Scaling the Memory Wall for Sparse Iterative Solvers

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University of Erlangen-Nuremberg

A “Bread & Butter” Simulation

https://energy.sandia.gov/programs/renewable-energy/

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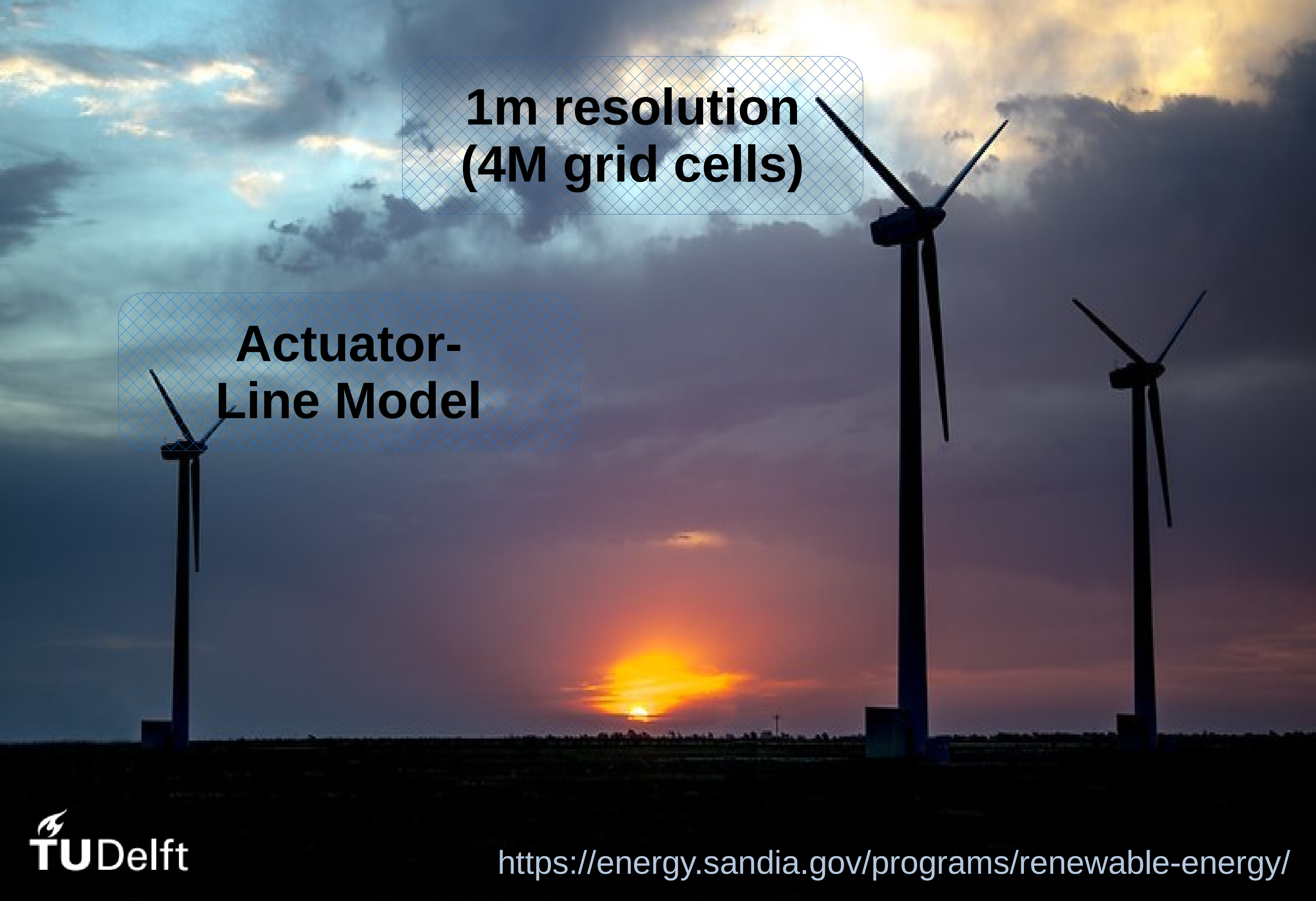
A “Bread & Butter” Simulation



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A “Bread & Butter” Simulation

1m resolution (4M grid cells)

Actuator-Line Model

Implicit Time-Stepping

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A “Bread & Butter” Simulation

**1m resolution
(4M grid cells)**

**Actuator-
Line Model**

**Implicit
Time-Stepping**

**Two Sparse
Systems
per Time-Step**

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GMRES for the Momentum Equations

Build orthogonal basis of a Krylov subspace

$$\mathcal{K}_m(A, r_0) = \mathrm{span}\{q_1, q_2, \ldots, q_m\}$$

Using the Arnoldi process

$$AQ_k = Q_{k+1}H_k.$$

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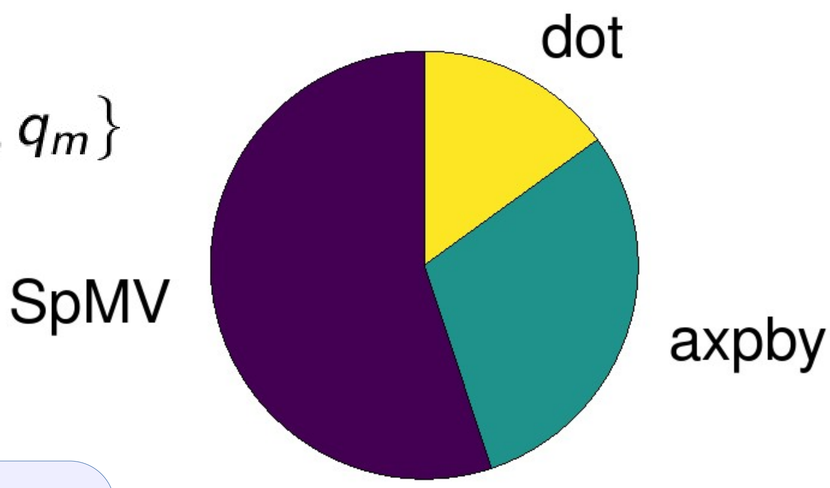
Runtime breakdown on 48-core Xeon
(1536 Flops/cycle)



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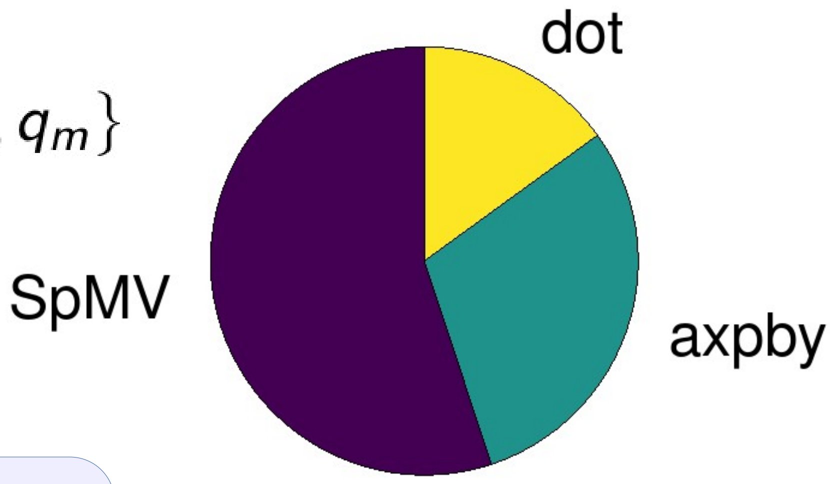

What is “Communication”, And how can it be “avoided”

?

“Communication Avoiding” Krylov

- Partially use polynomial with constant coefficients
- Fewer orthogonalization operations
- More compute-intensive ‘tall&skinny’ operations
- Bundle reductions
- **Glue SpMV’s together (Matrix-Power Kernel):**

$$y^k = \sum_{k=1}^{s} \alpha_k A^k x$$

“Communication Avoiding” Krylov

Synchronization Points

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s-step methods

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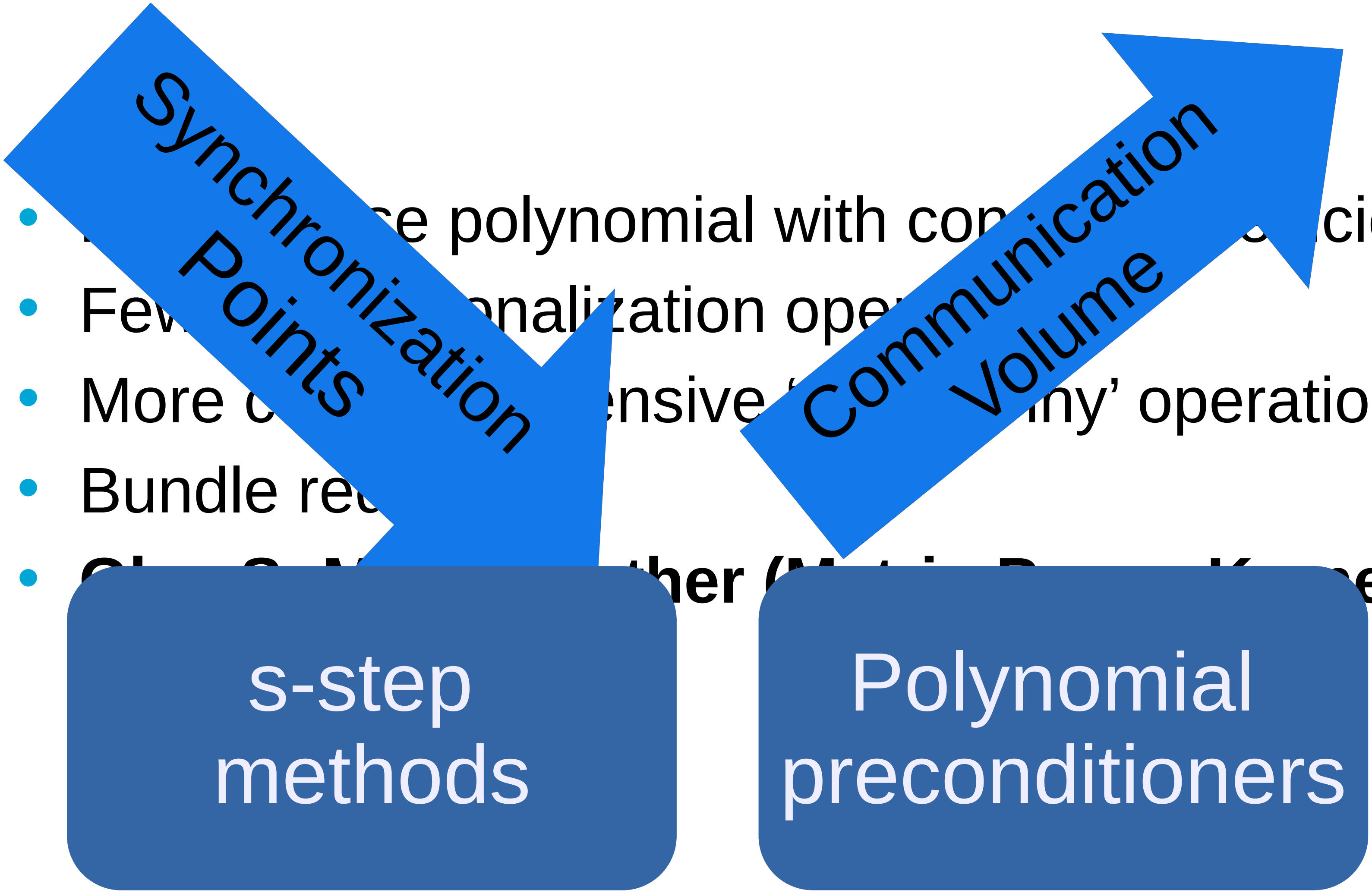

