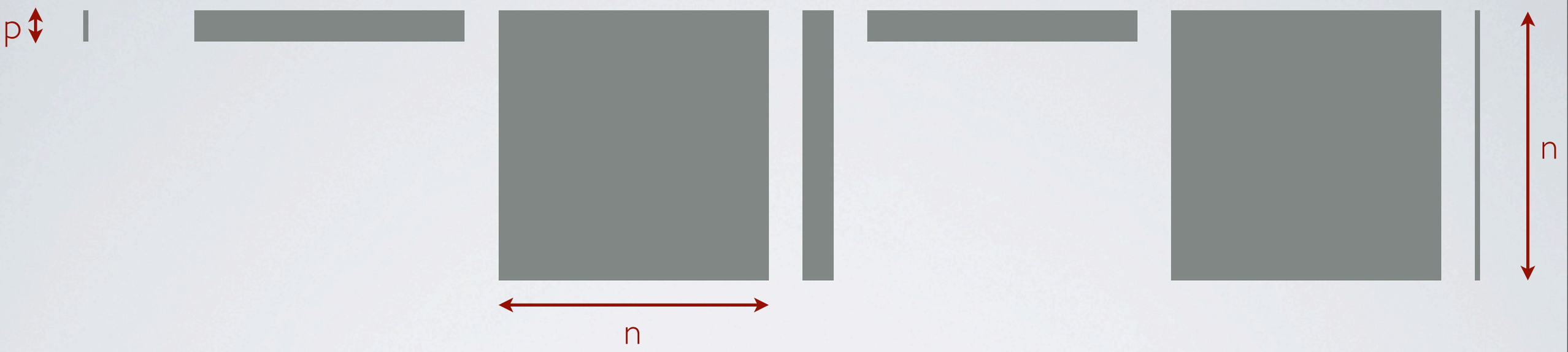

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output	$r_i \in \mathbb{R}^p$	relations between phenotype and genome variations

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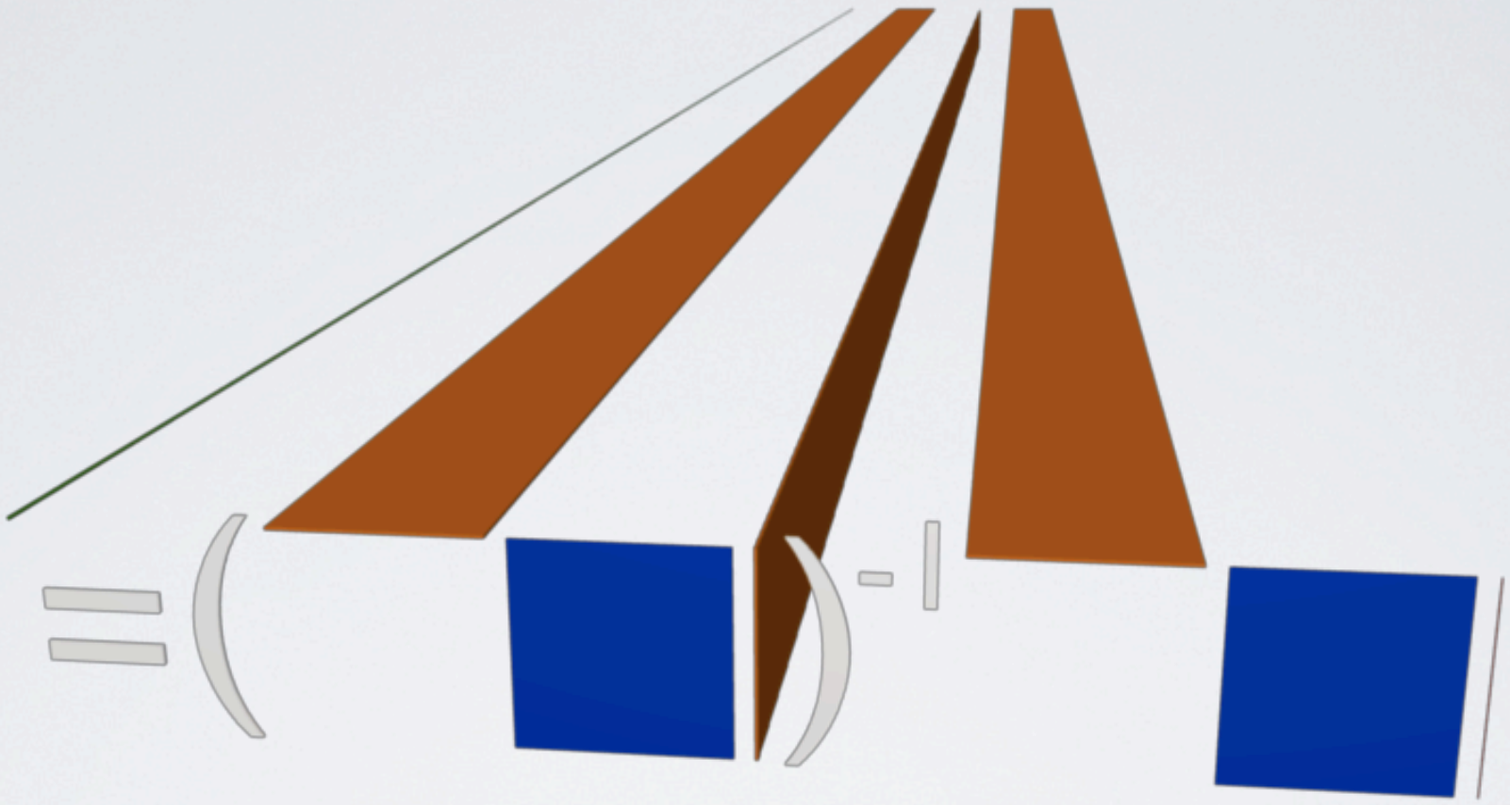
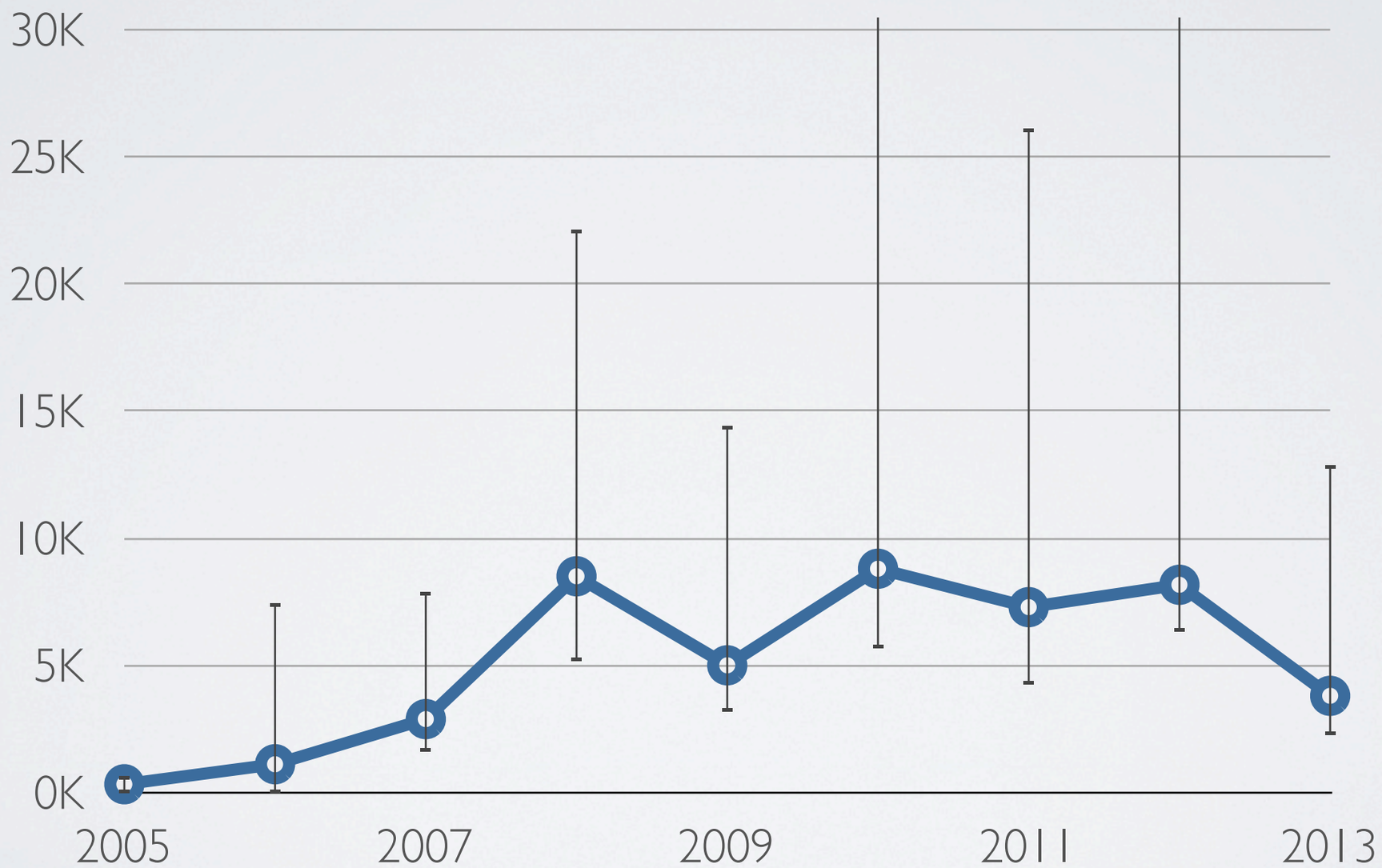
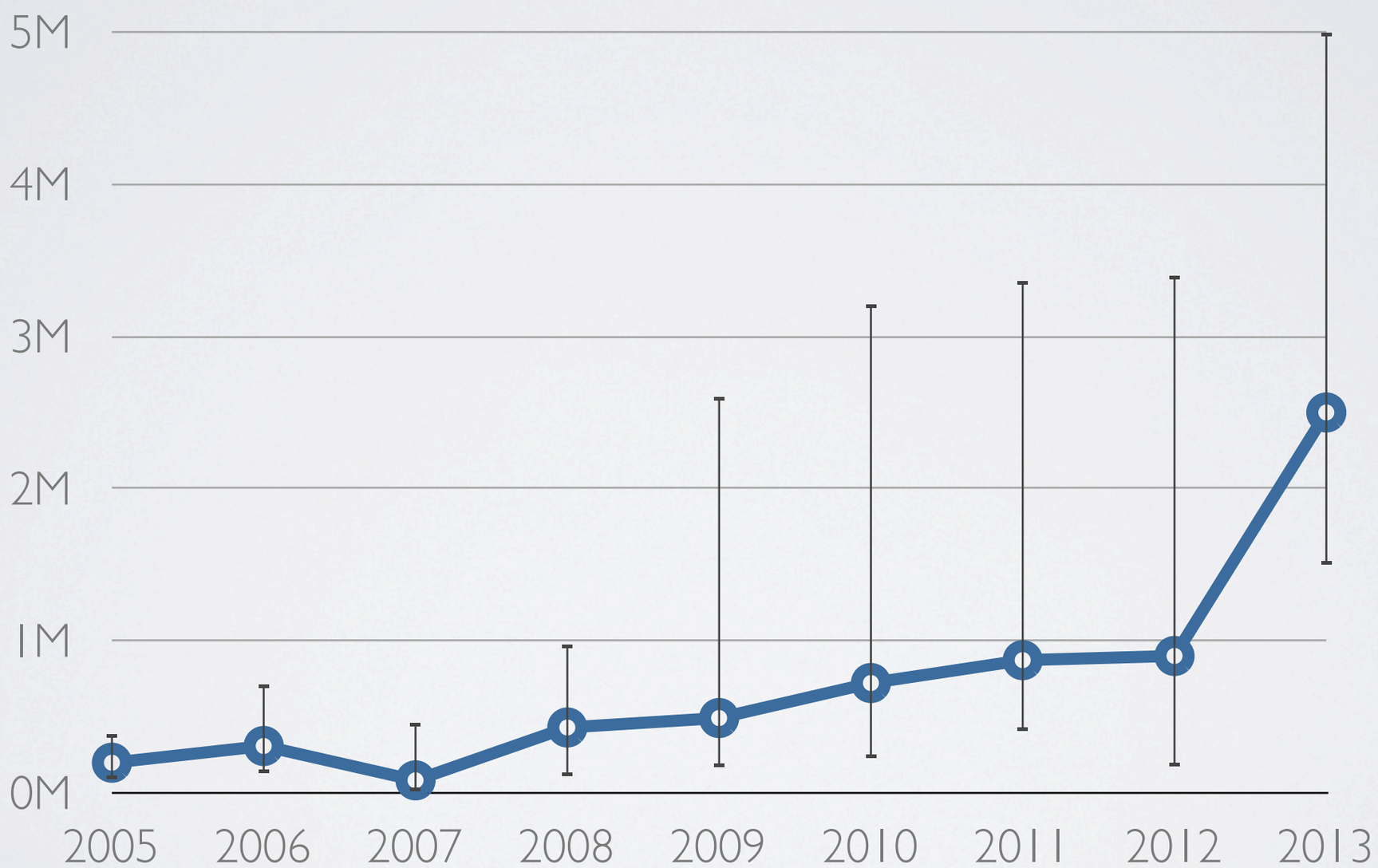


GWAS STATS


Sample size n (# of people)
30K
25K
20K
15K
10K
5K
0K
2005
2007
2009
2011
2013

GWAS STATS


#SNPs m (passing QC)
5M
4M
3M
2M
1M
0M
2005
2006
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2010
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2012
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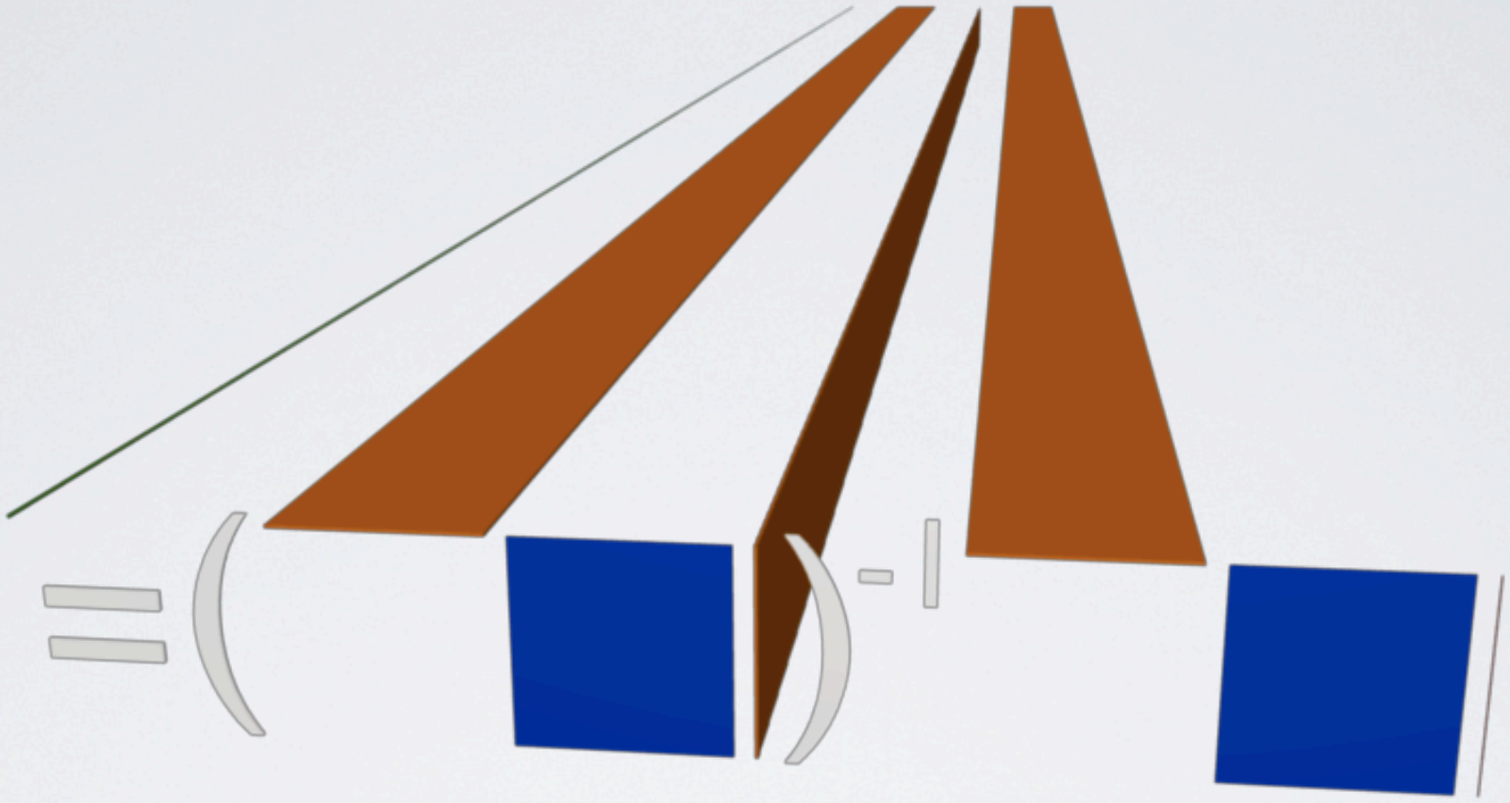
GWAS STATS

Largest #SNPs m (passing QC)

$$r_i \leftarrow (X_i^T M^{-1} X_i)^{-1} X_i^T M^{-1} y$$



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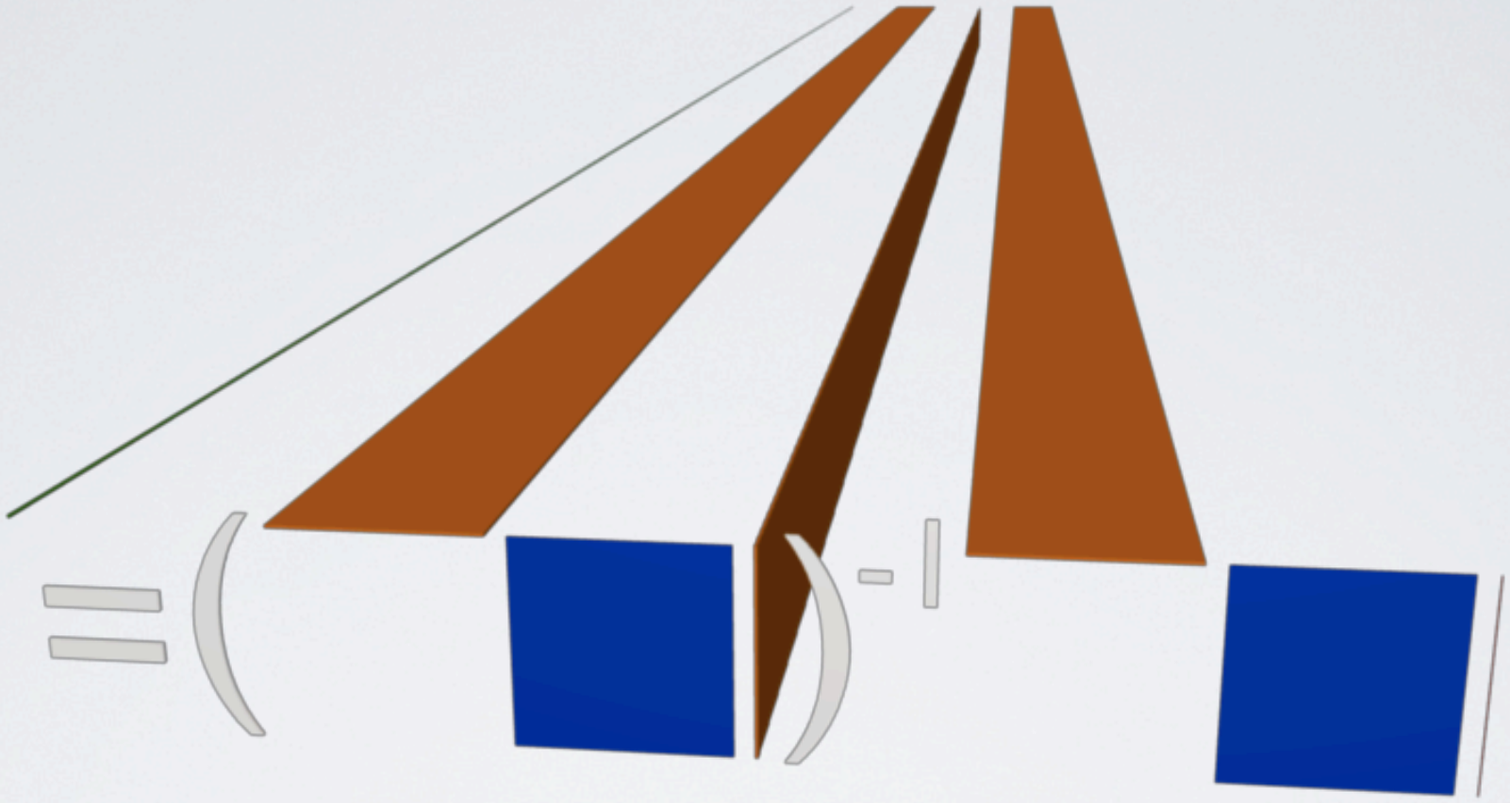

THE NUMBERS

# DNA fragments (nucleotides)	$m \sim 48 - 250$ million
# samples	$n \sim 10\,000$
# covariates	$p = 20$

$\Rightarrow$

$y \in \mathbb{R}^n$	80 MB
$M \in \mathbb{R}^{n \times n}$	800 MB
$r \in \mathbb{R}^{p \times m}$	7-40 GB
$X \in \mathbb{R}^{n \times p \times m}$	72 TB – 373 TB

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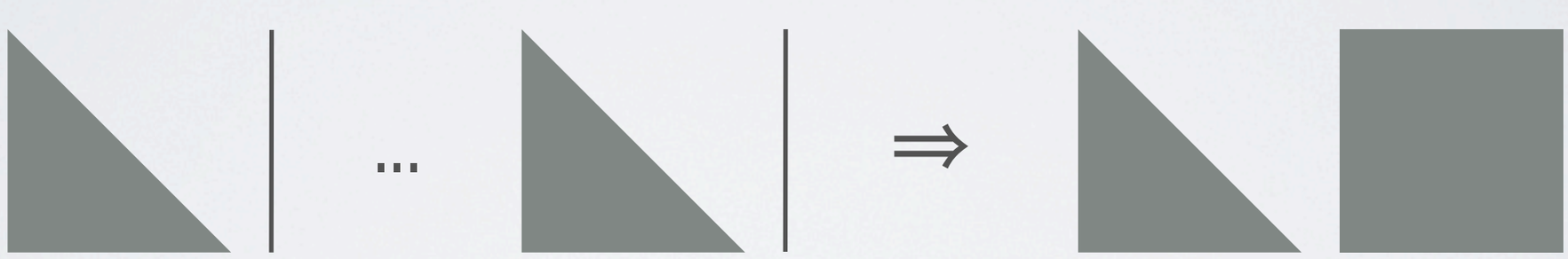
OPTIMIZATIONS

- Blocking in i
  - many small trsms vs. one big trsm



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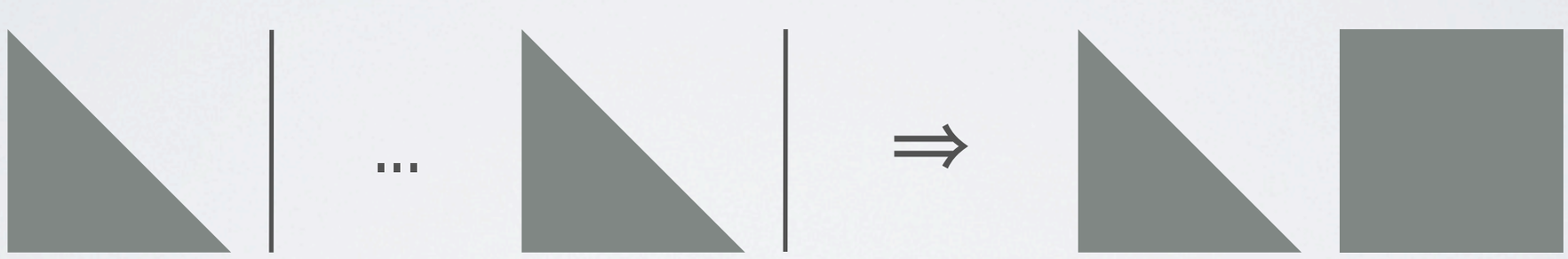
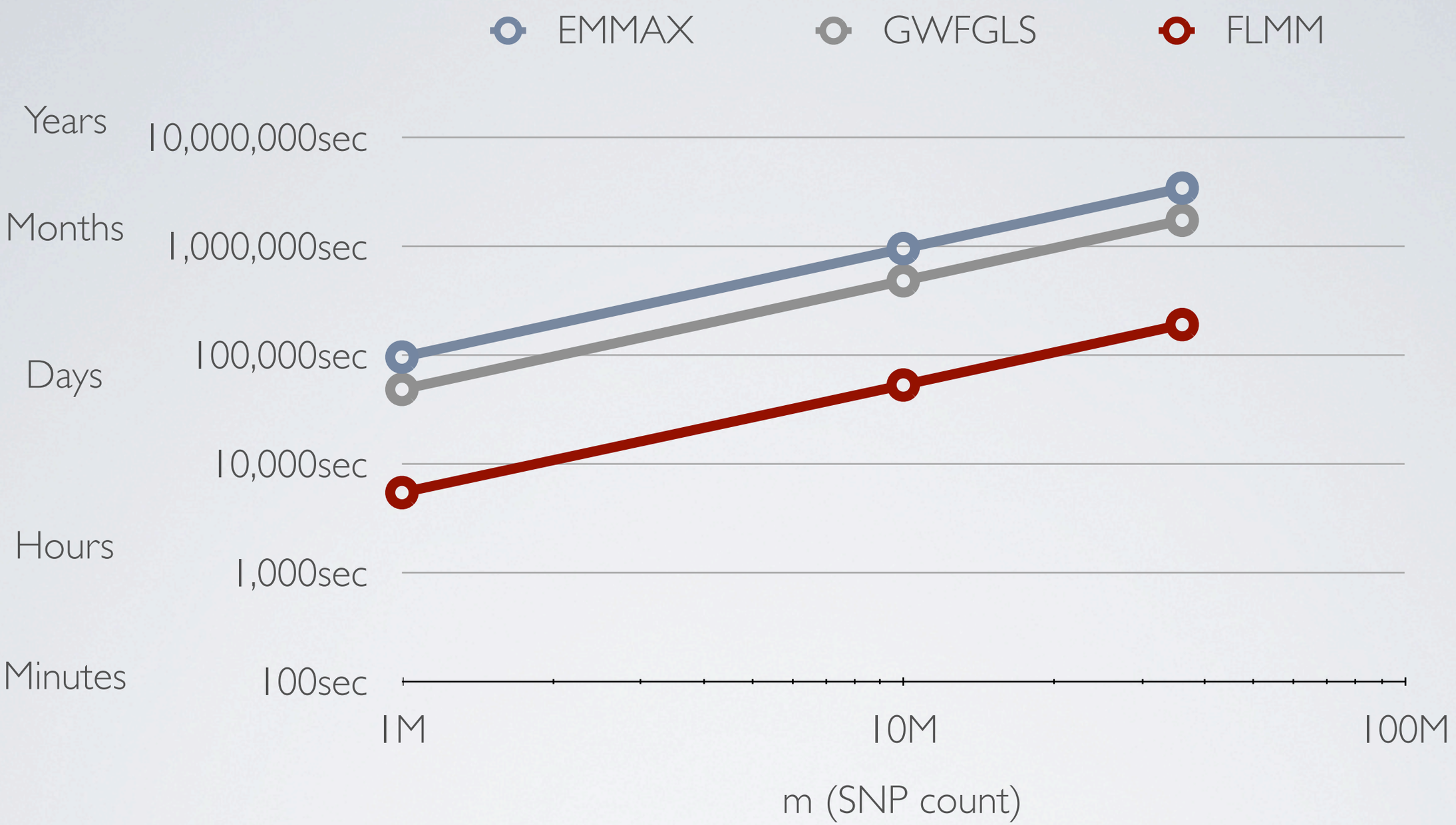
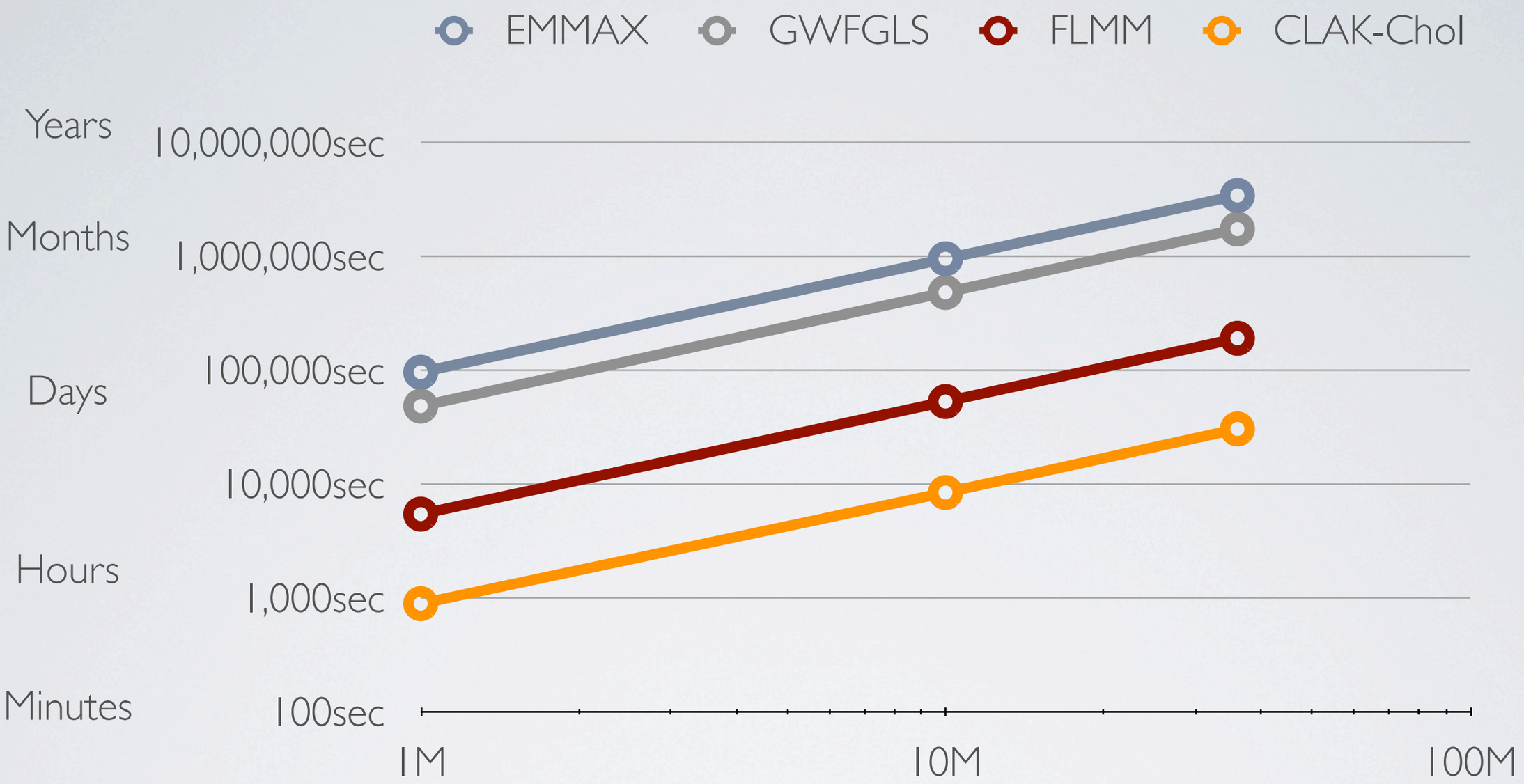


- Out-of-core algorithm
  - read block b_{+1} while computing block b
  - double-buffering technique necessary



PERFORMANCE

From years/months down to weeks/days



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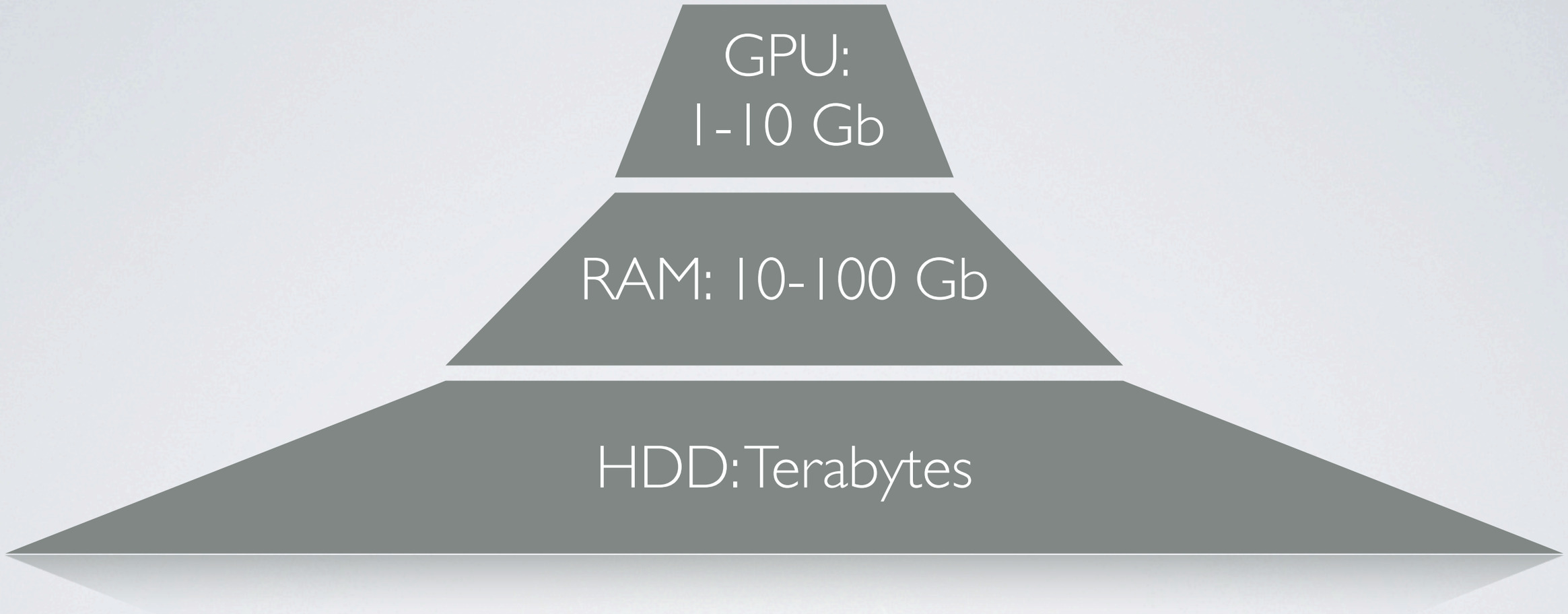
CAN GPUs HELP GO FURTHER?