Simple Example:
Neumann Polynomial Preconditioner

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Neumann series

$$\frac{1}{x} \approx \sum_{k=1}^{s} \left(1 - x\right)^{k}$$

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Jacobi splitting

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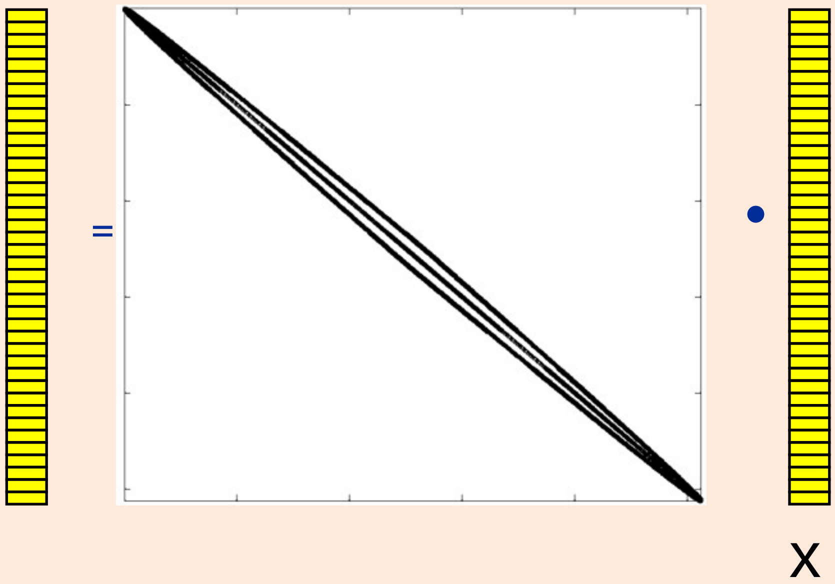
Degree-s preconditioner

$$(D^{-1}A)^{-1} v \approx [D^{-1}(L+U)]^s D^{-1} v$$

Matrix Power Kernel

“Back to back” SpMVs



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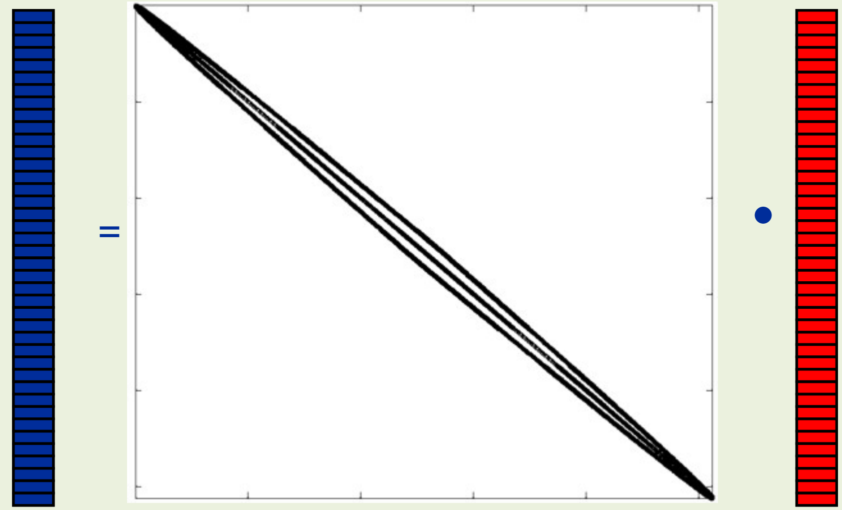

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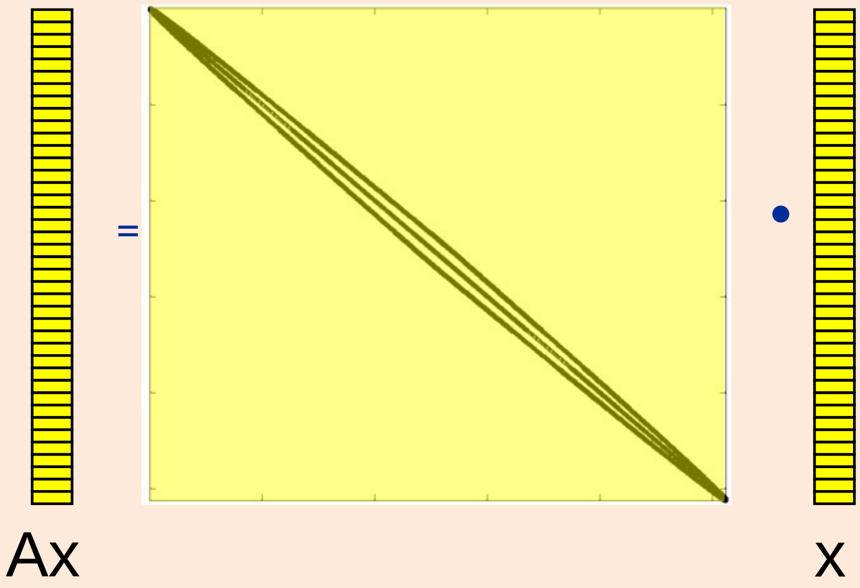

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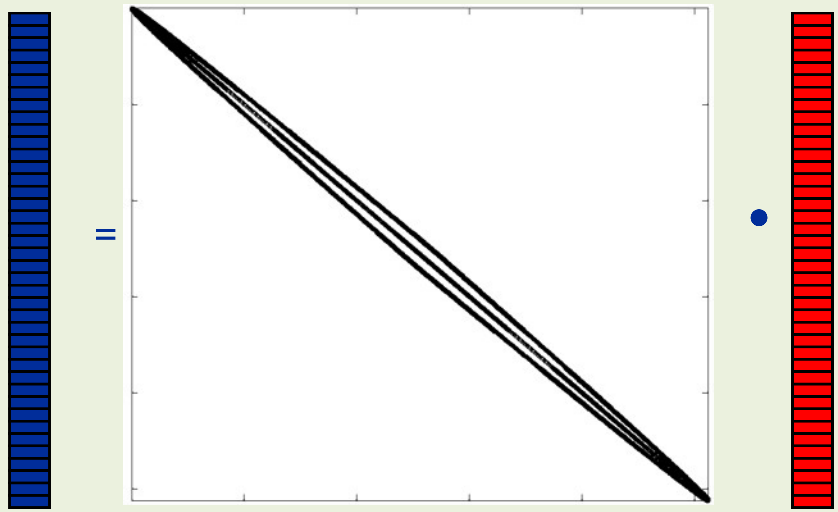

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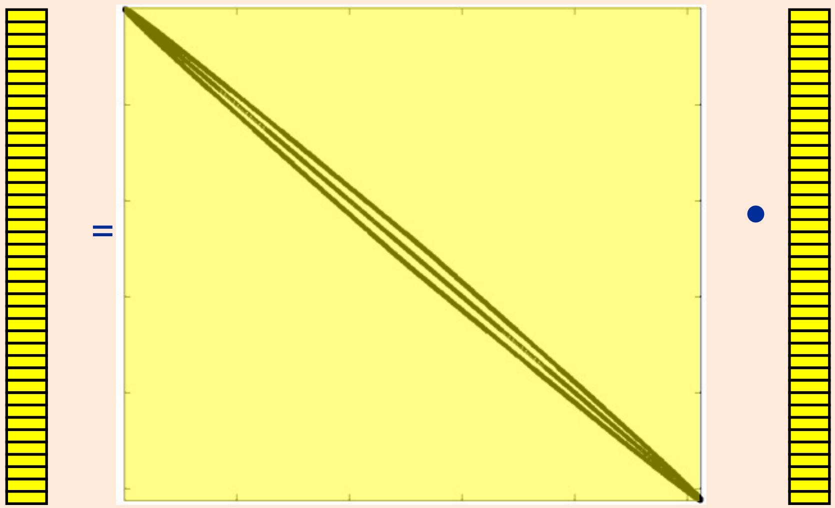

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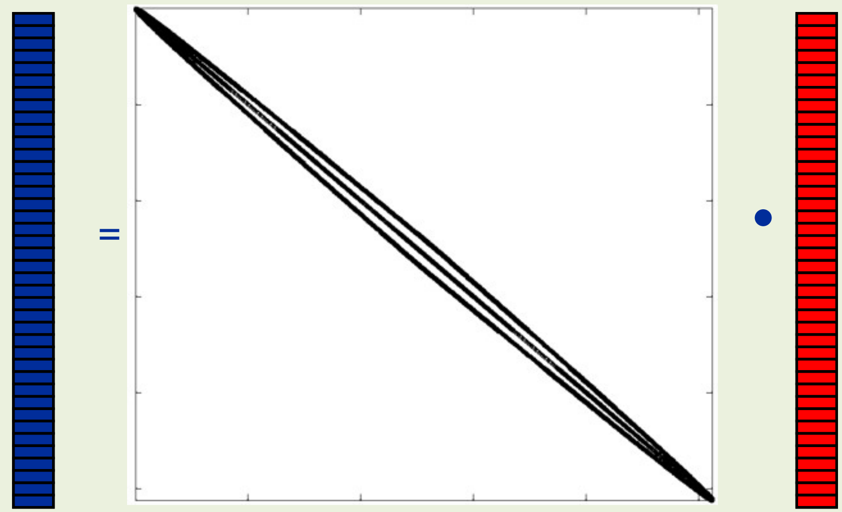

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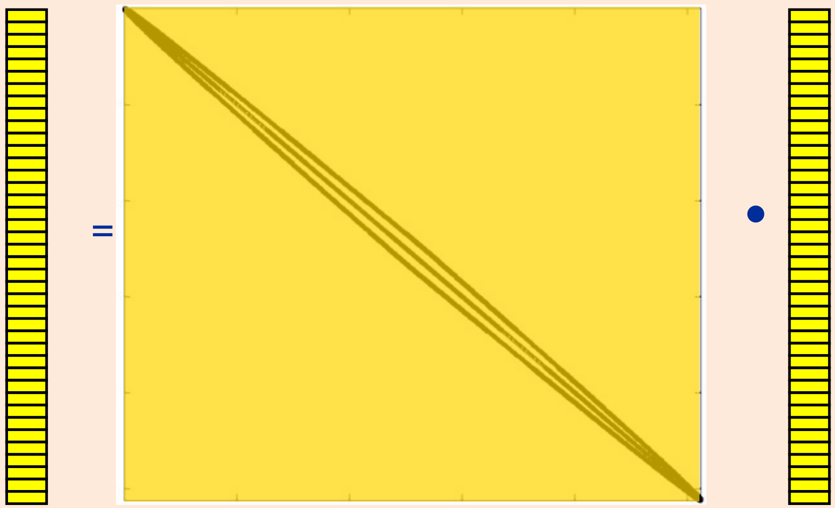
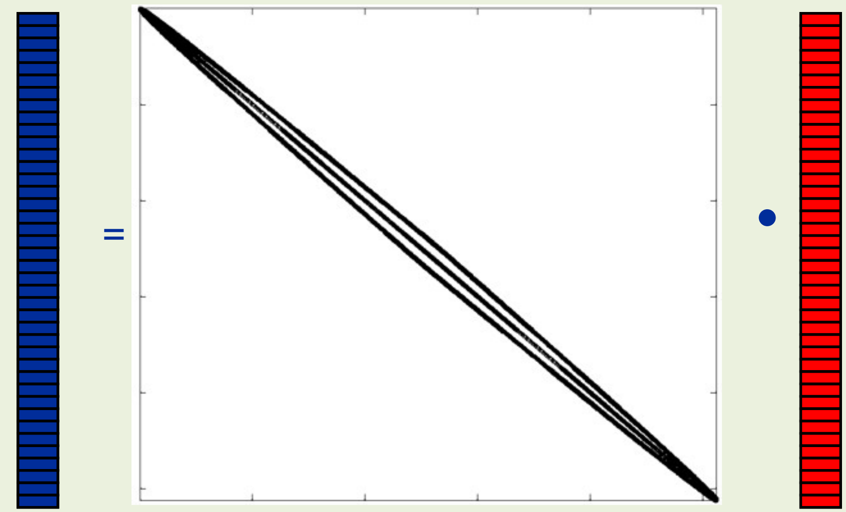


A^2x

RACE MPK



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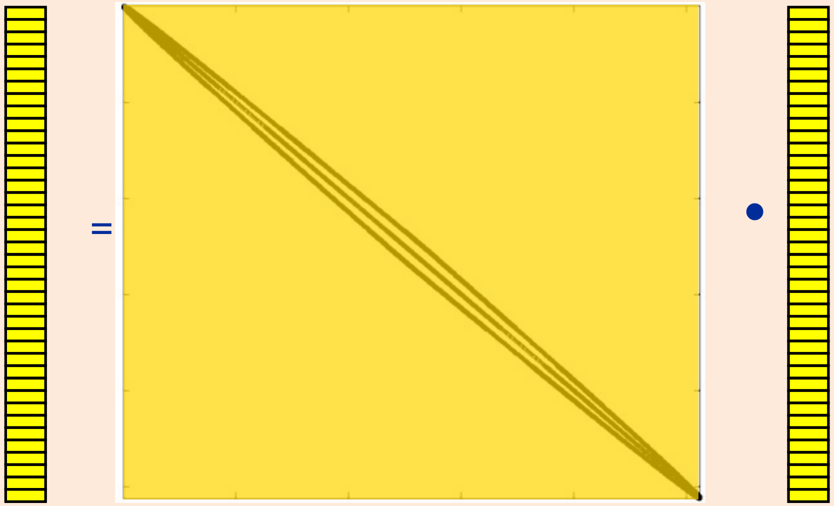