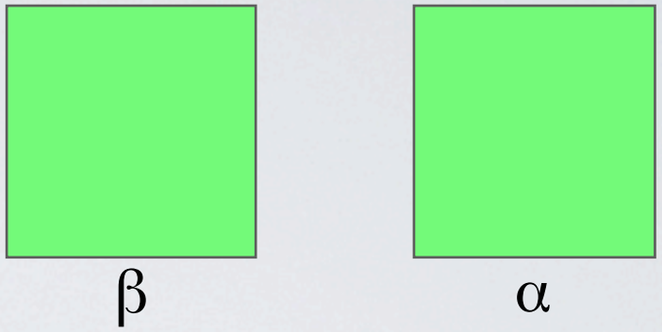
- trsm takes 90-95% of time
  - compute on the GPU
- while GPU computes:
  - CPU computations
  - CPU ⇄ GPU transfers
- our cluster: nVidia Fermi ☞



MEMORY PYRAMID

Need for two levels of streaming

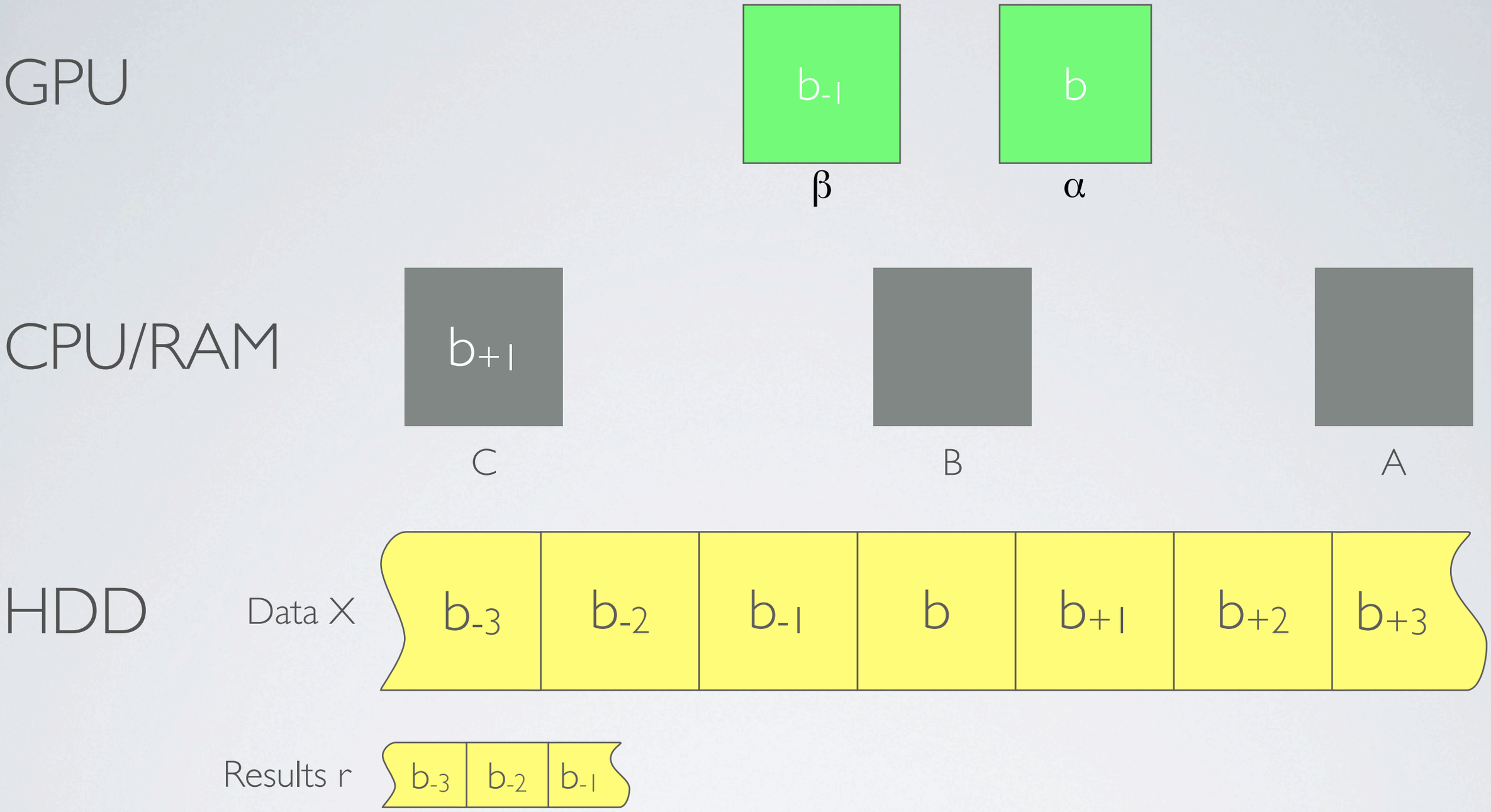
GPU



CPU/RAM

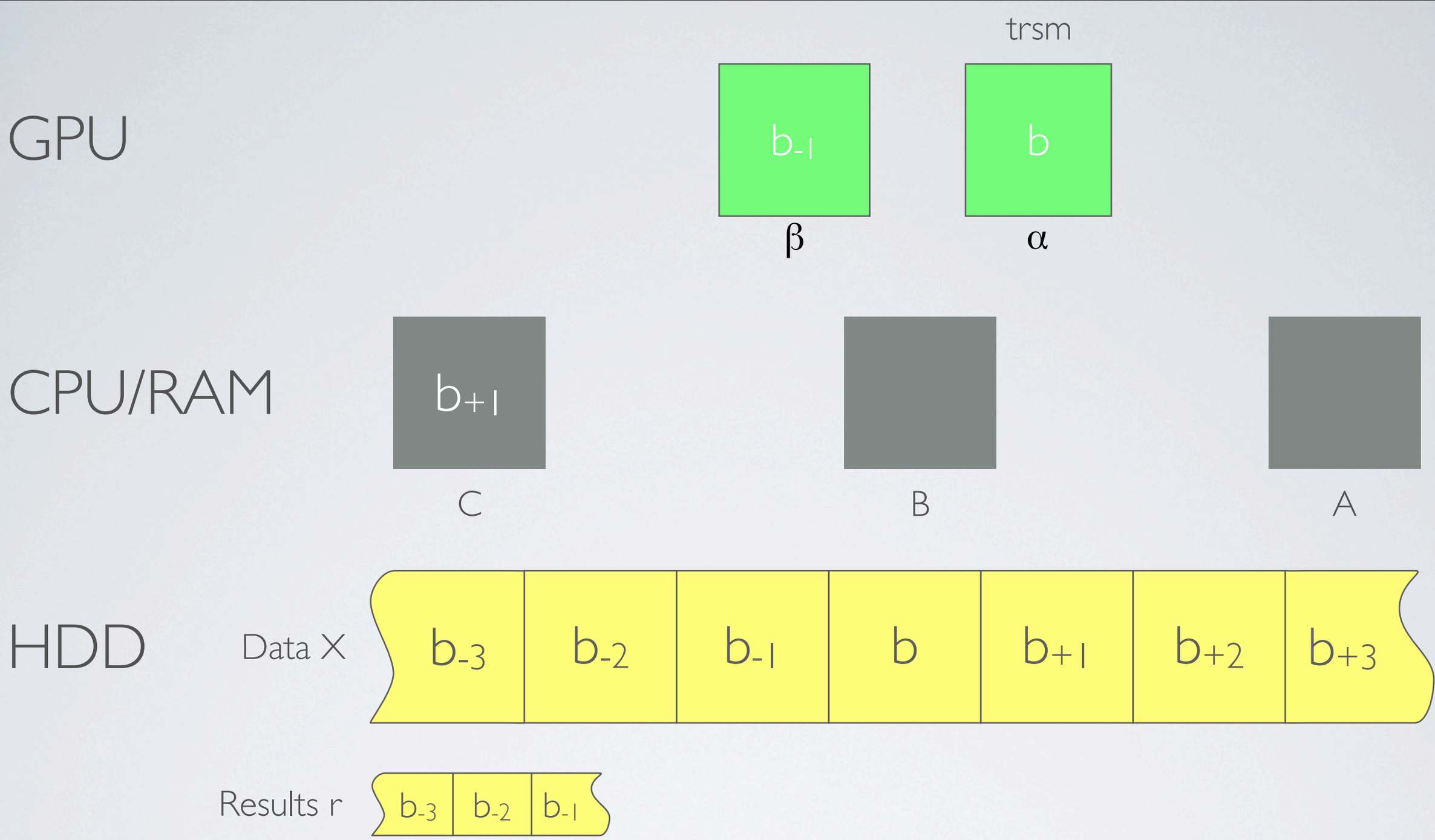
HDD

2-LEVEL TRIPLE-DOUBLE-BUFFERING



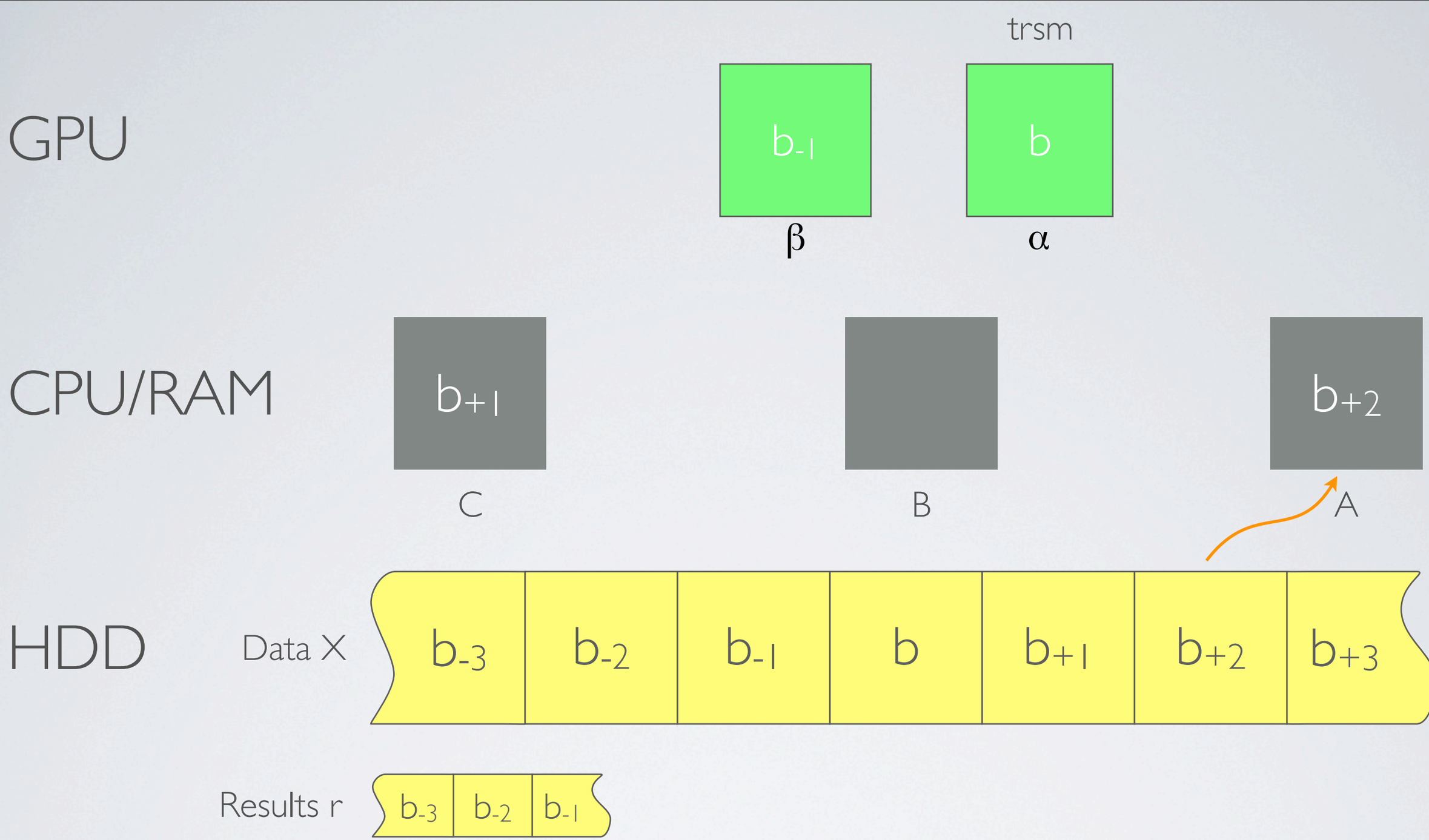
2-LEVEL TRIPLE-DOUBLE-BUFFERING

Assume the GPU holds b and is done with b-1



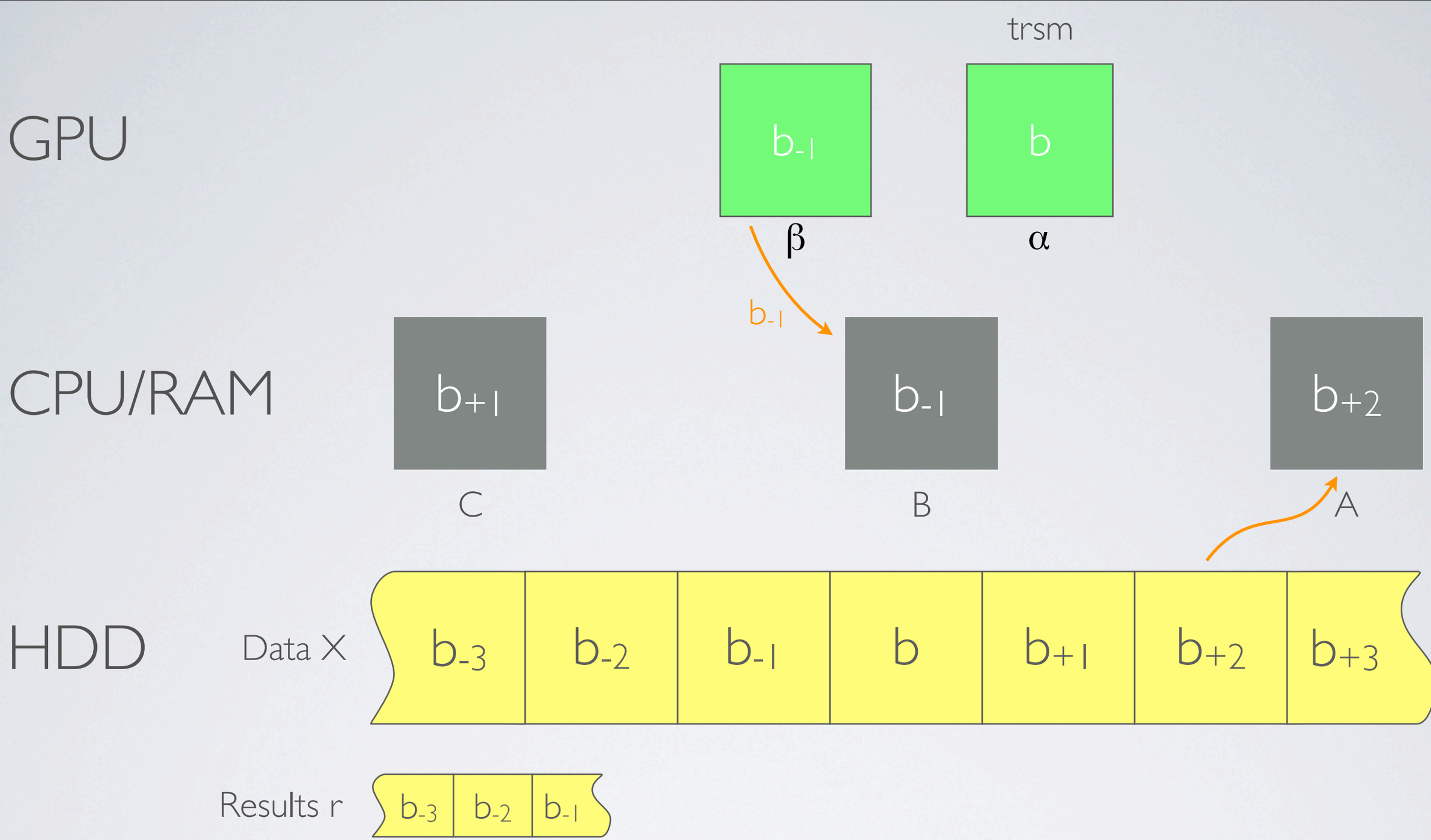
2-LEVEL TRIPLE-DOUBLE-BUFFERING

(1) TRSM of b on GPU



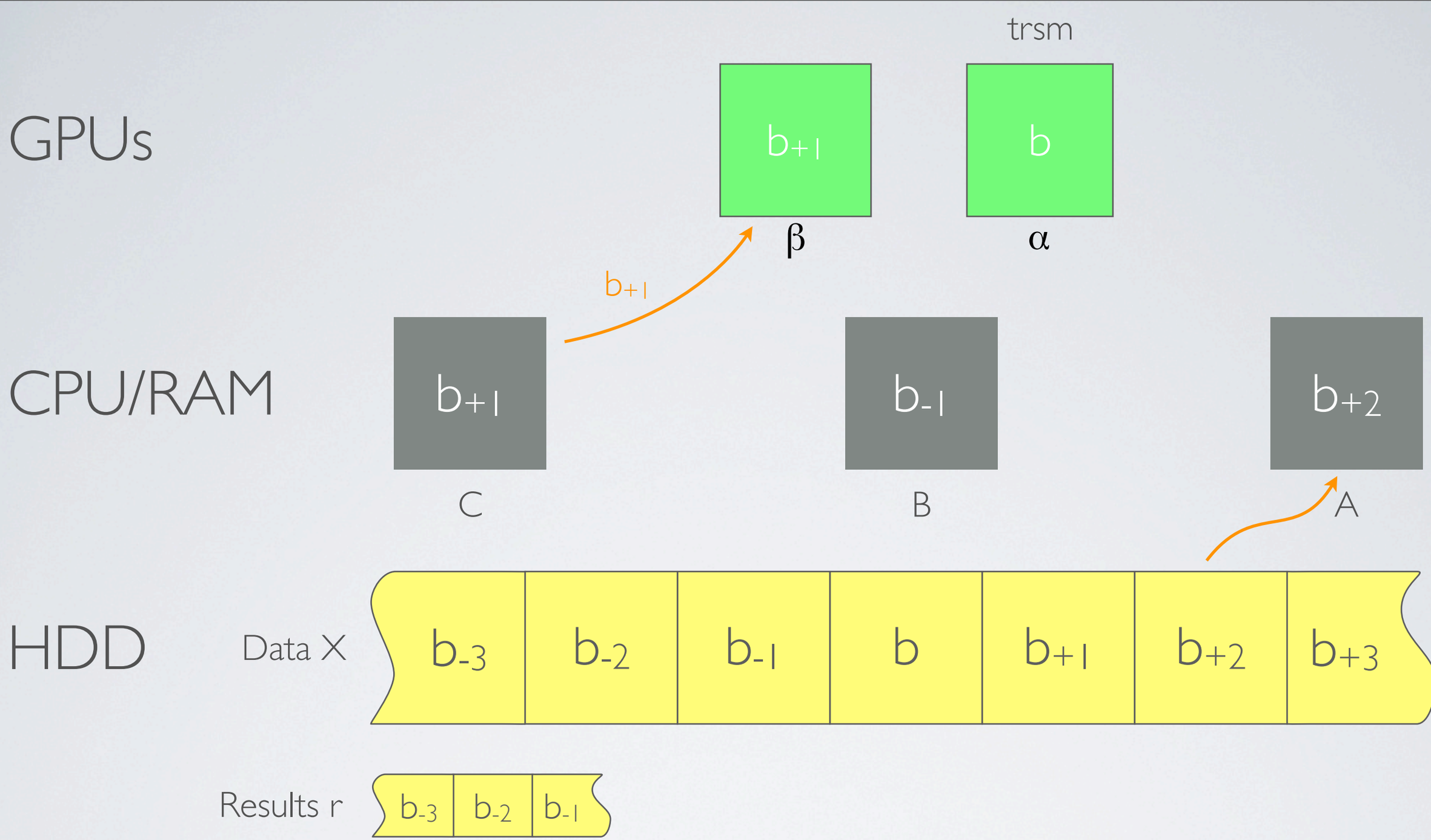
2-LEVEL TRIPLE-DOUBLE-BUFFERING