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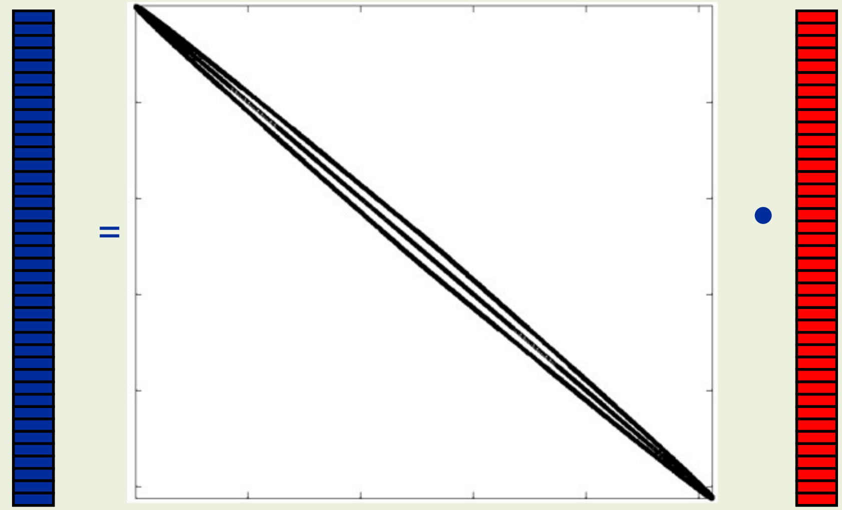

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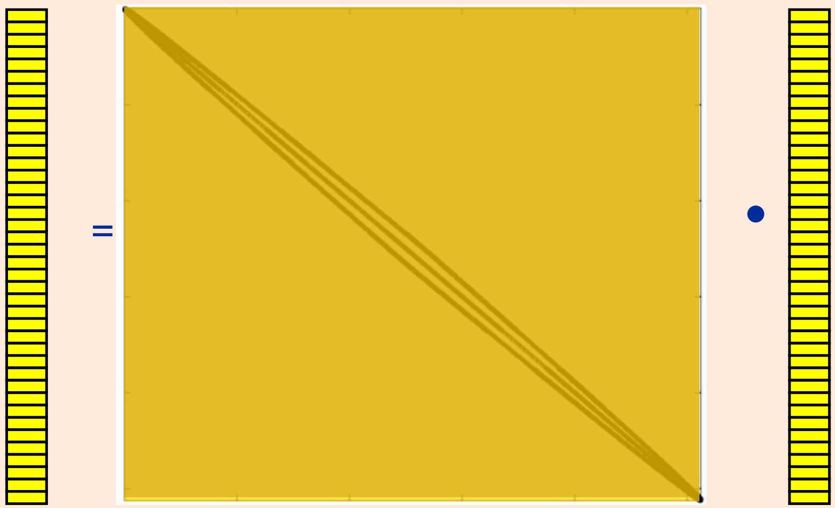

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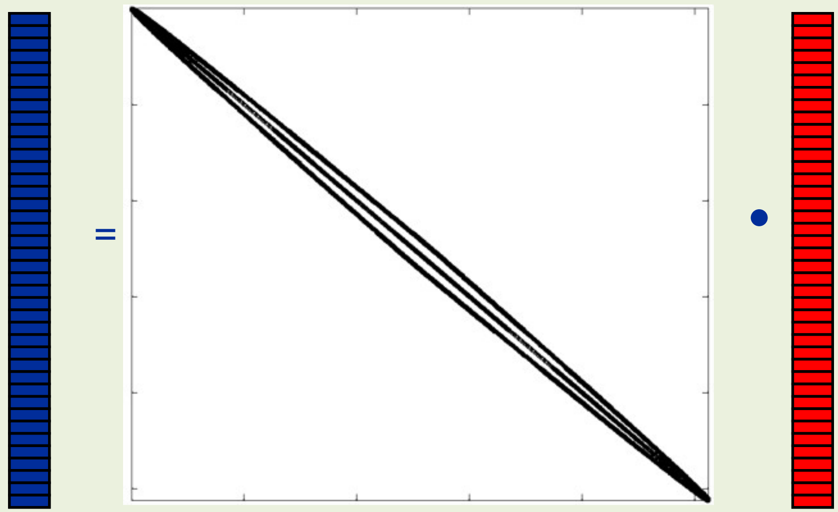

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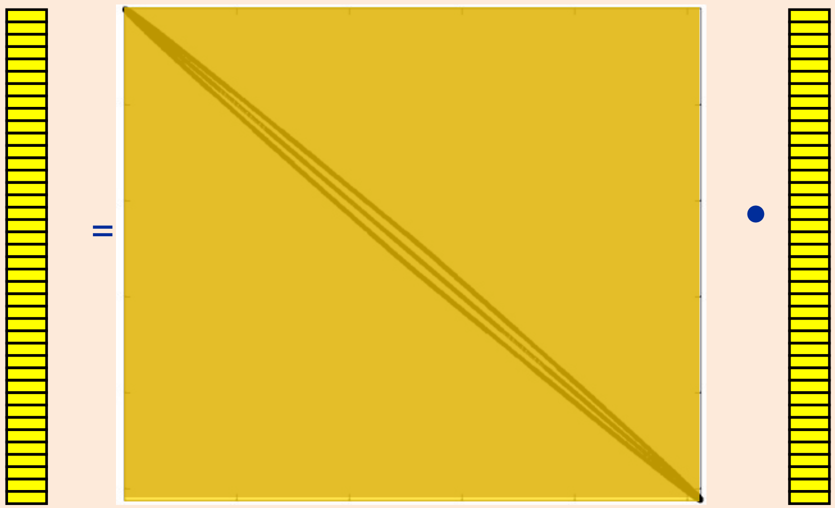

Matrix accessed 3 times from memory

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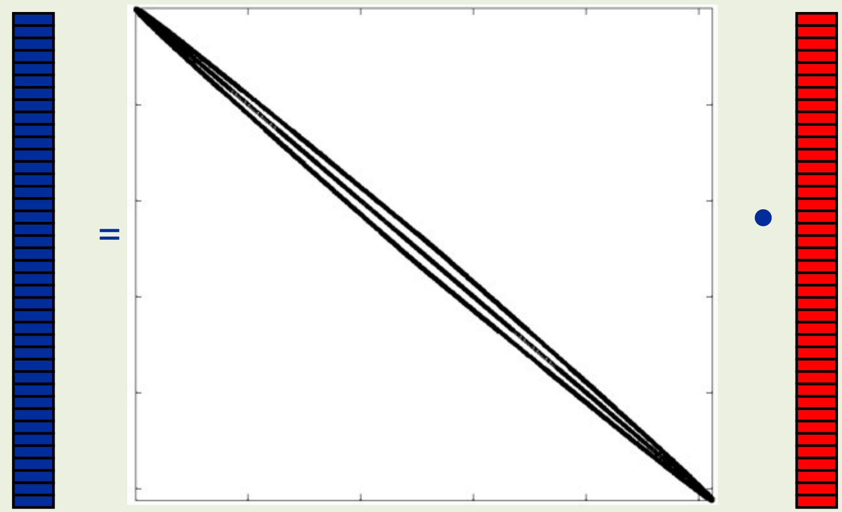

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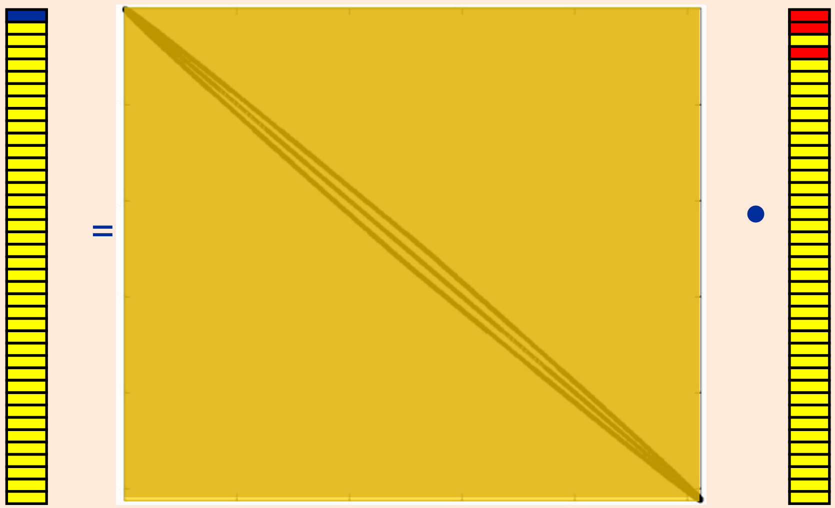

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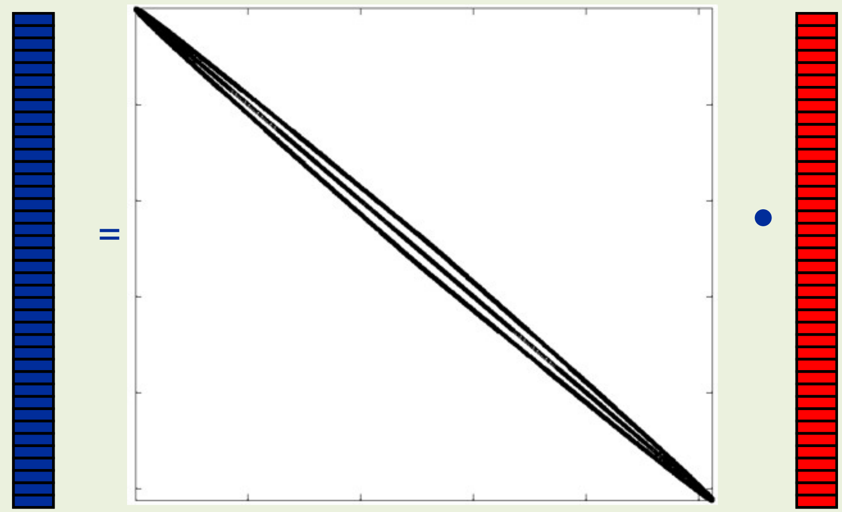

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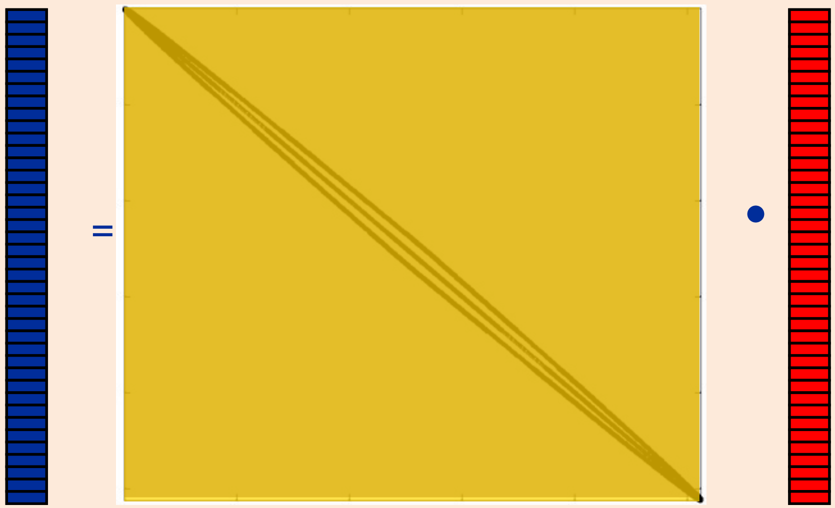

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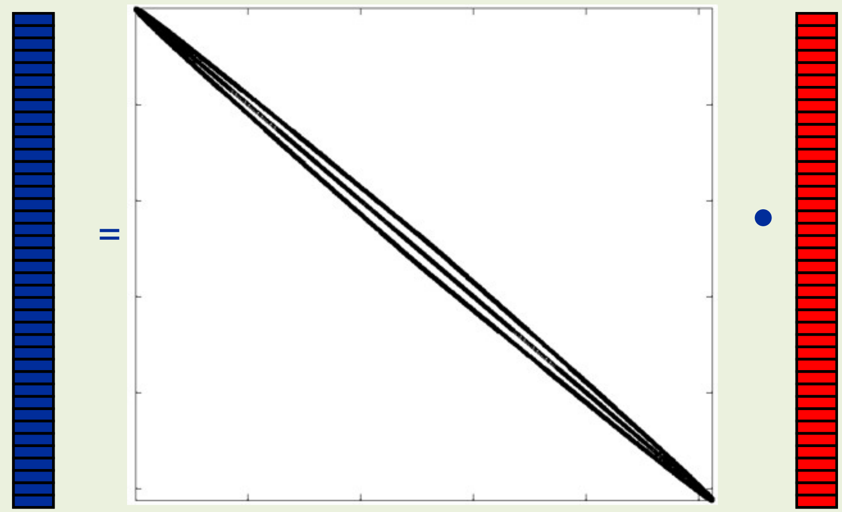