(2) start reading second-next block from HDD



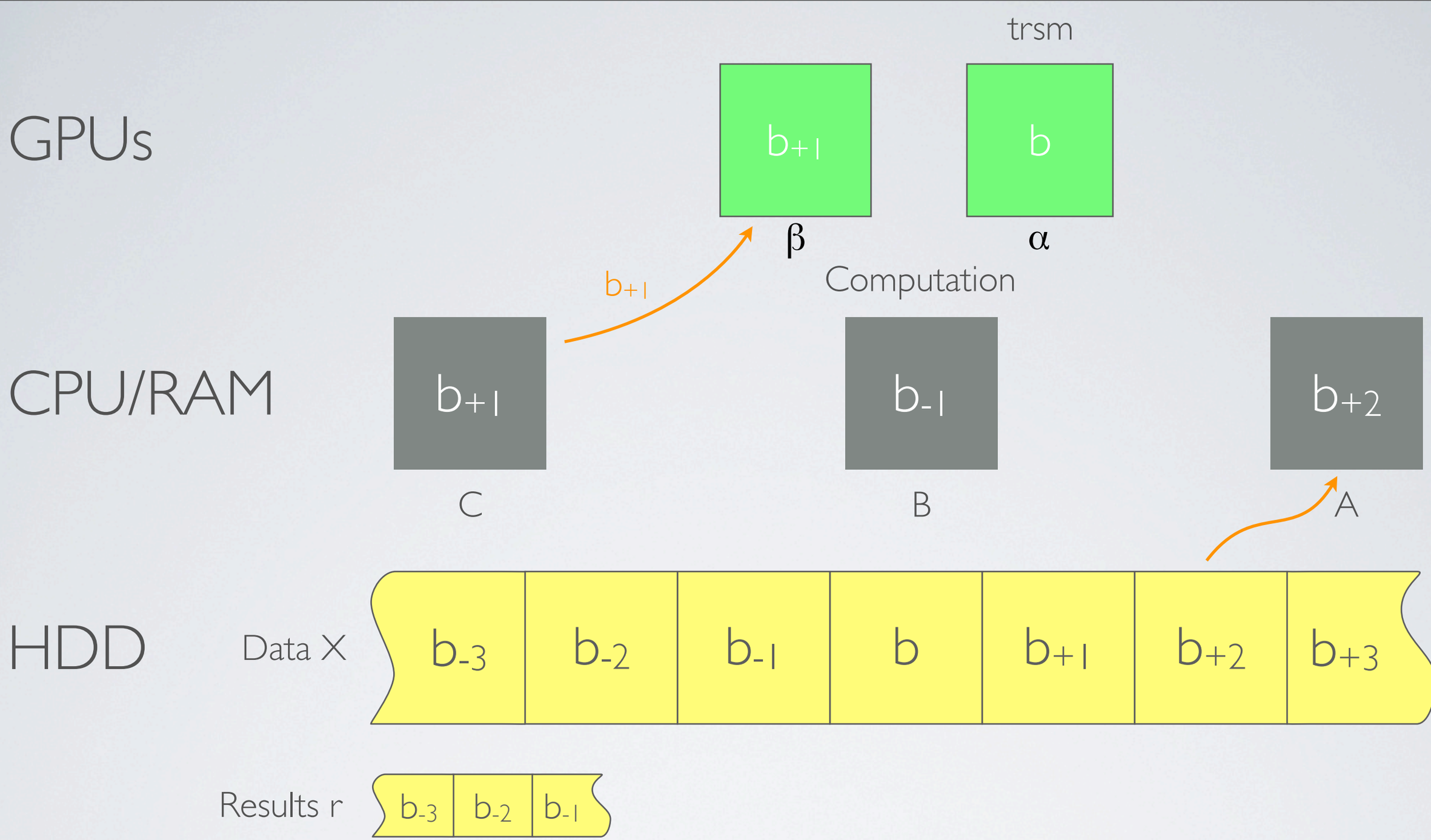
2-LEVEL TRIPLE-DOUBLE-BUFFERING

(3) Retrieve previous results from GPU



2-LEVEL TRIPLE-DOUBLE-BUFFERING

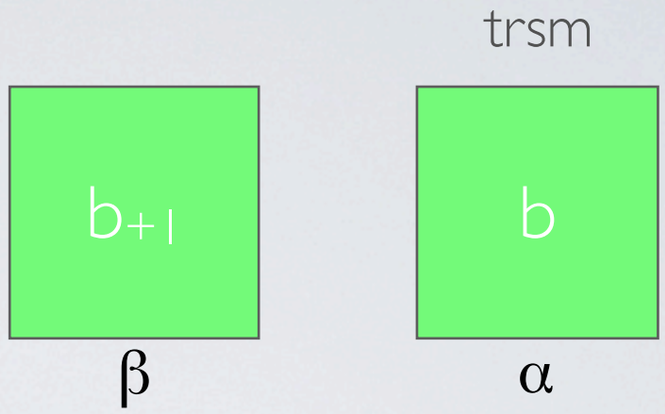
(4) Send next block to GPU



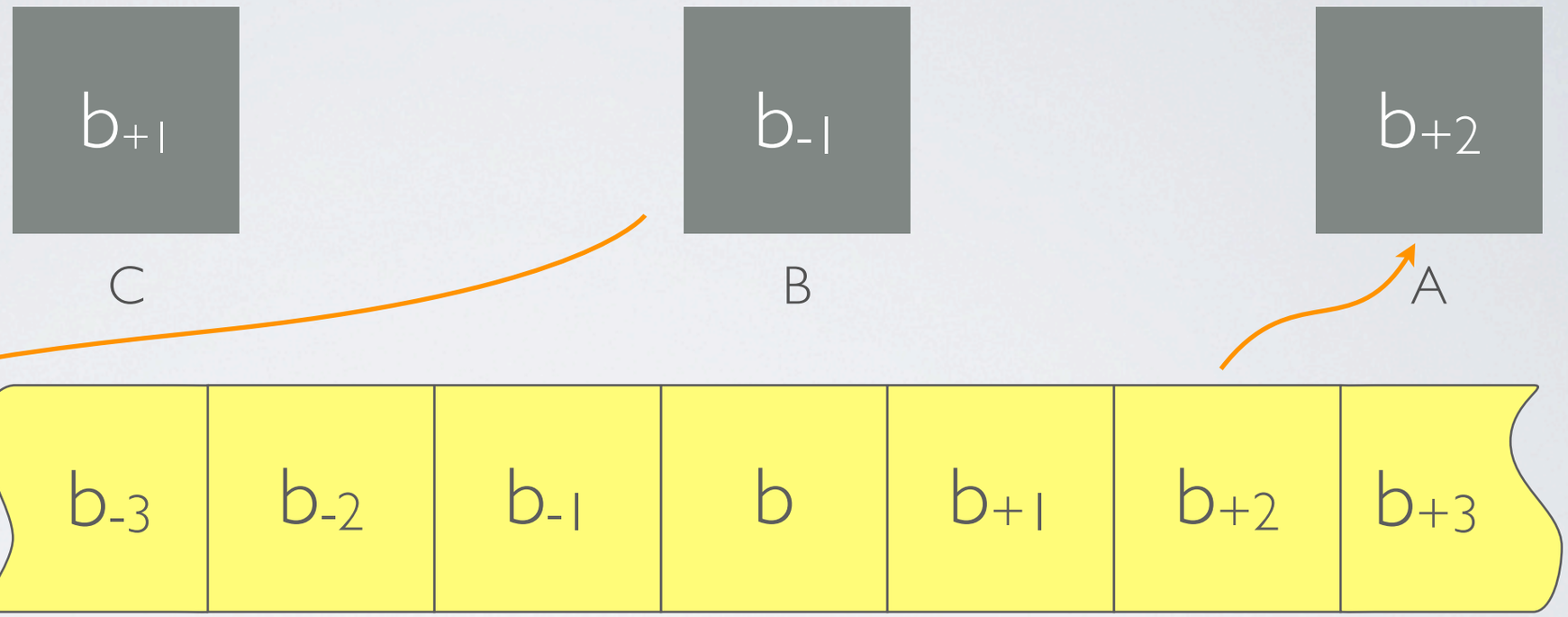
2-LEVEL TRIPLE-DOUBLE-BUFFERING

(5) start CPU computation of least-squares

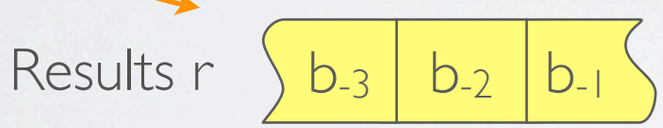
GPUs



CPU/RAM



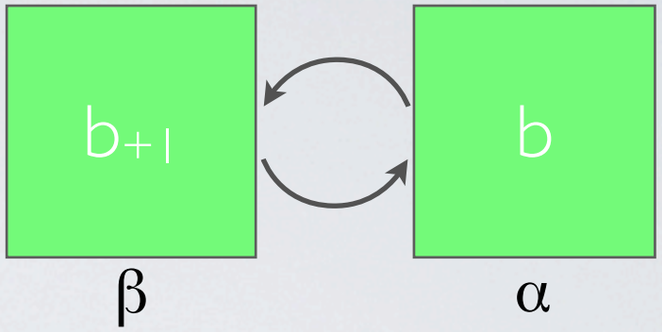
HDD



2-LEVEL TRIPLE-DOUBLE-BUFFERING

(6) Write results to disk (fast because small)

GPUs



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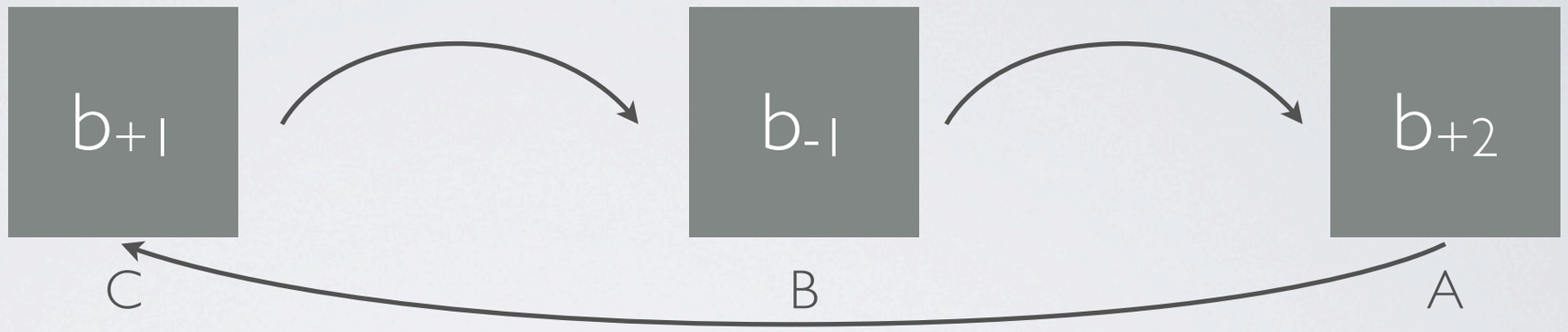

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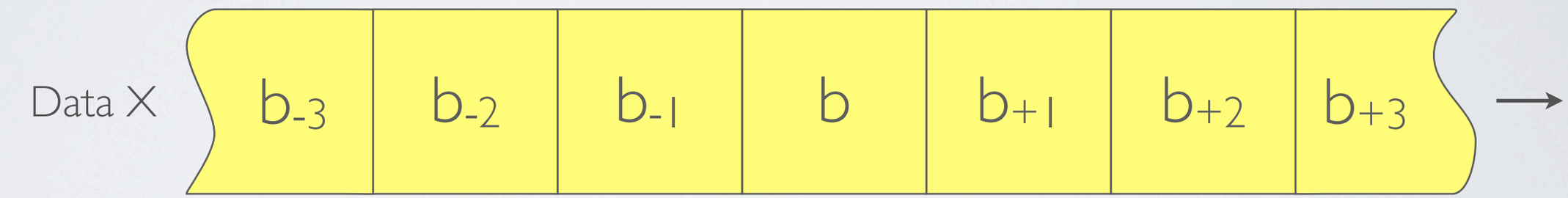
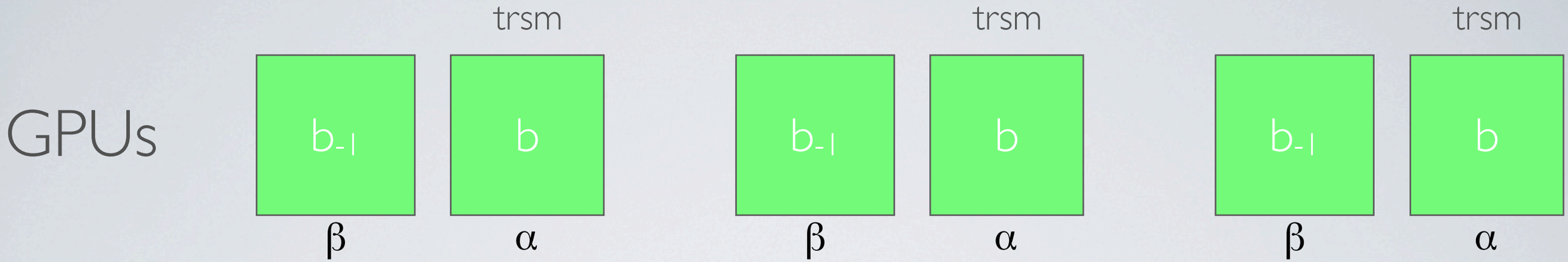


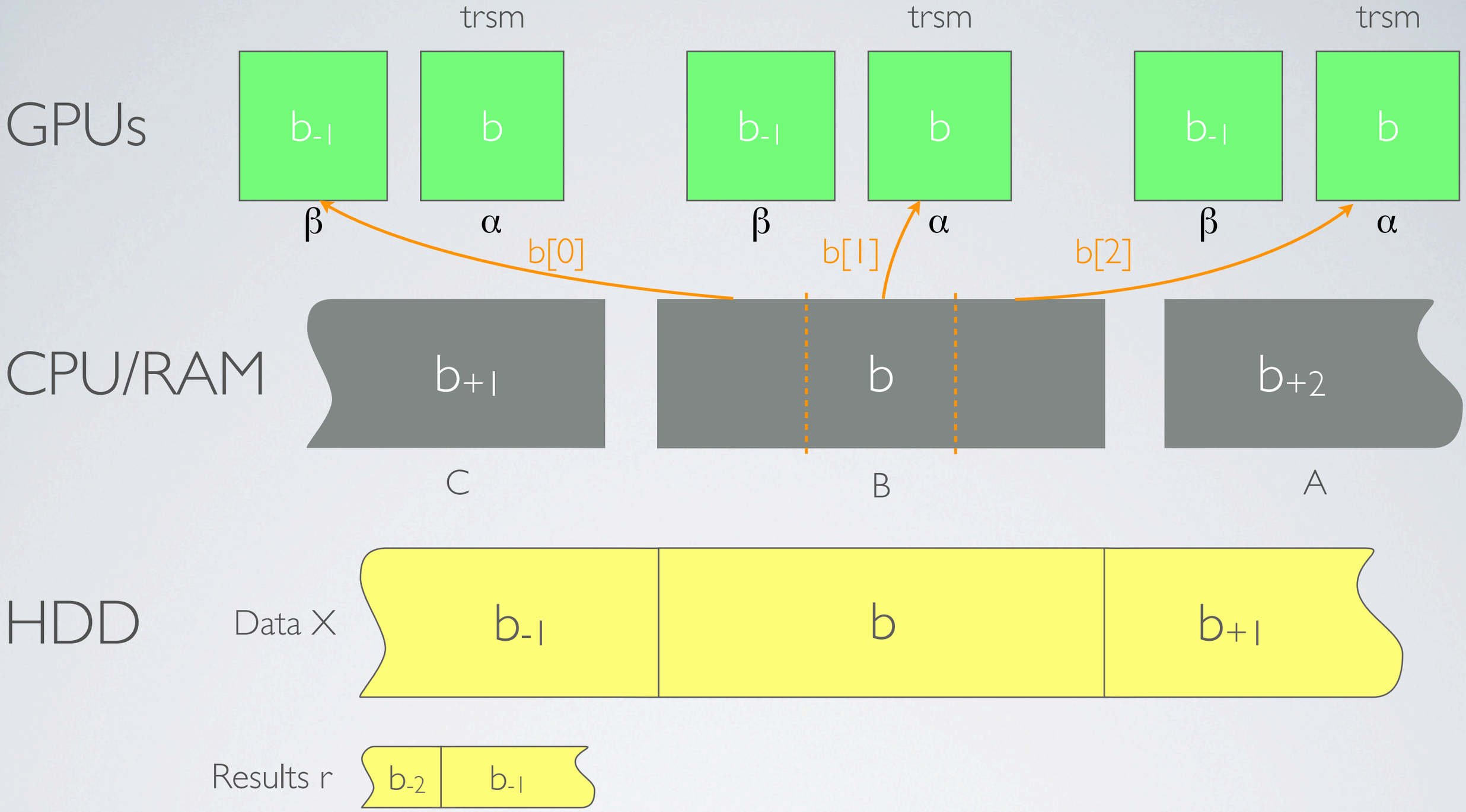
2-LEVEL TRIPLE-DOUBLE-BUFFERING

(7) Rotate buffers, iterate, smile



WITH MULTIPLE GPUs

Increase CPU's block size



WITH MULTIPLE GPUs

Increase CPU's block size

TIMELINE

Parallelism on the vertical axis

Heavy use of asynchronous dispatching

CPU ⇄ GPU transfer

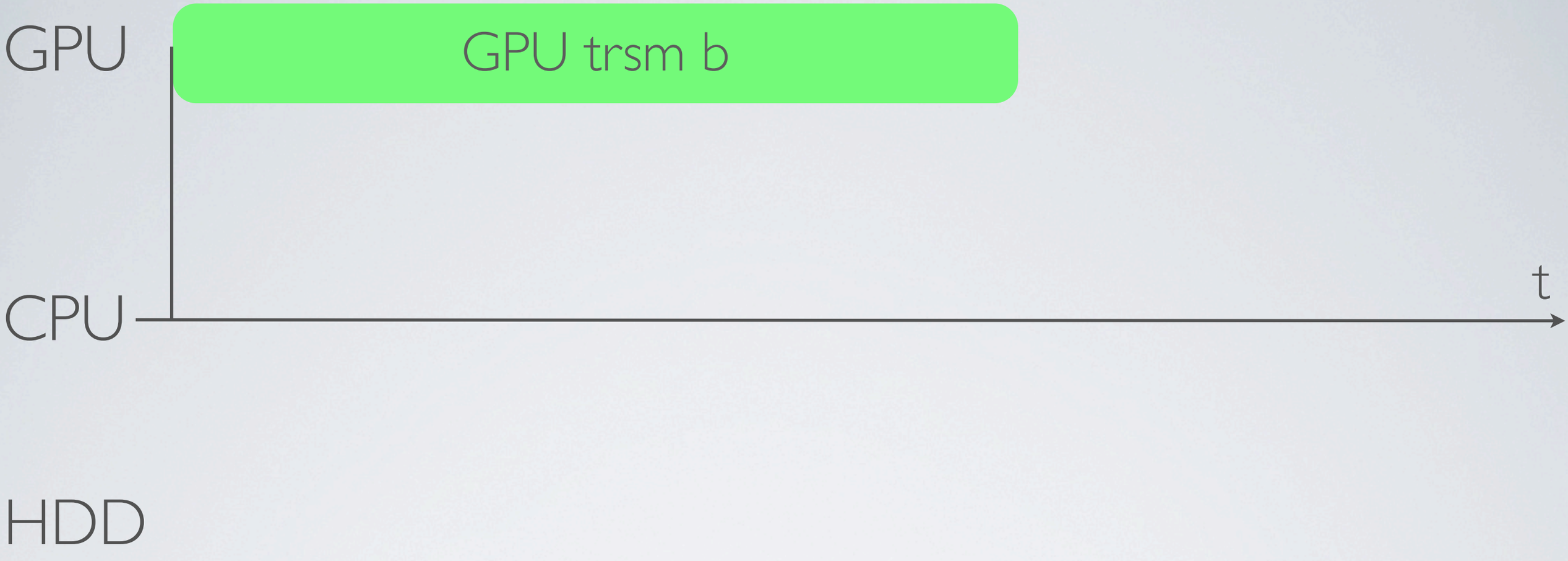
HDD ⇄ CPU transfer

GPU computation

CPU computation

Data dependencies

Asynchronous dispatch



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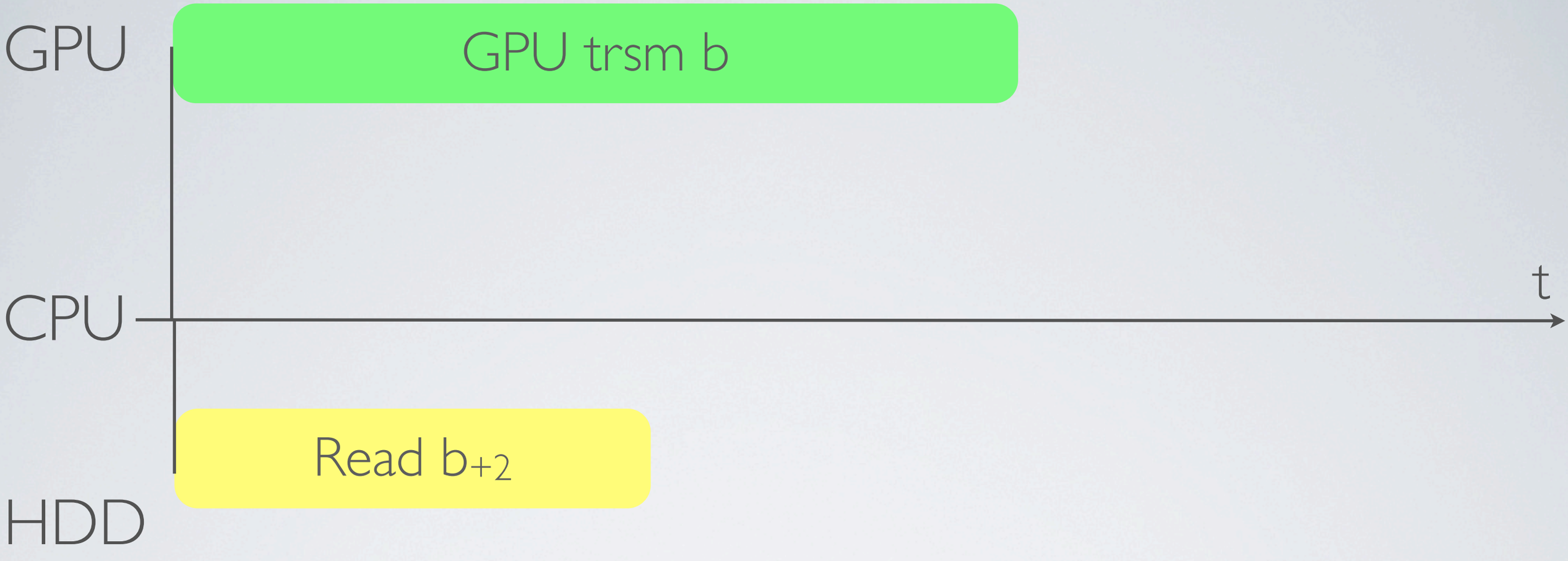

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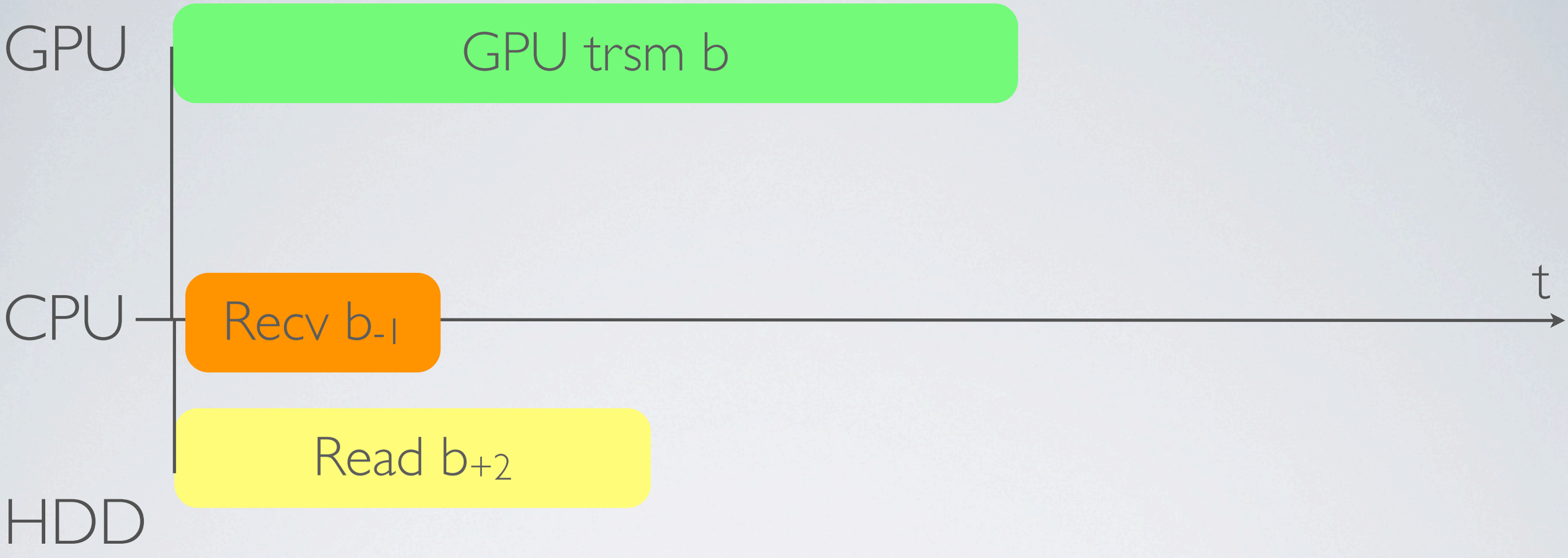