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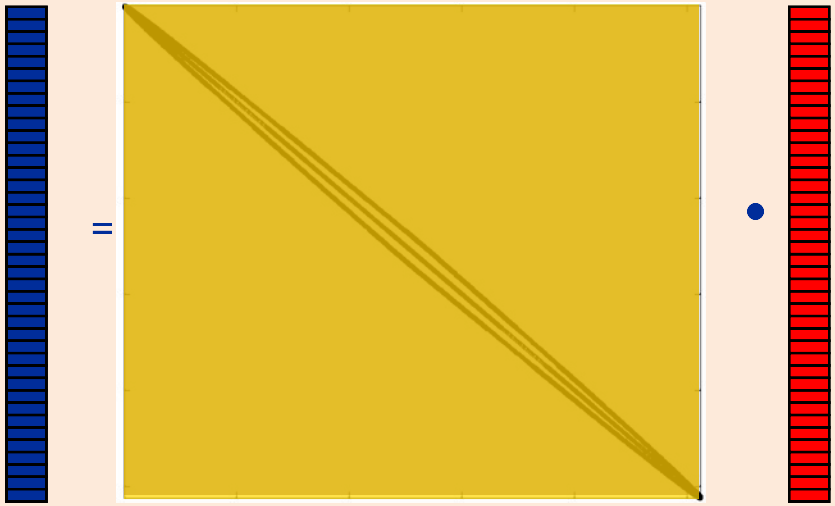

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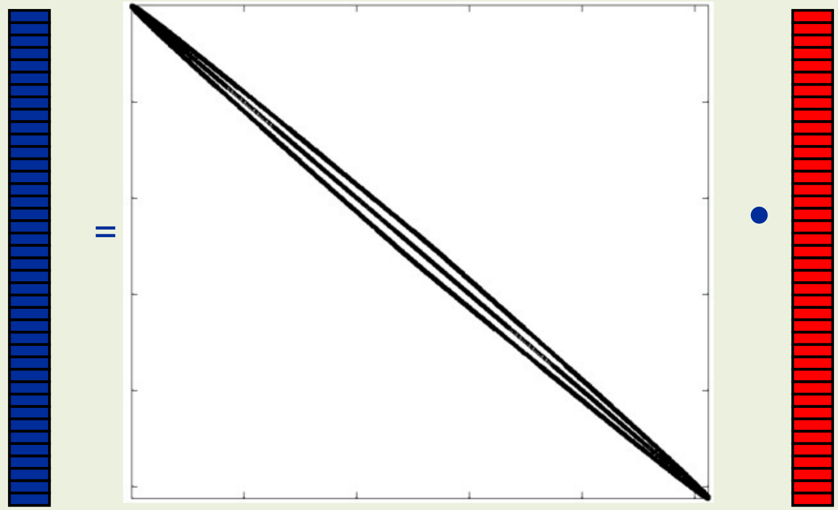

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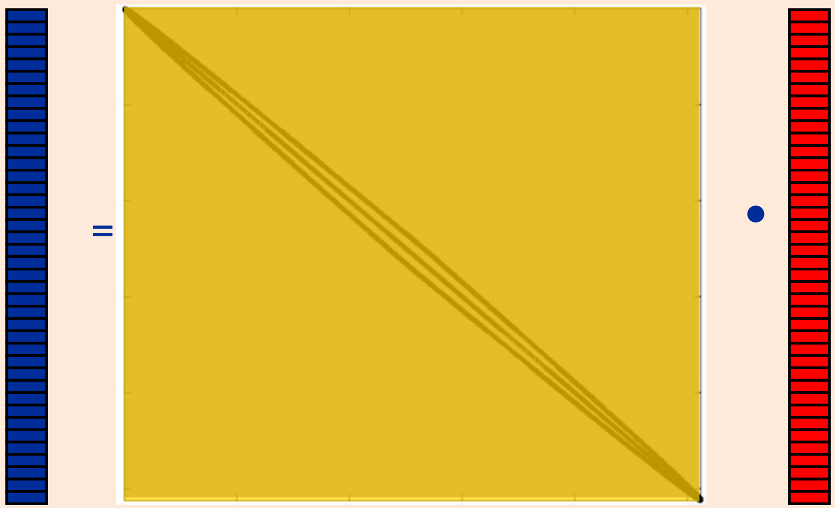

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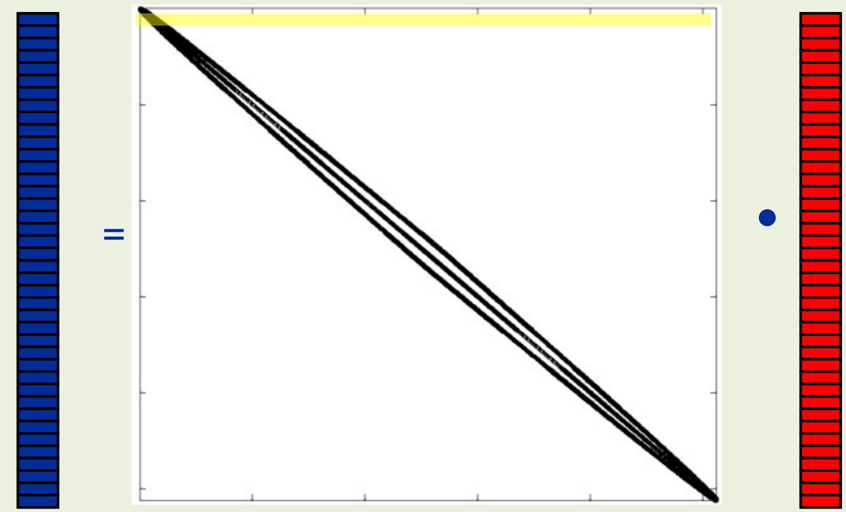

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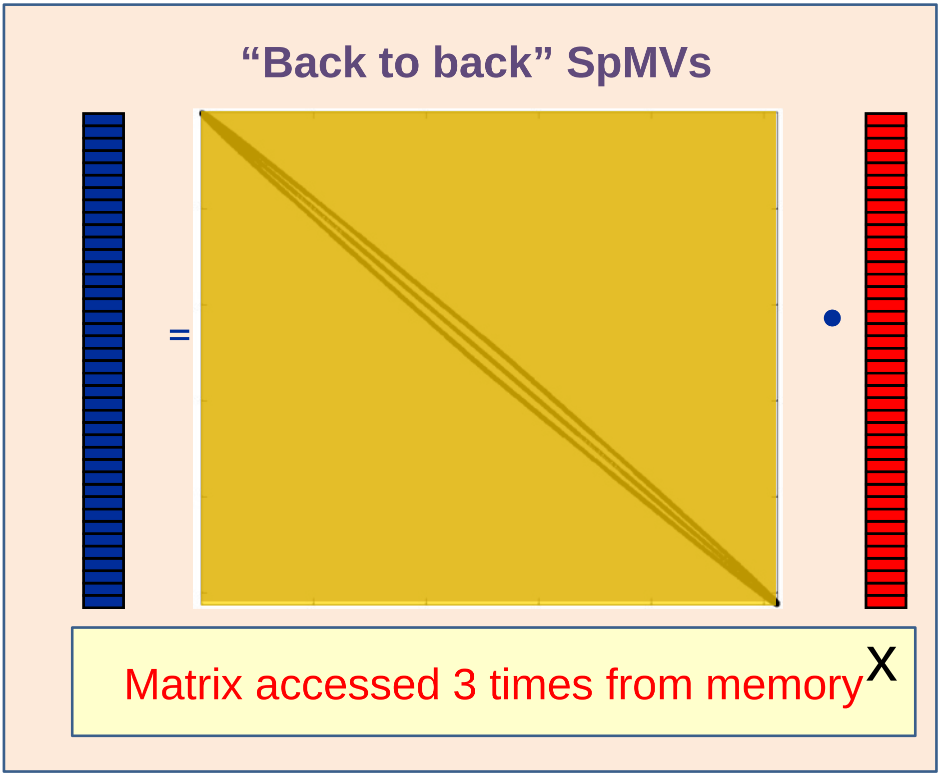

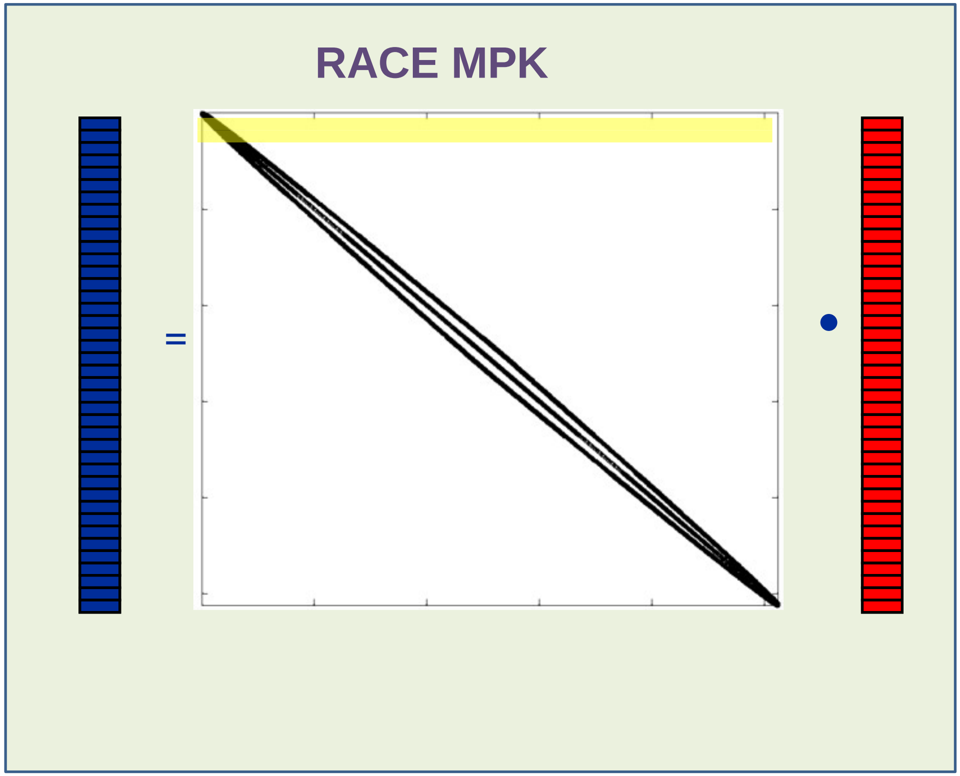

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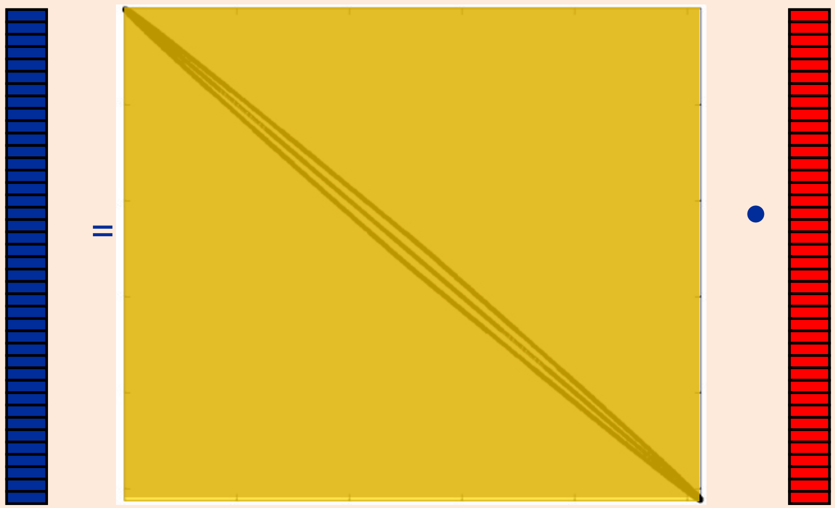

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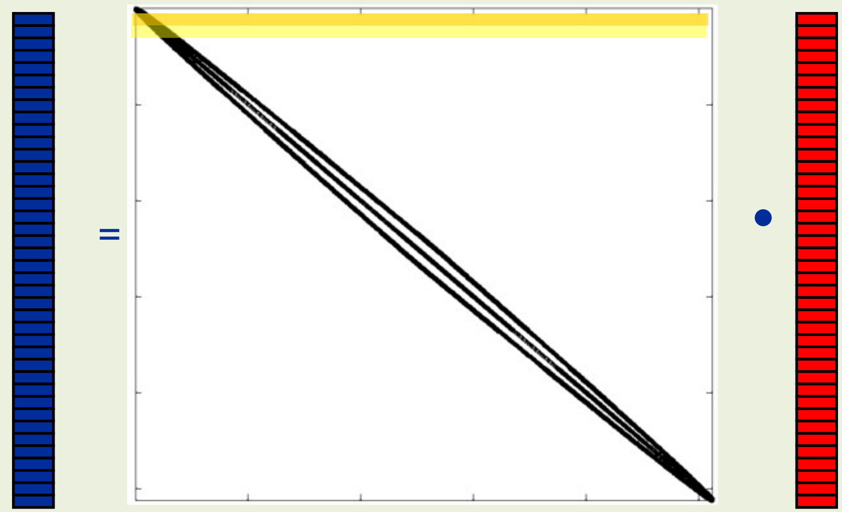