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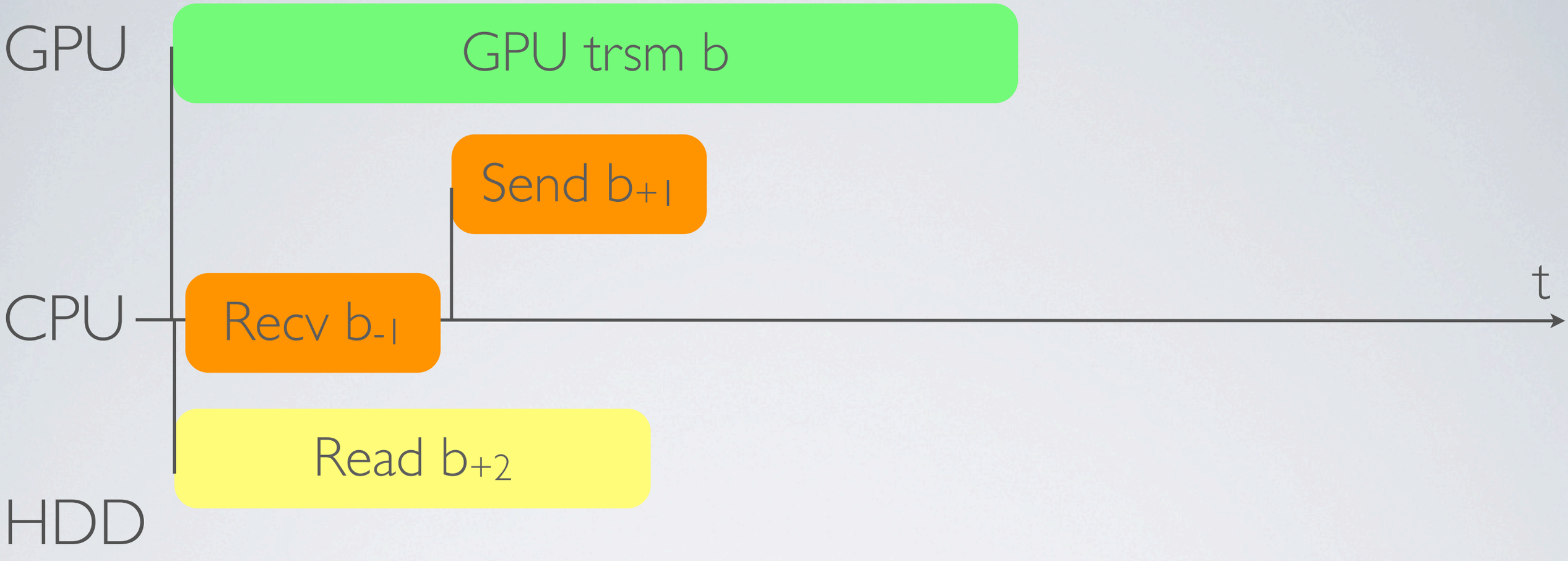

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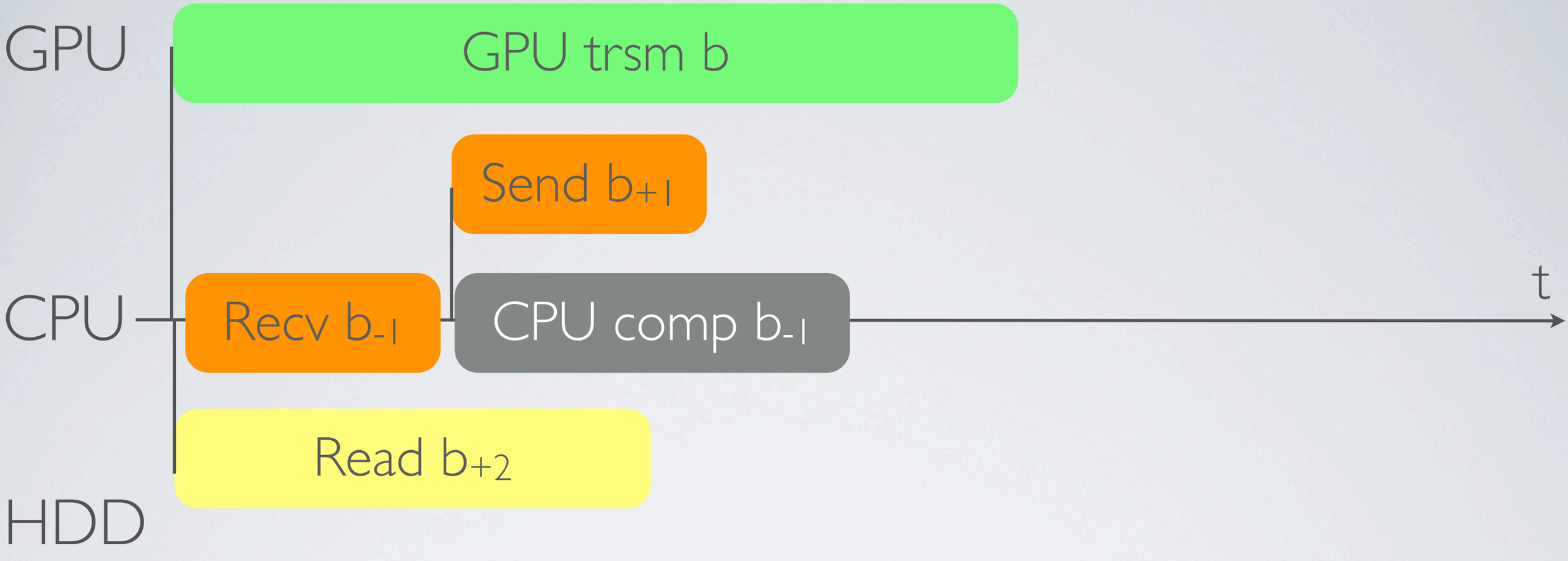


TIMELINE

Parallelism on the vertical axis

Heavy use of asynchronous dispatching

CPU ⇄ GPU transfer

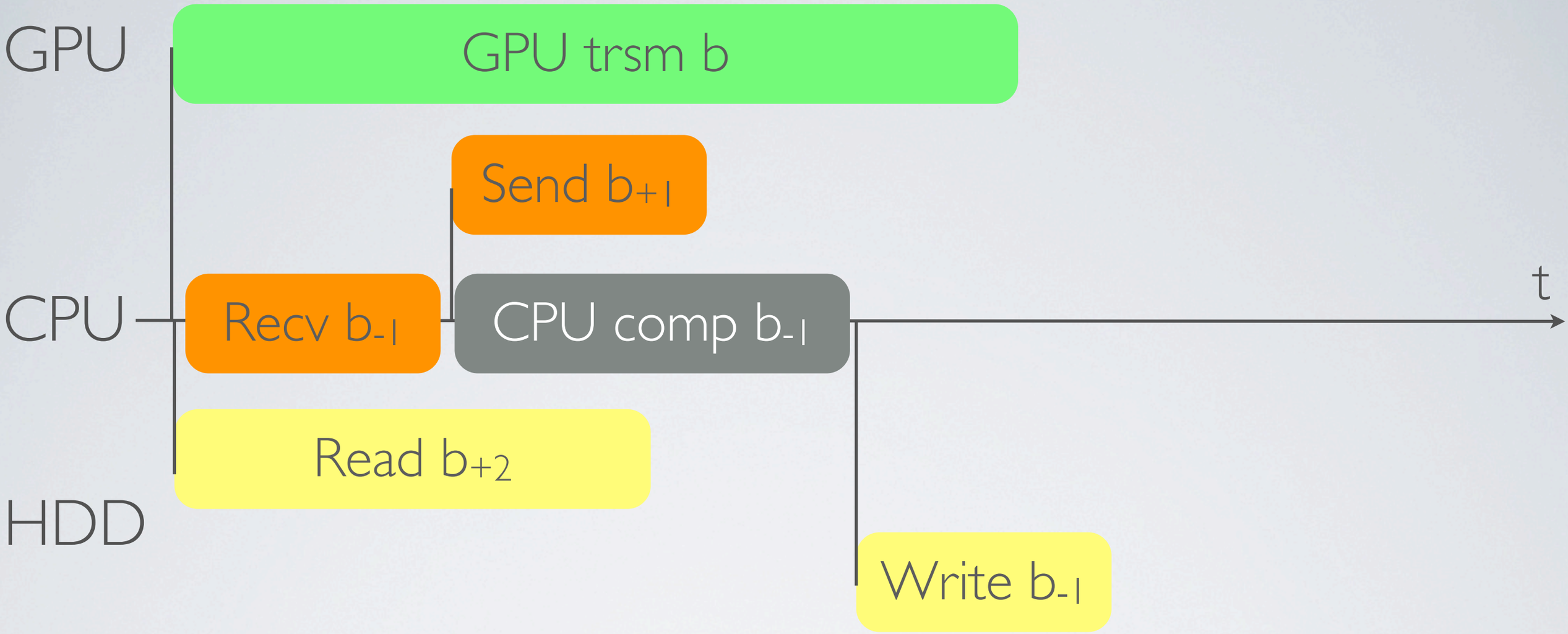
HDD ⇄ CPU transfer

GPU computation

CPU computation

Data dependencies

Asynchronous dispatch



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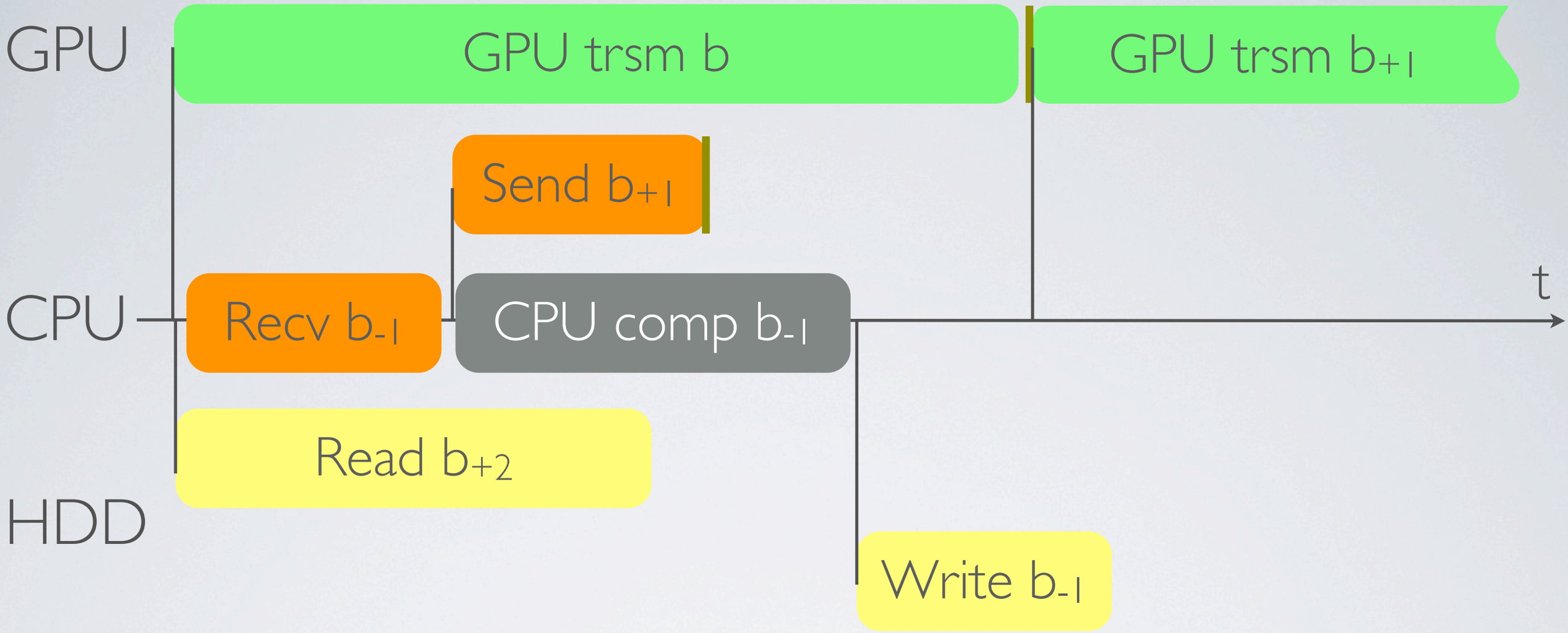

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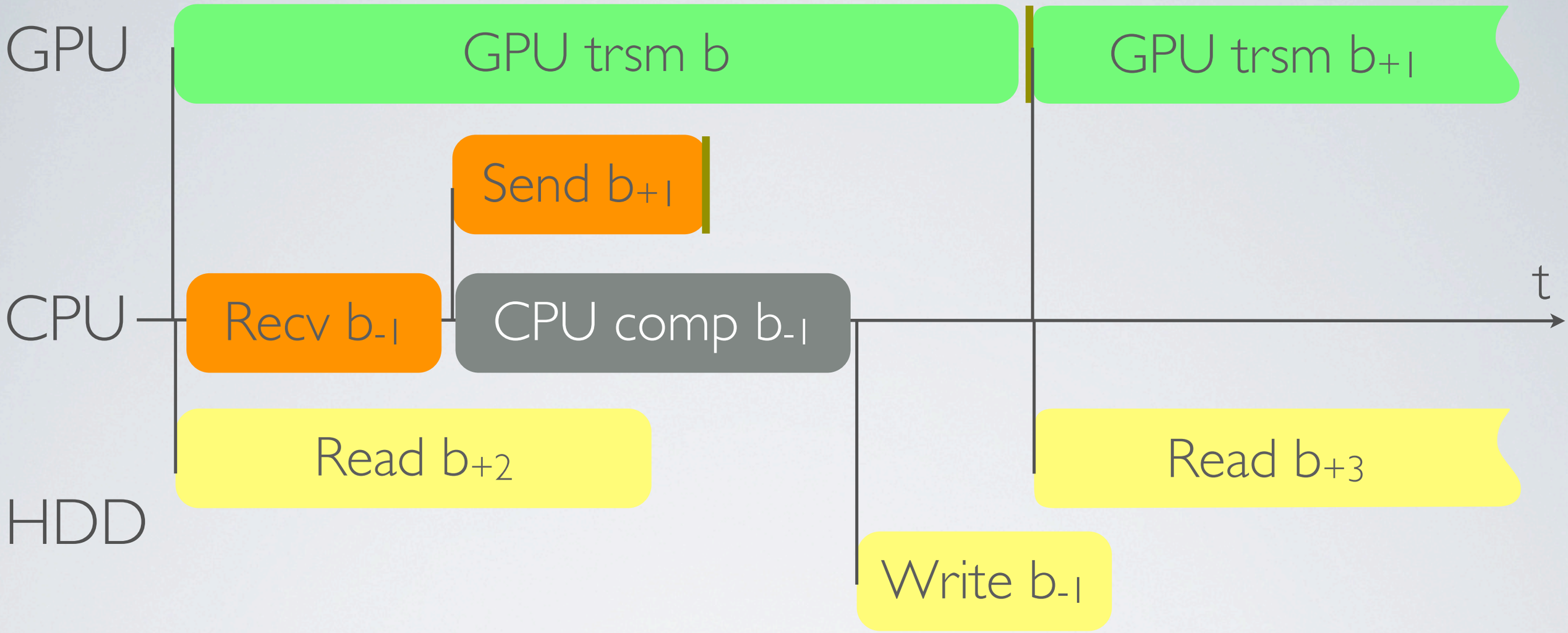

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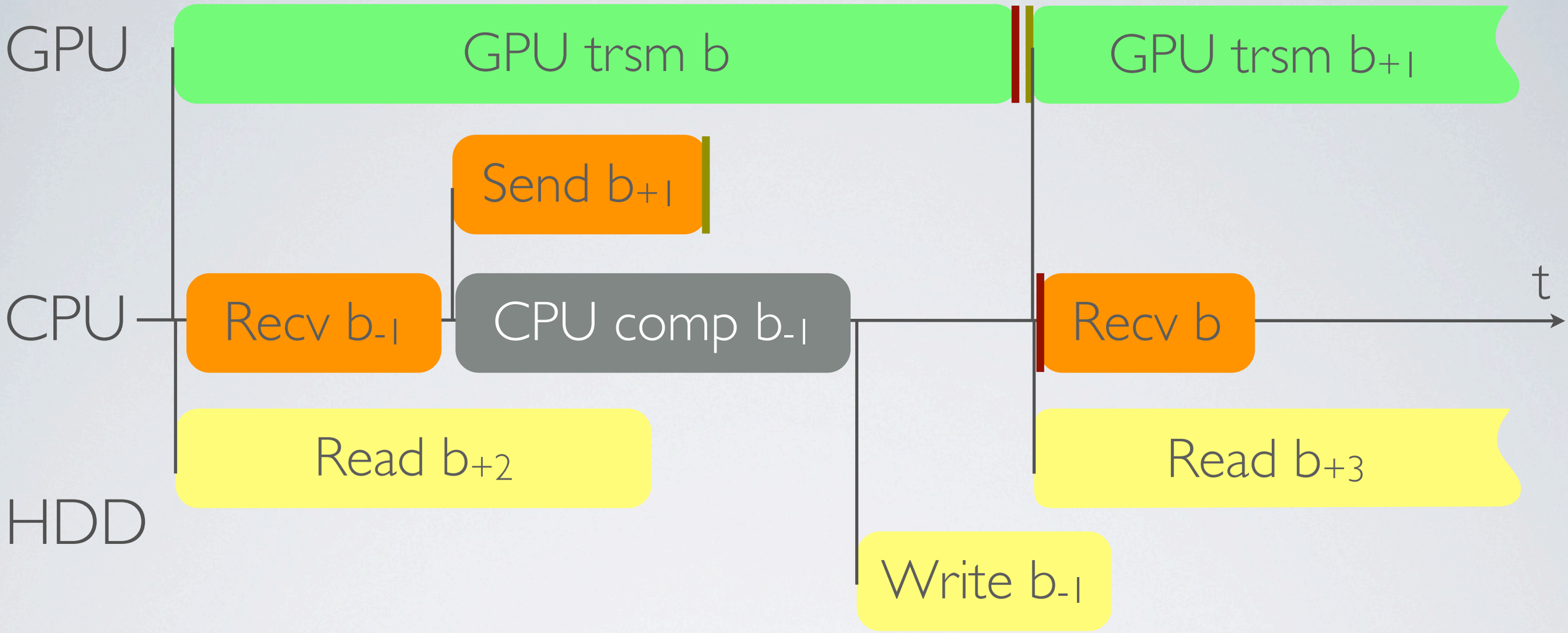