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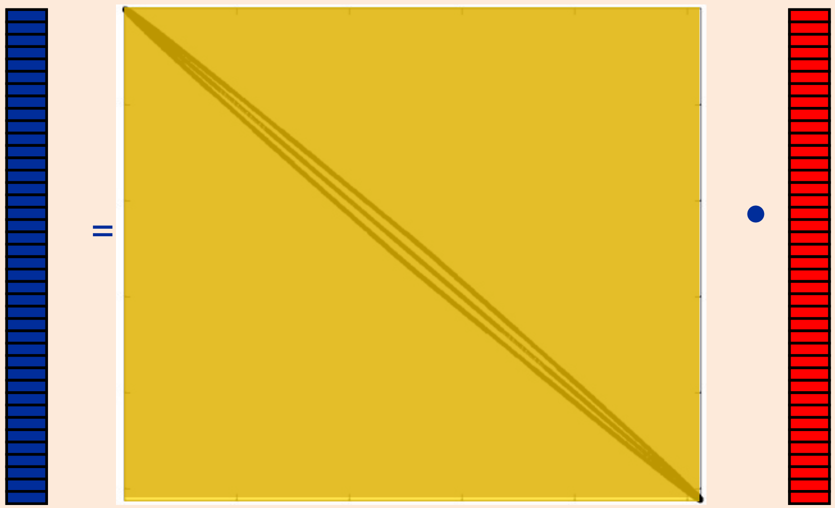

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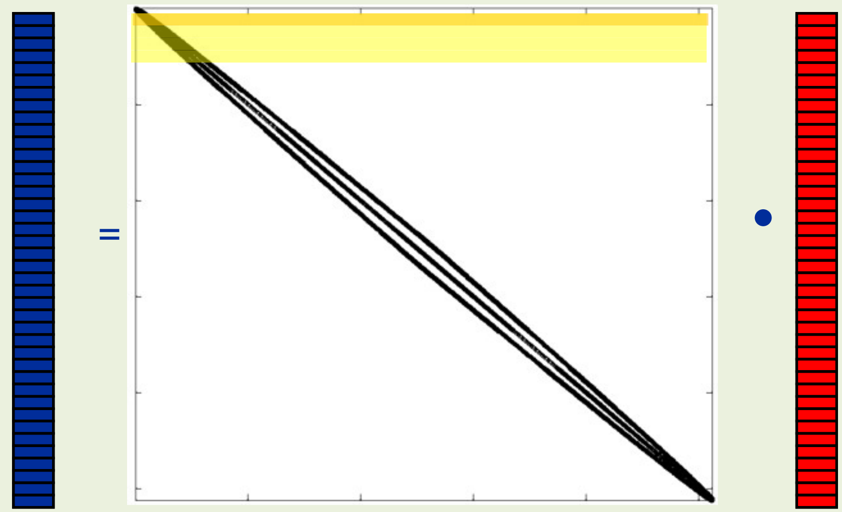

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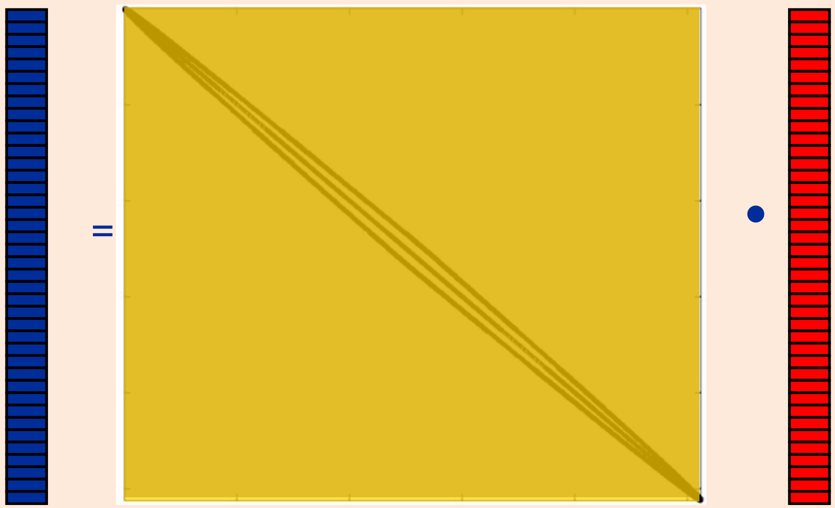

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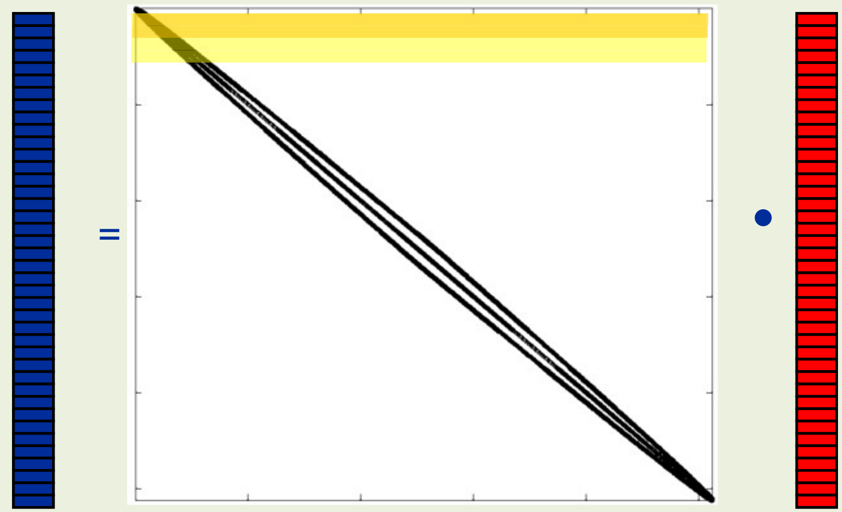

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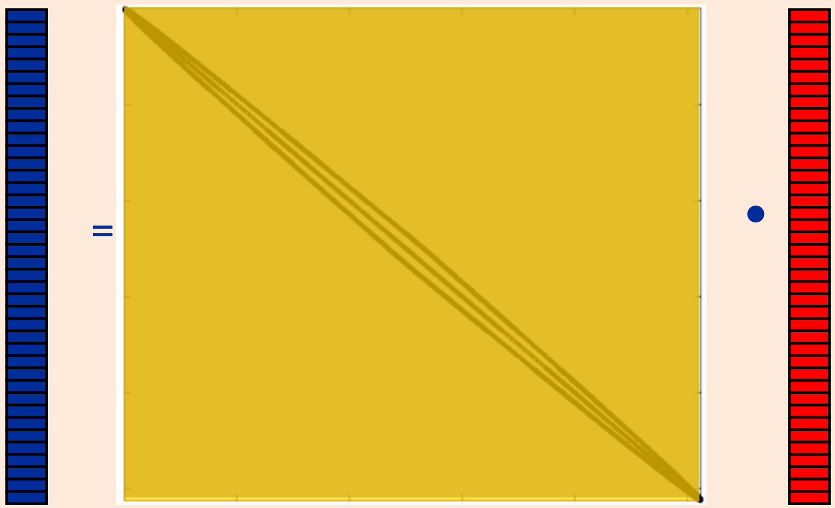

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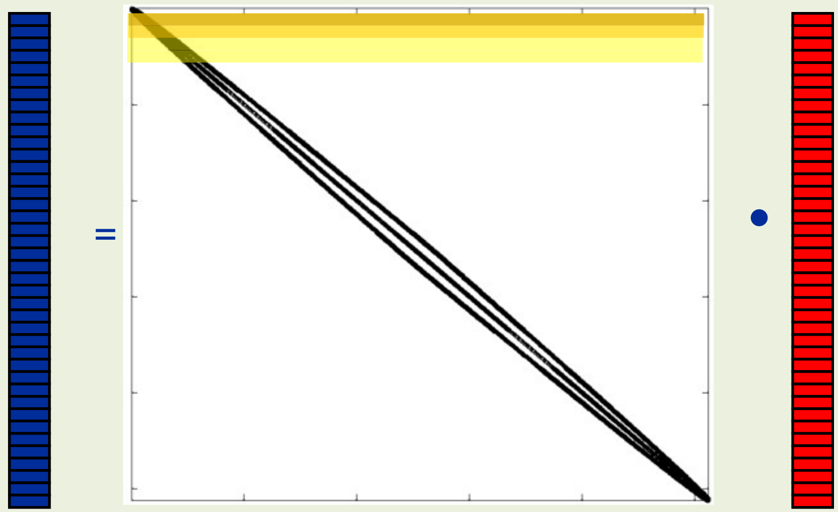

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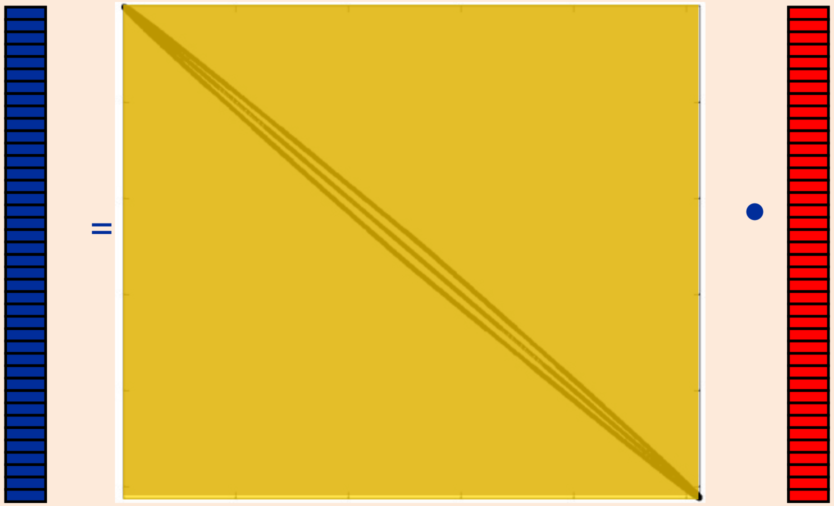

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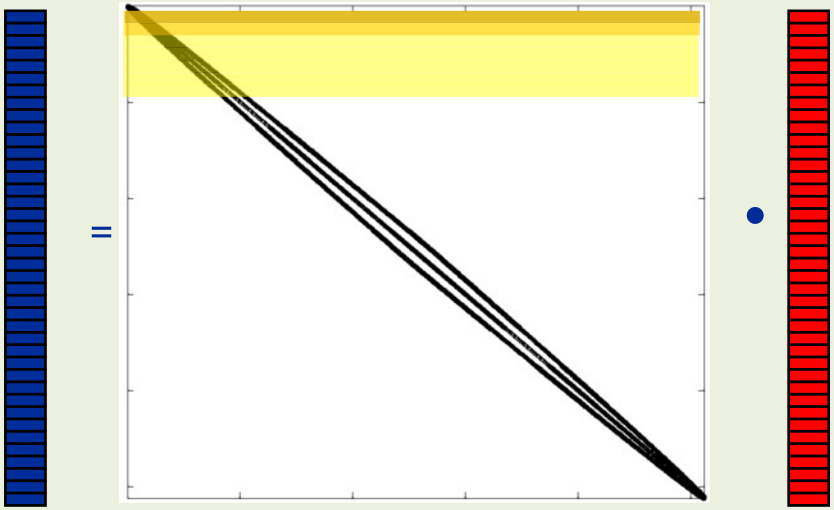

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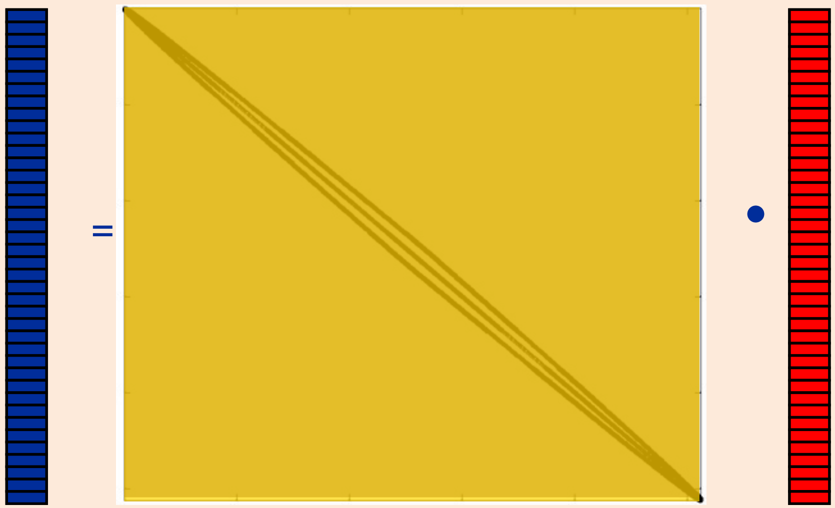