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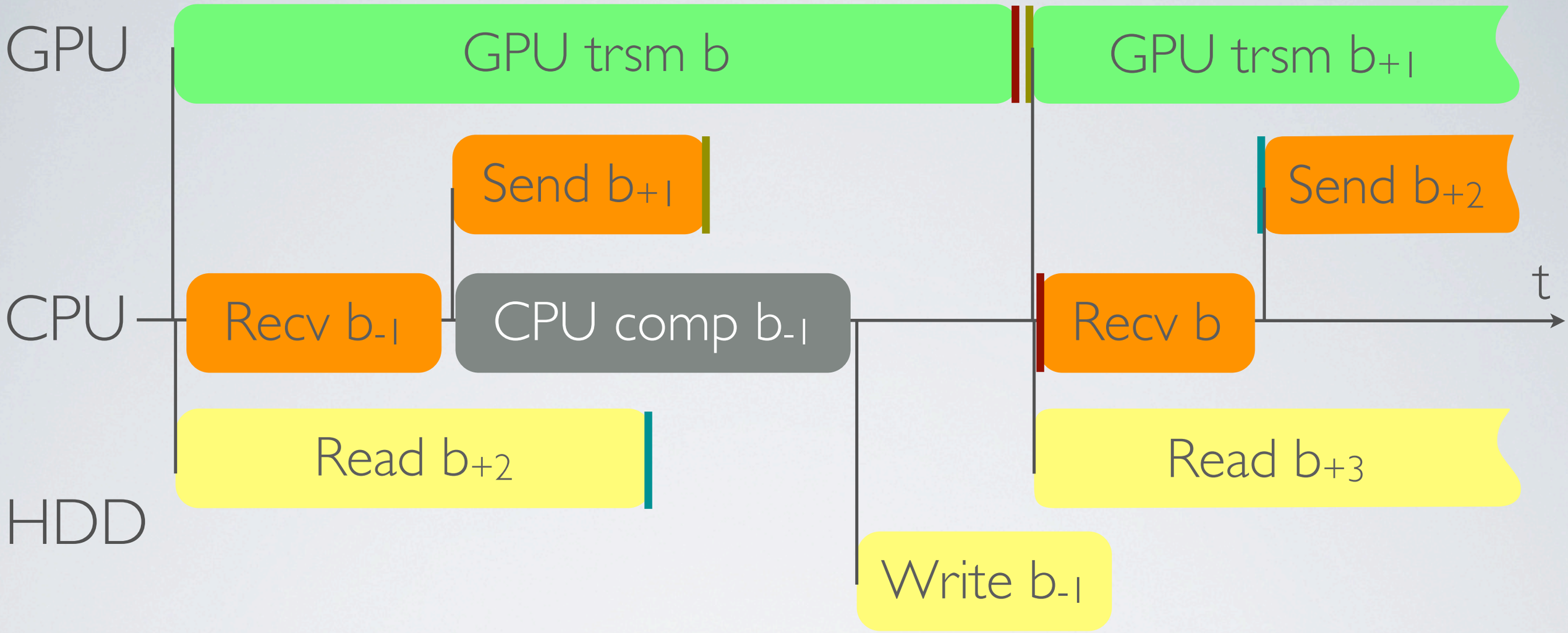

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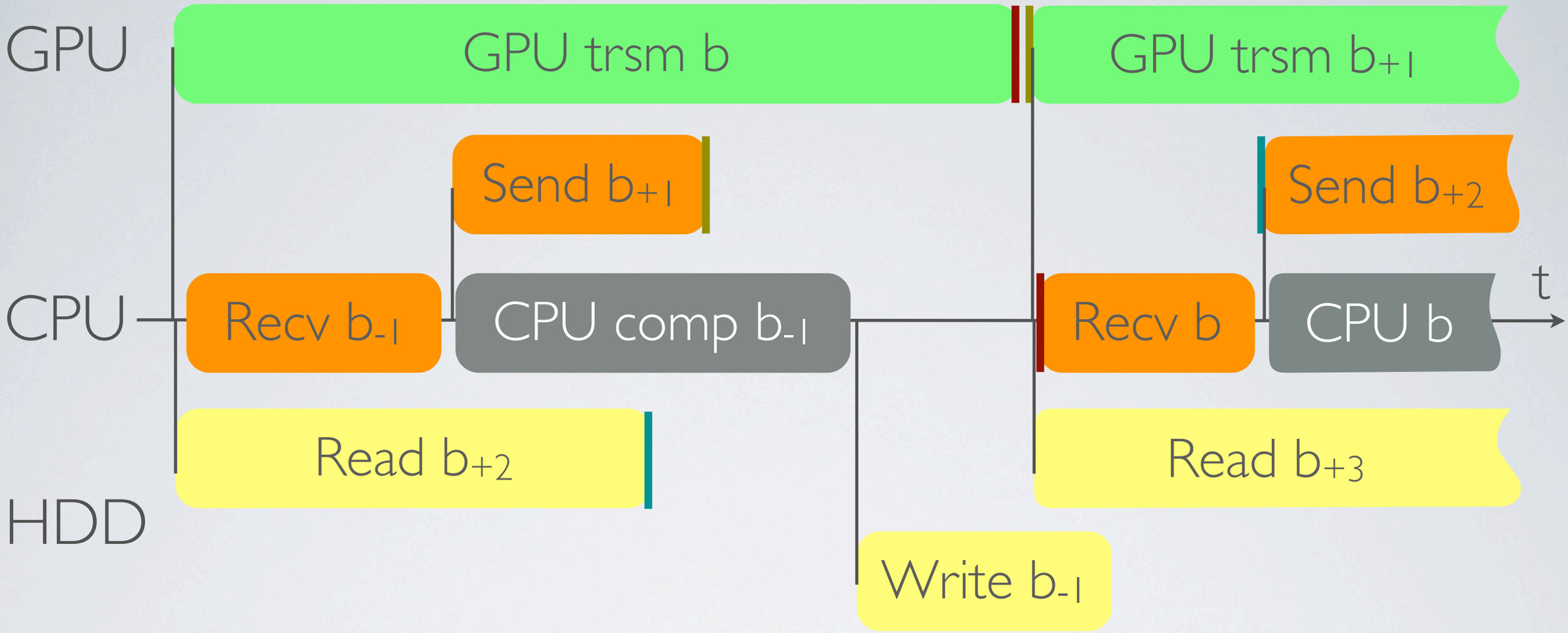

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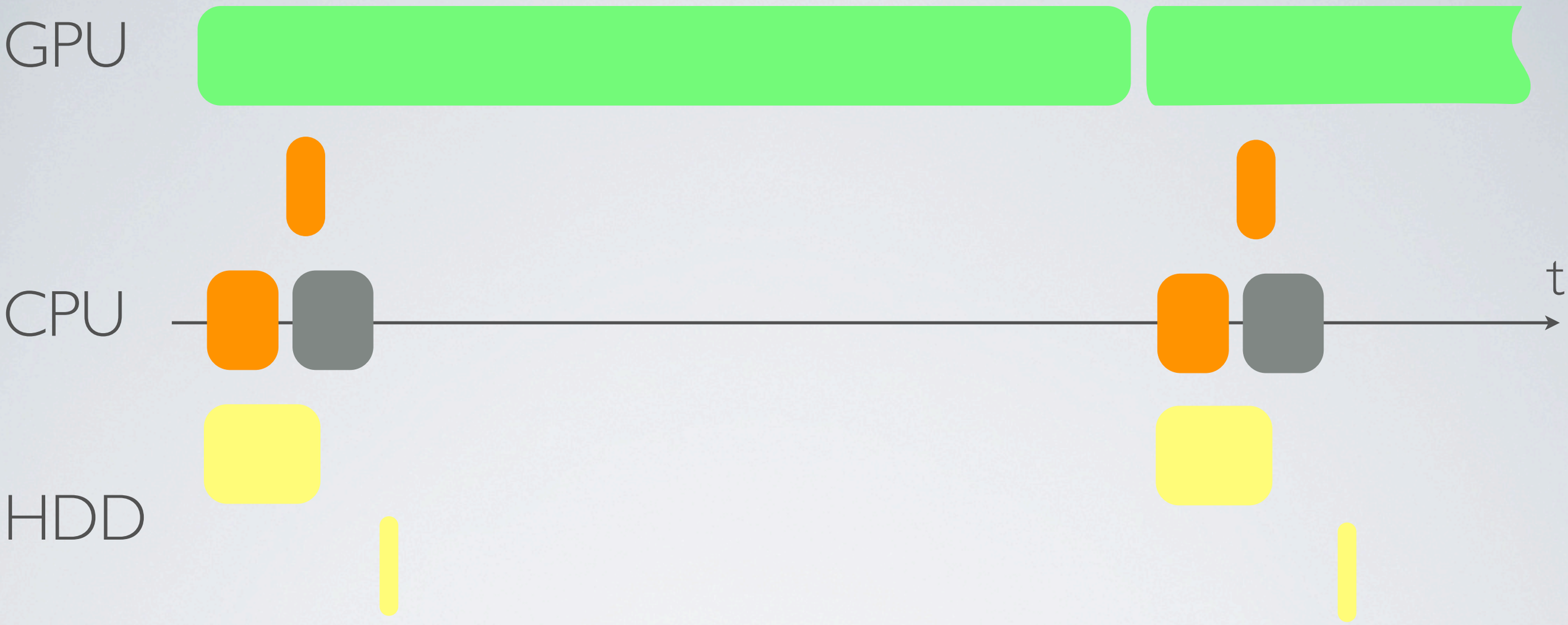


TIMELINE, TO SCALE

problem sizes: n=10k, m=100k, block=10k

GPU: **2x** nVidia Quadro 6000 (Fermi, 515 GFlops **each**, 6GB memory) = 10.000$
CPU: 2x Intel Xeon X5650 (6cores, 128 GFlops, 24GB memory) = 2000$

CPU ⇄ GPU transfer

HDD ⇄ CPU transfer

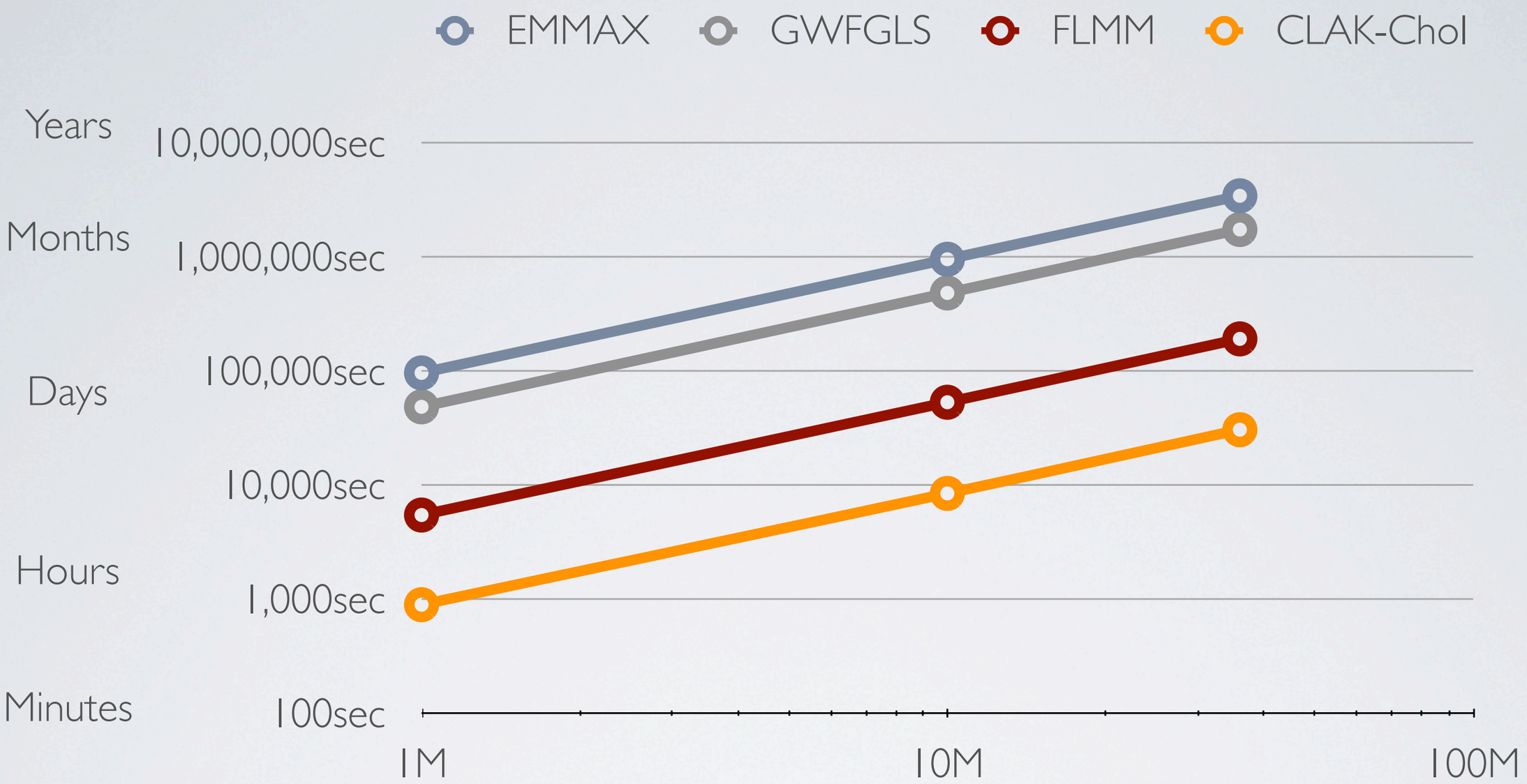
GPU computation

CPU computation

Blas: Intel MKL 10.2
Compiler: icc 12.1

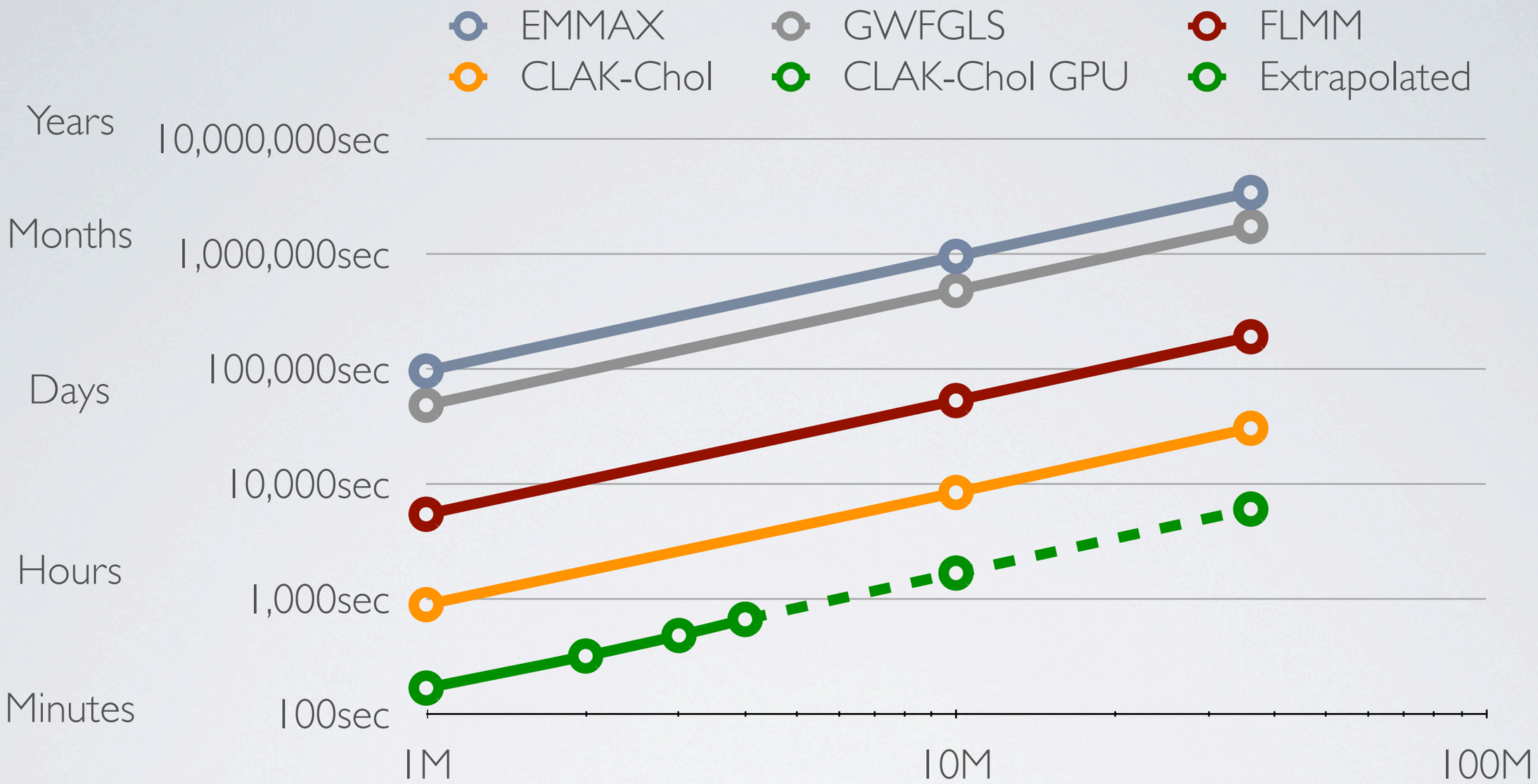
OUTLINE

- Intoduction and motivation
- Problem description
- CPU-only algorithm
- Leveraging the GPU
- Results and conclusion