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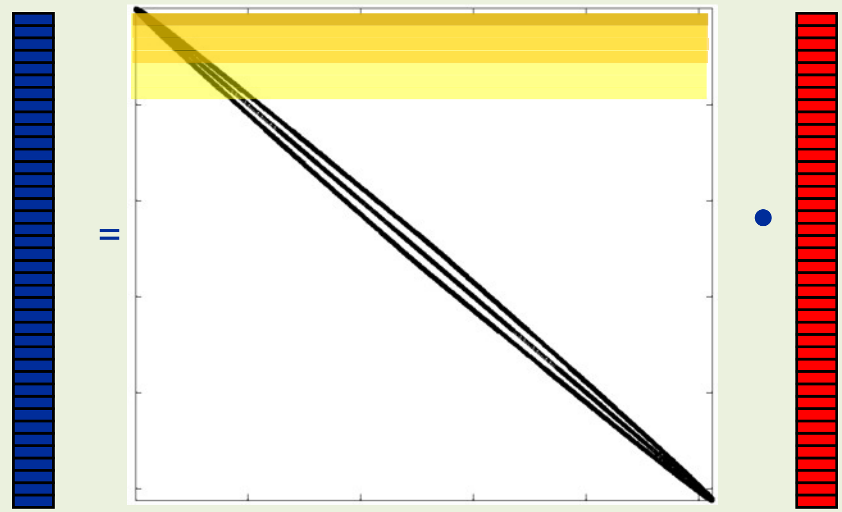

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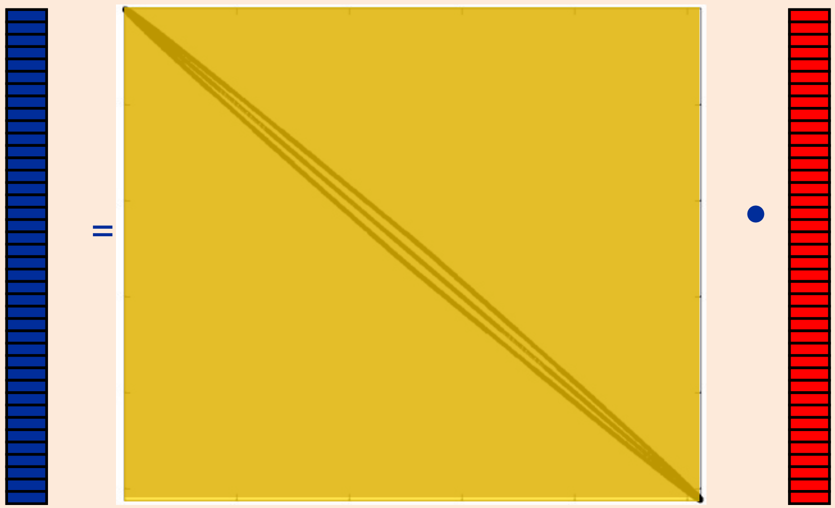

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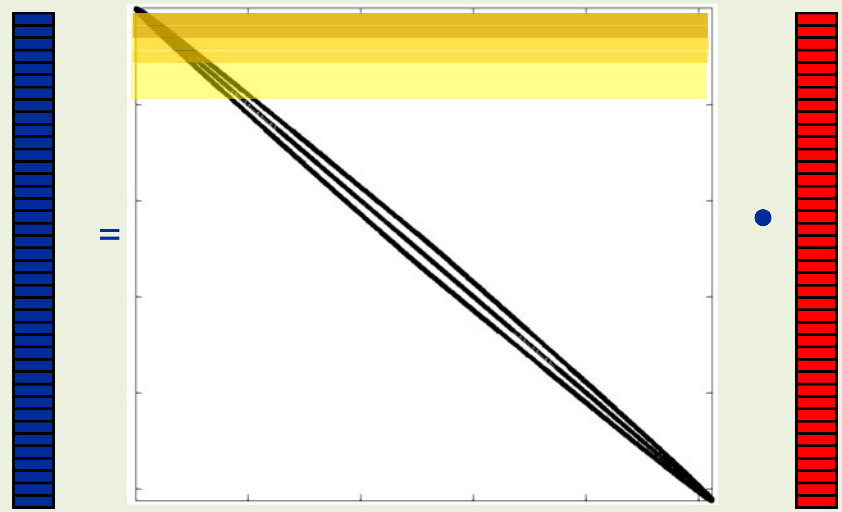

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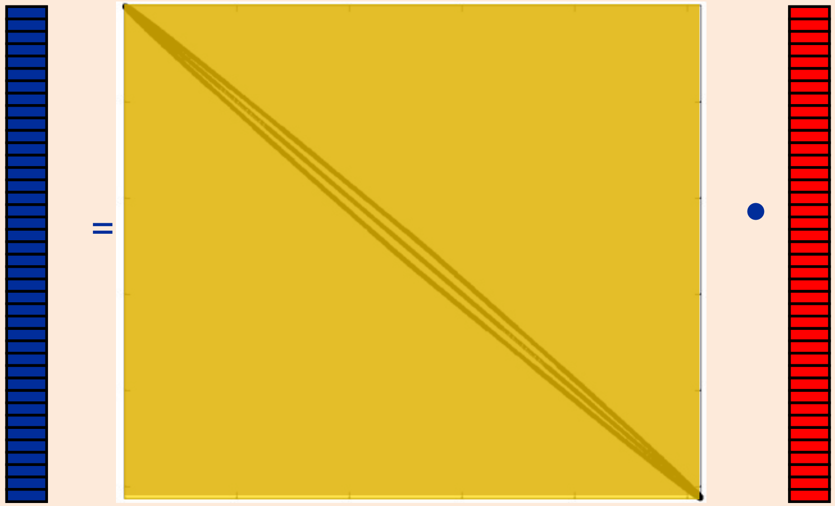

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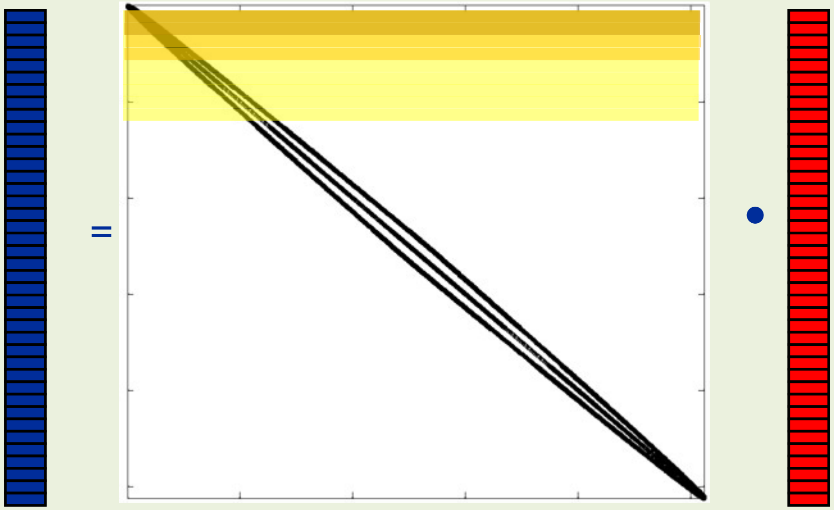

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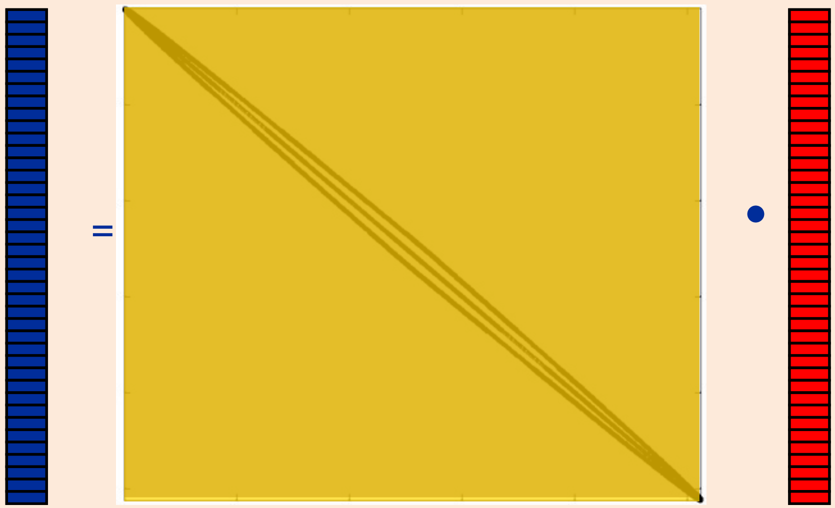

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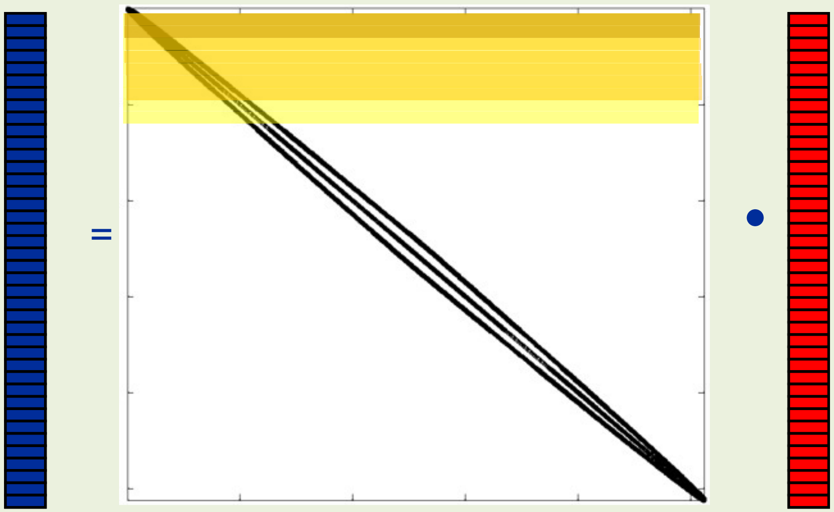

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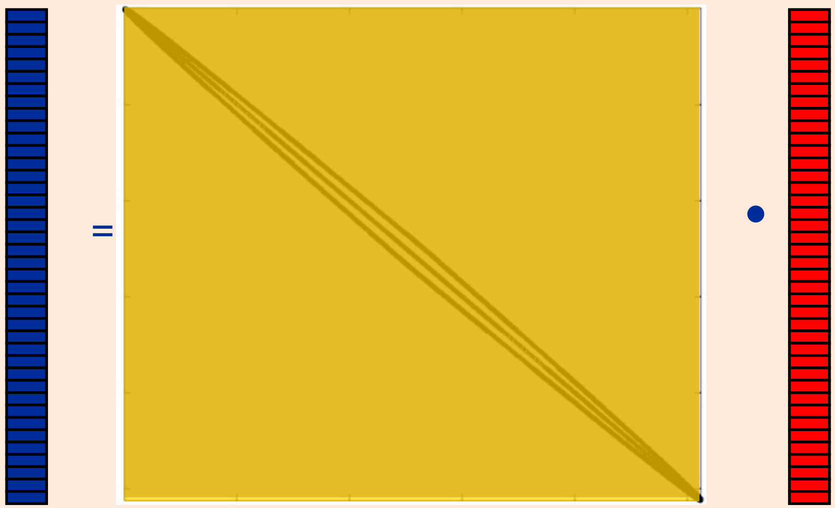

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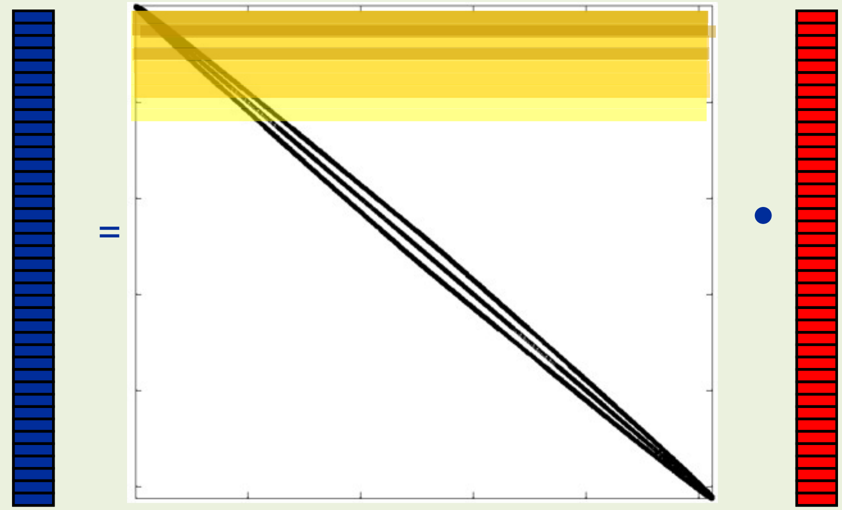

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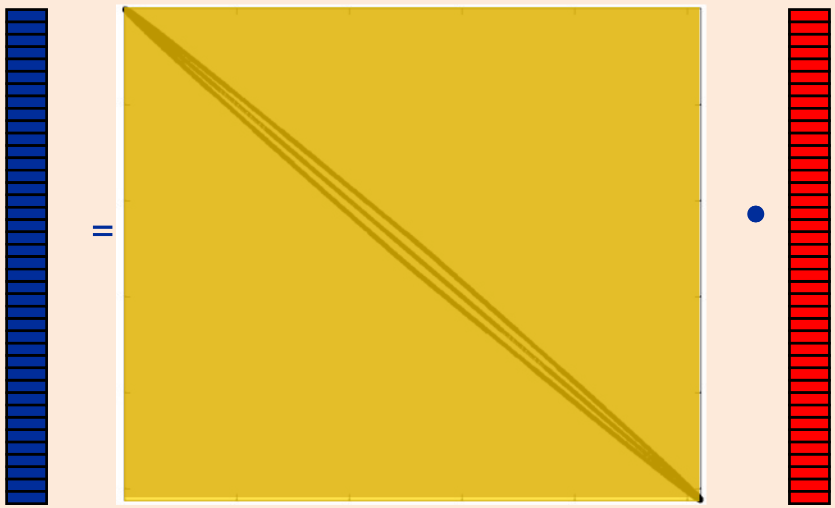

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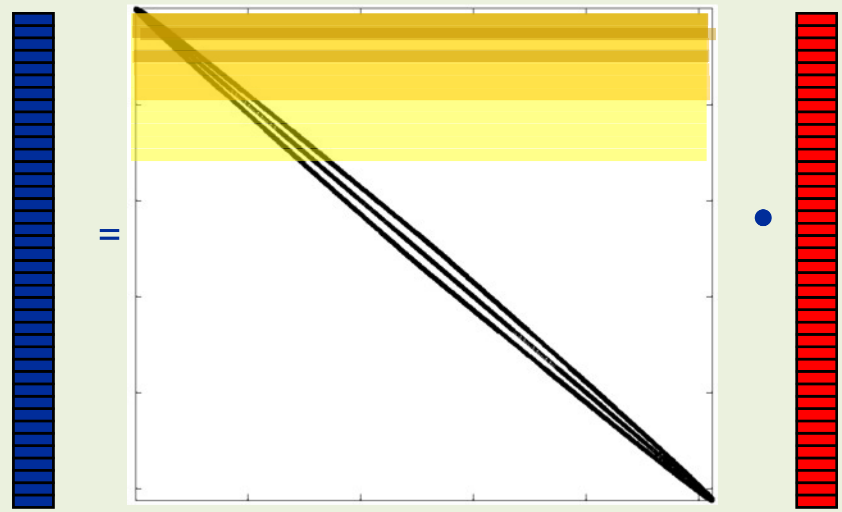

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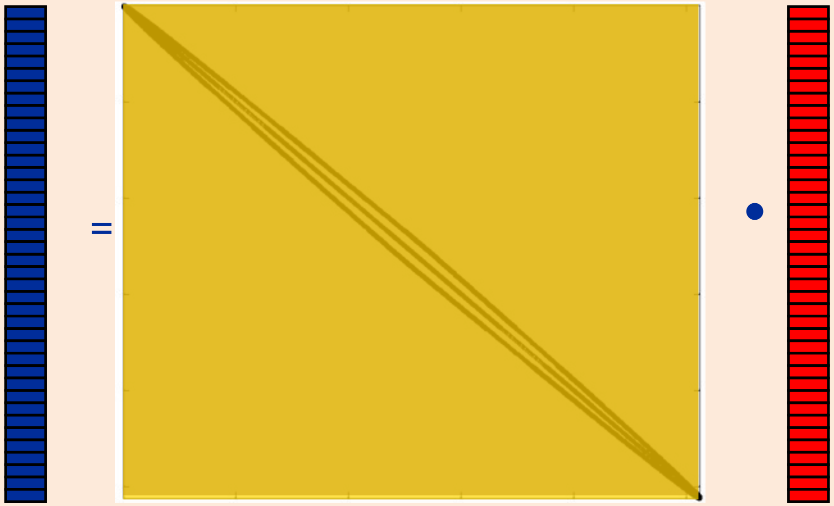

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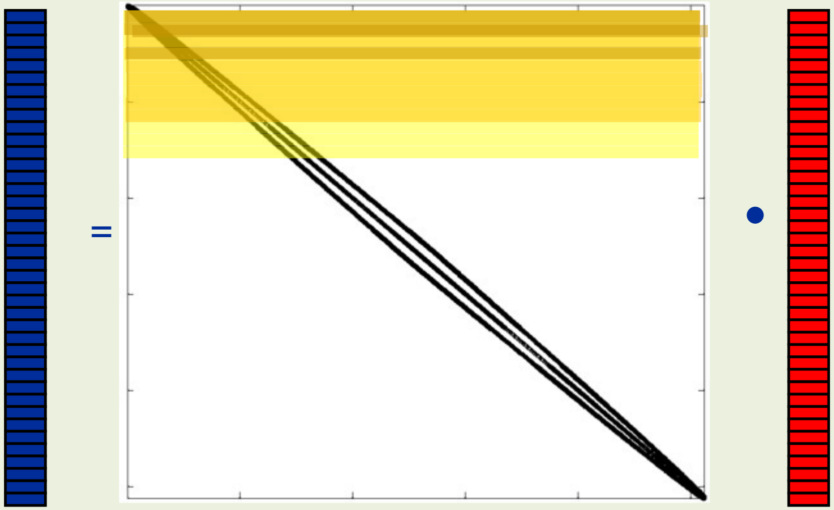

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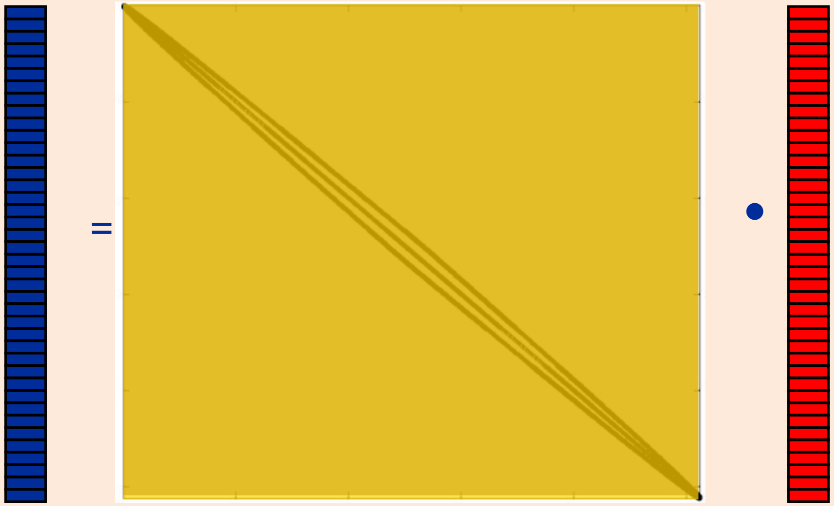

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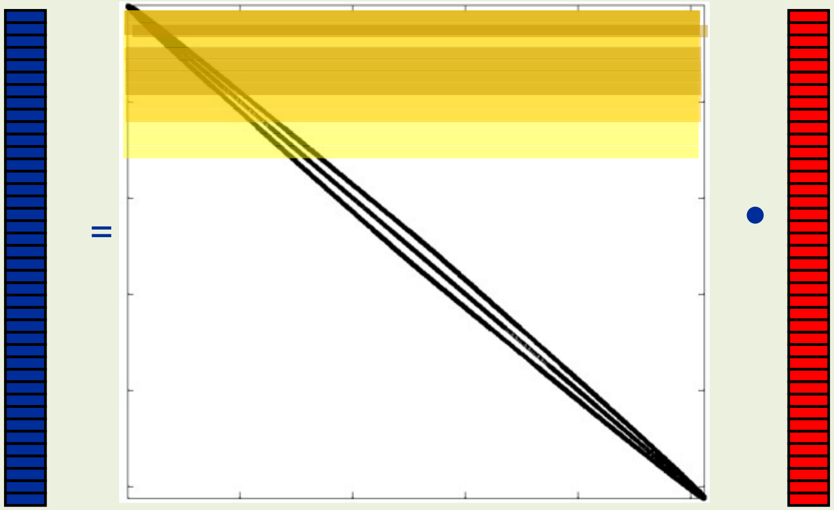

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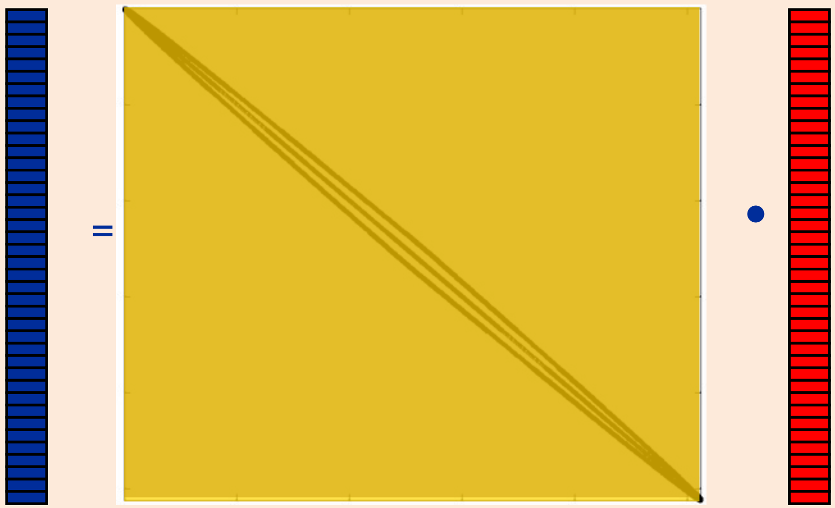

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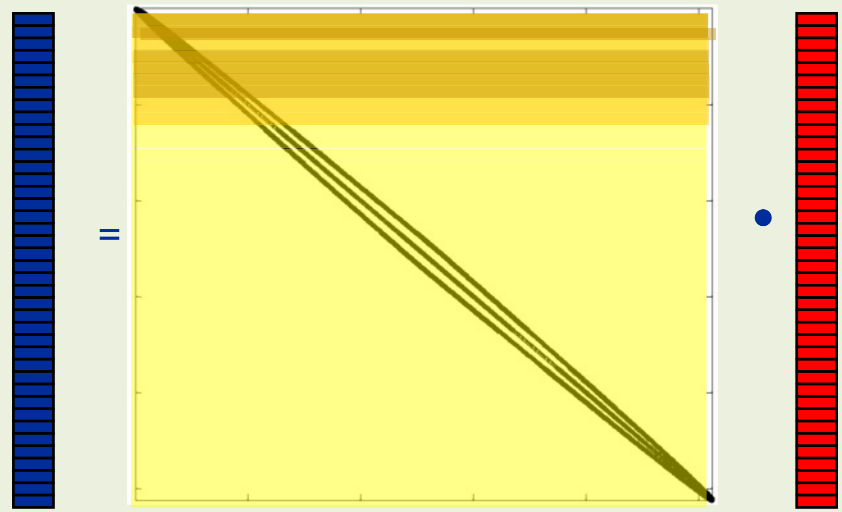
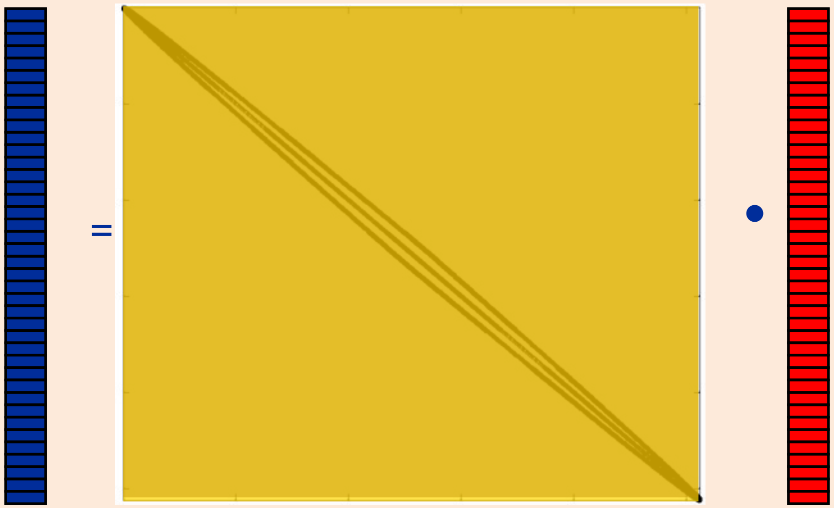