PERFORMANCE

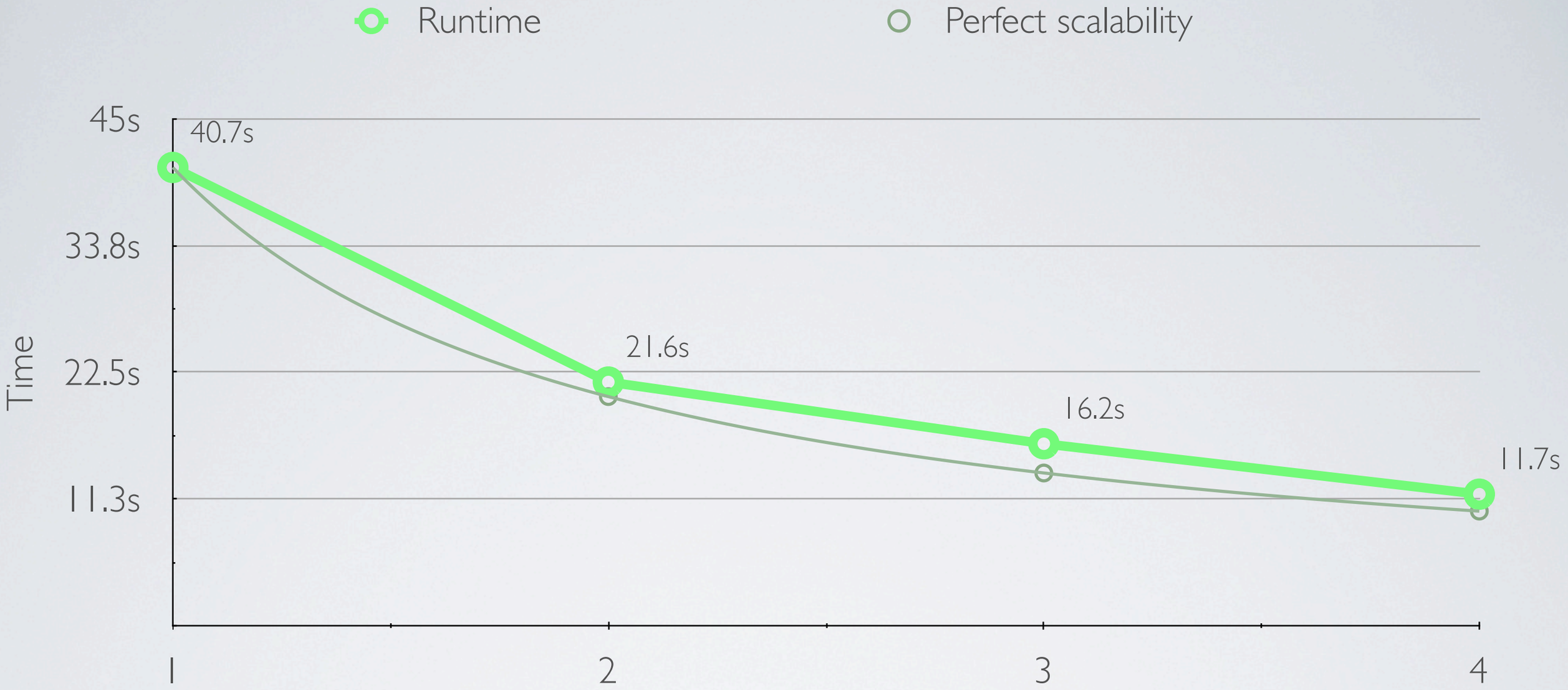
From years/months down to hours



PERFORMANCE

From years/months down to hours

12 CPU cores vs. 12 CPU cores + 4 GPUs



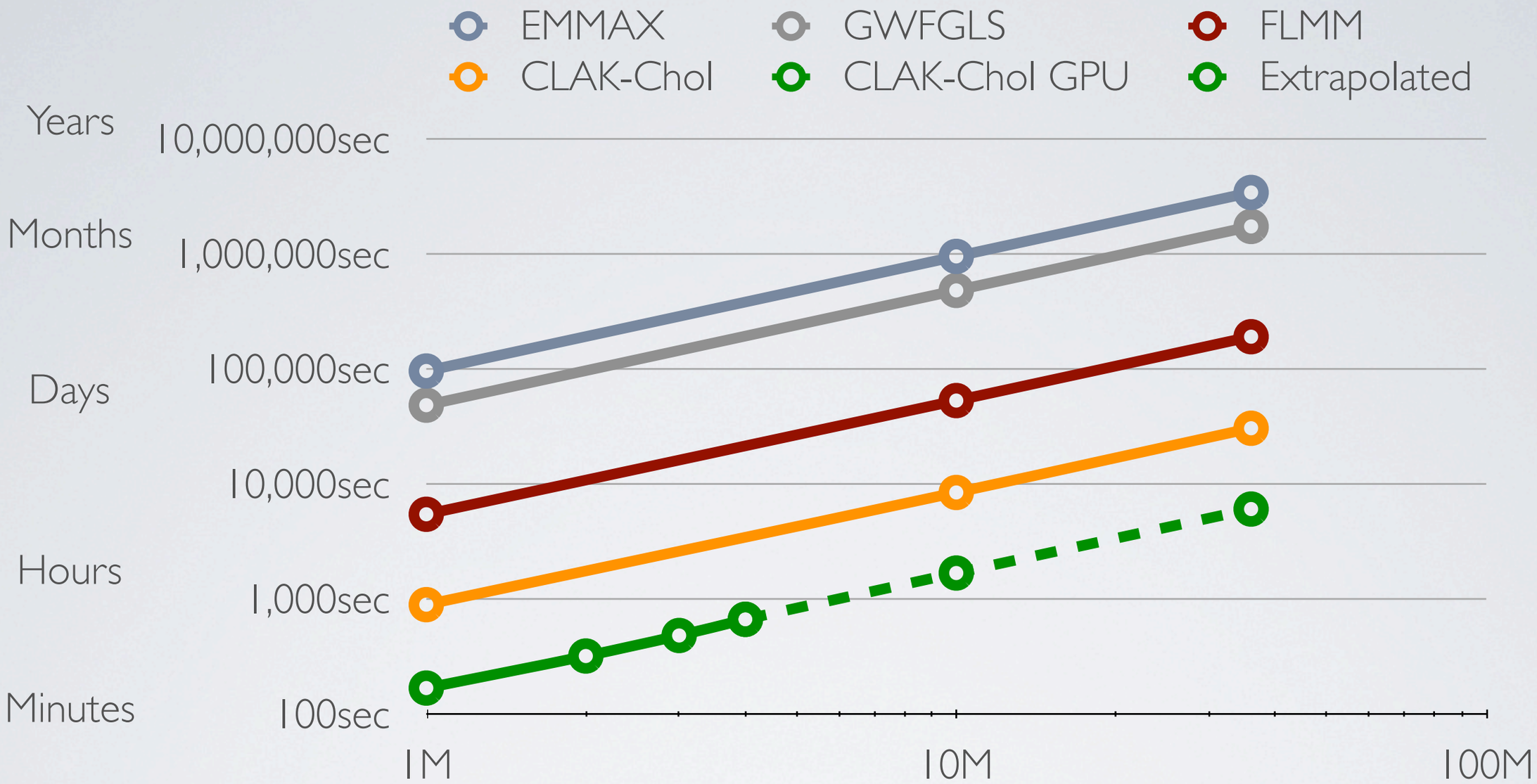
SCALABILITY

#GPUs x2 ⇒ time x0.54

Almost perfect

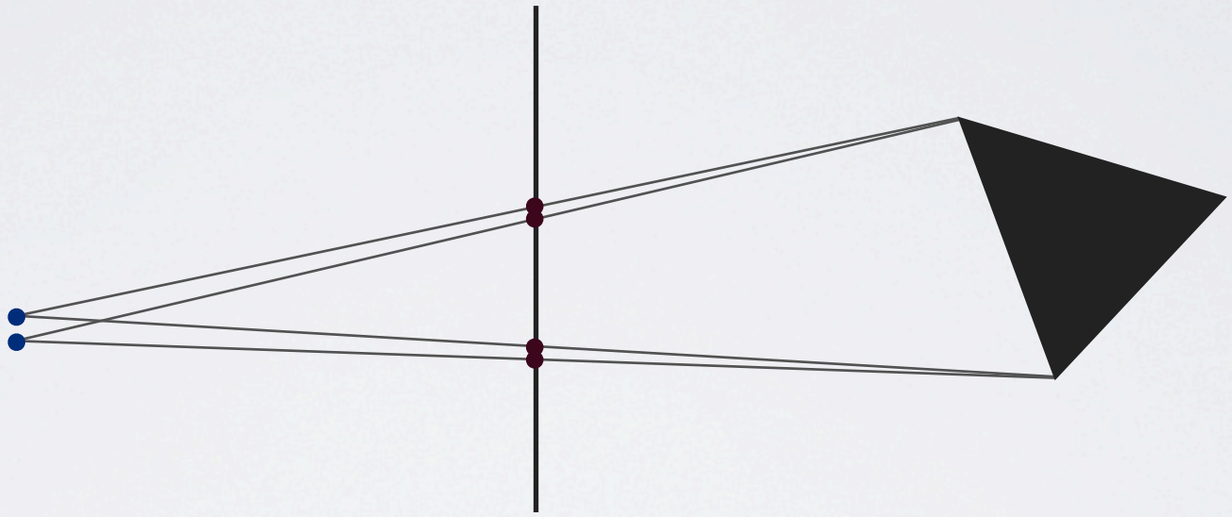
CONCLUSION

- ~2.6x Speedup per *additional* GPU (~10x for 4 GPUs)
- Don't replace the CPU by GPU; combine them
- Hide data transfer latency by overlapping with computation
  - Double/triple-buffering: GPU never stops computing
- one GPU order of magnitude faster?
  - Faster than what?
  - Victor W. Lee et al. («Debunking the 100X GPU vs. CPU Myth: An Evaluation of Throughput Computing on CPU and GPU», 2010)

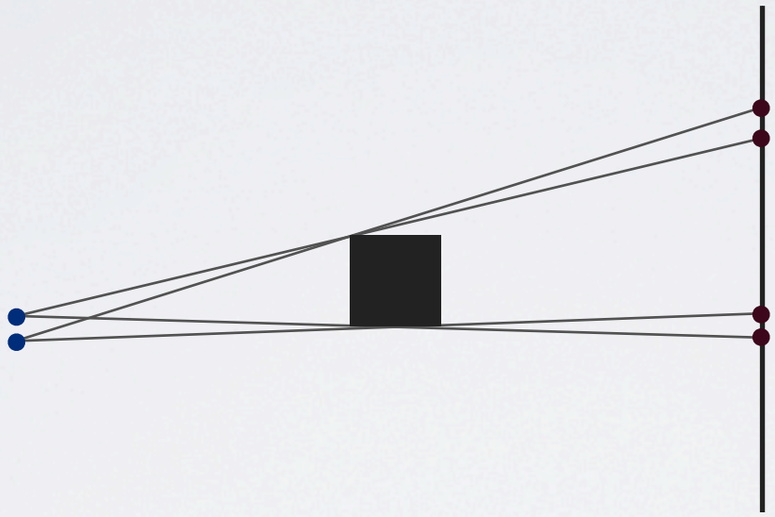


QUESTIONS?

lucasb.eyer.be

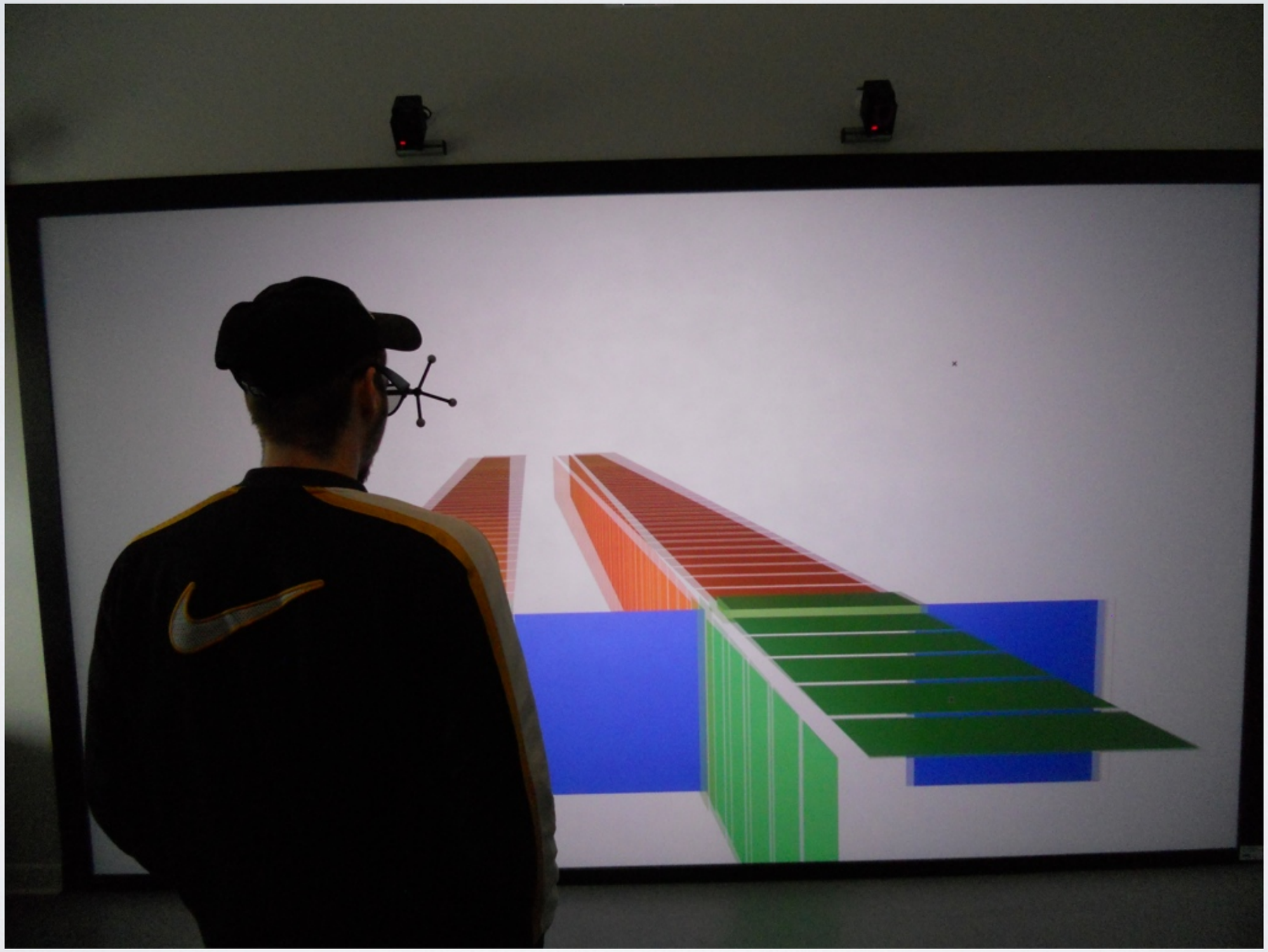


Viewer's eyes Projection surface 3D scene



Viewer's eyes 3D scene Projection surface

VISUALIZATION



FUTURE WORK

- Solution for L too big for GPU memory
- Apply similar technique to similar problems
- Extension to multiple phenotypes (y)