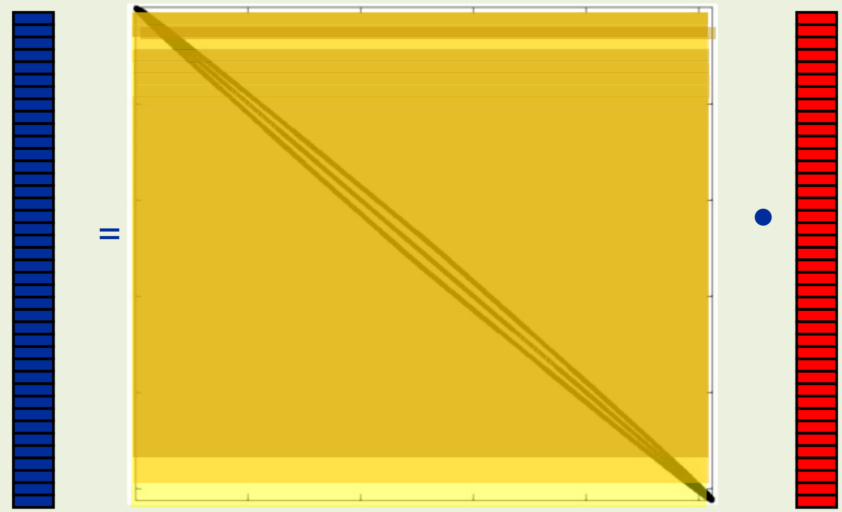
Matrix Power Kernel

“Back to back” SpMVs



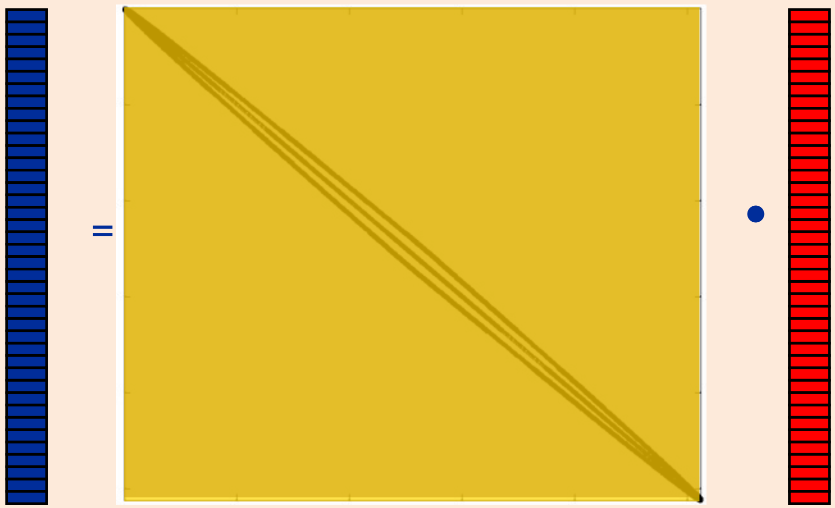
Matrix accessed 3 times from memory X

RACE MPK



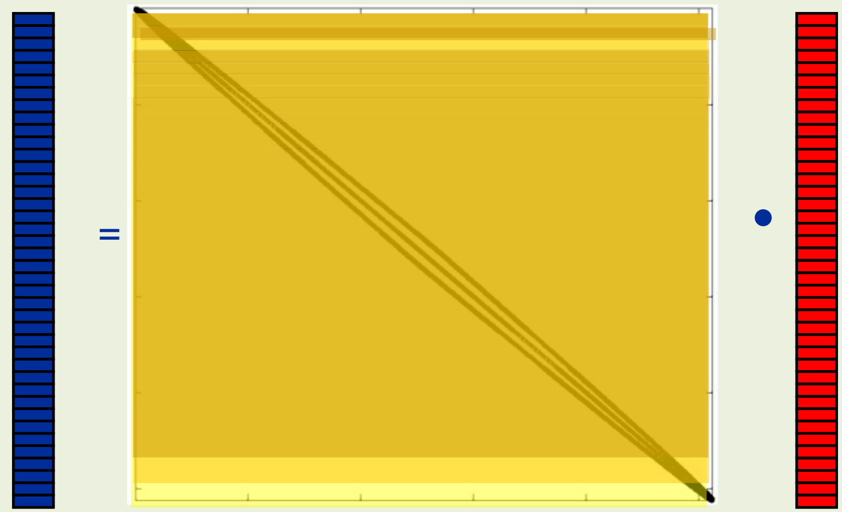
Matrix Power Kernel

“Back to back” SpMVs



Matrix accessed 3 times from memory X

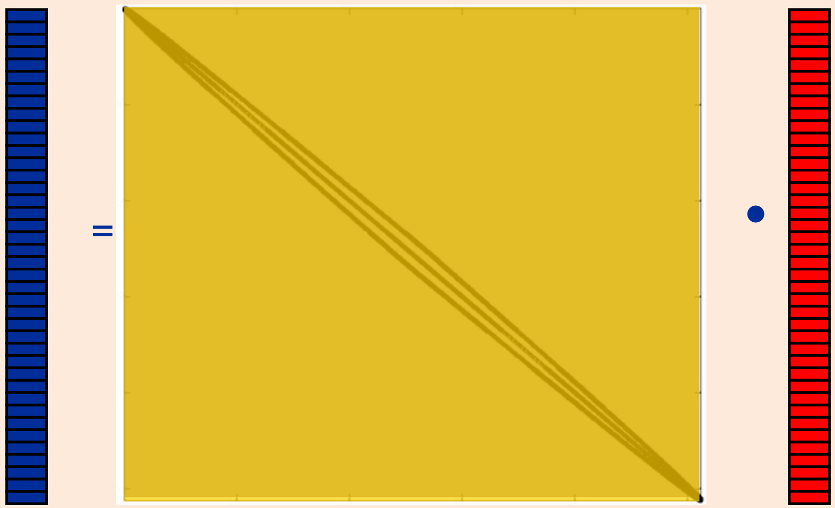
RACE MPK



Matrix accessed 1 time from memory

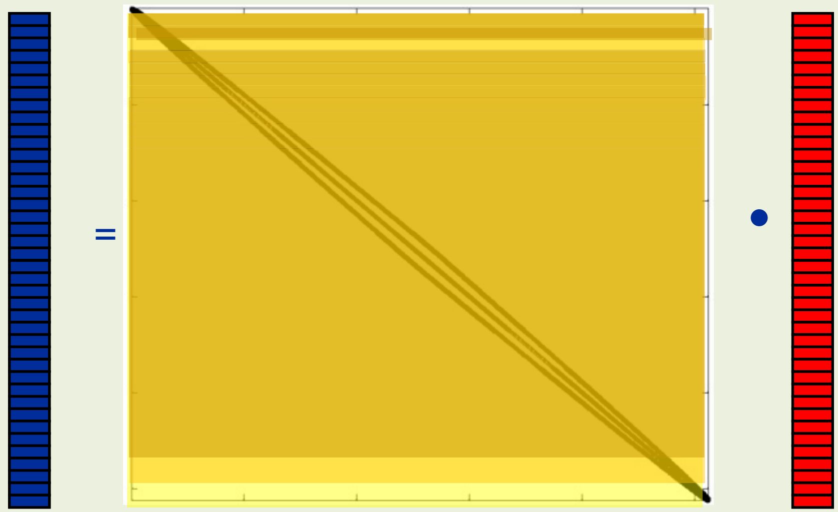
Matrix Power Kernel

"Back to back" SpMVs



Matrix accessed 3 times from memory X

RACE MPK



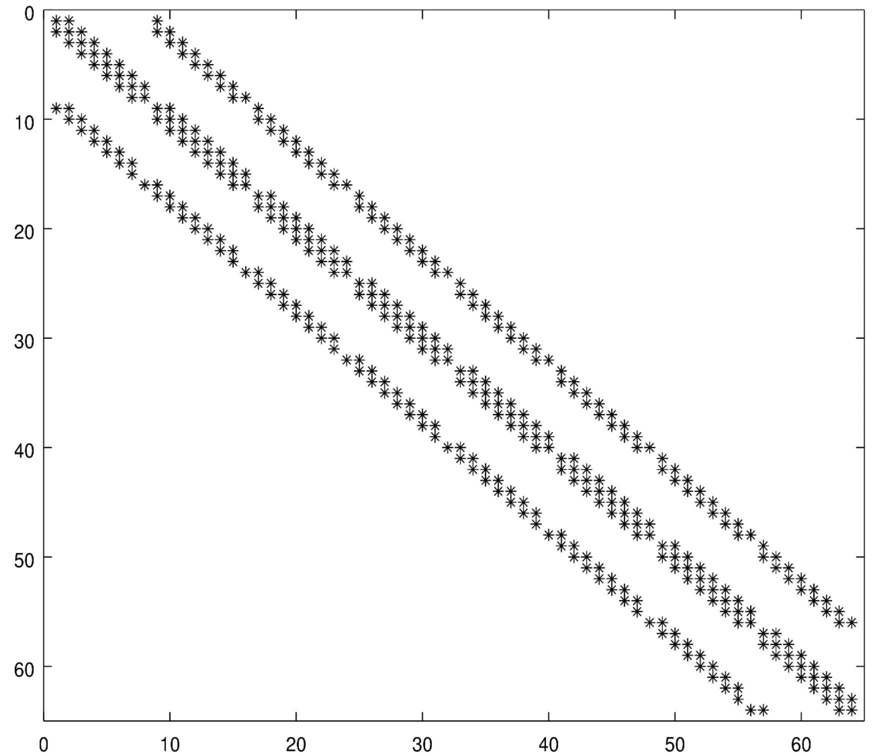
Matrix accessed 1 time from memory

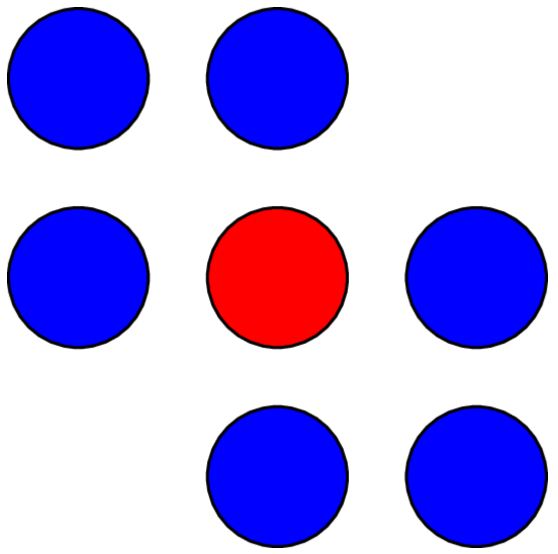
Alappat et al, "Level-Based Blocking for Sparse Matrices: Sparse Matrix-Power-Vector Multiplication," in *IEEE Transactions on Parallel and Distributed Systems*, 2023, doi: 10.1109/TPDS.2022.3223512.

Wavefront passing through matrix.

- More complicated than the Regular example seen here!

Sparse Matrix ✉ Graph





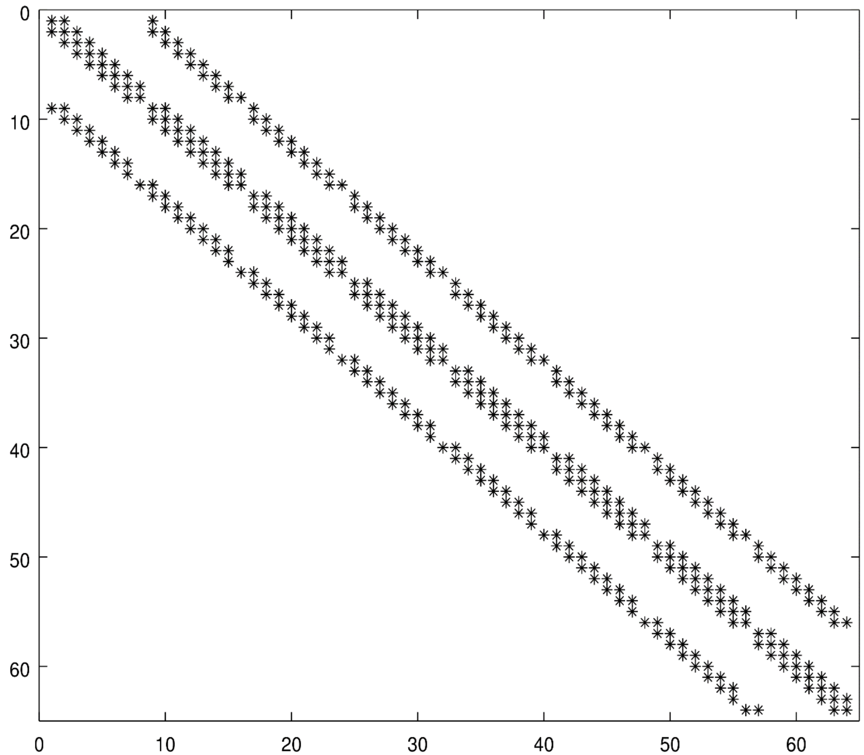
Stencil

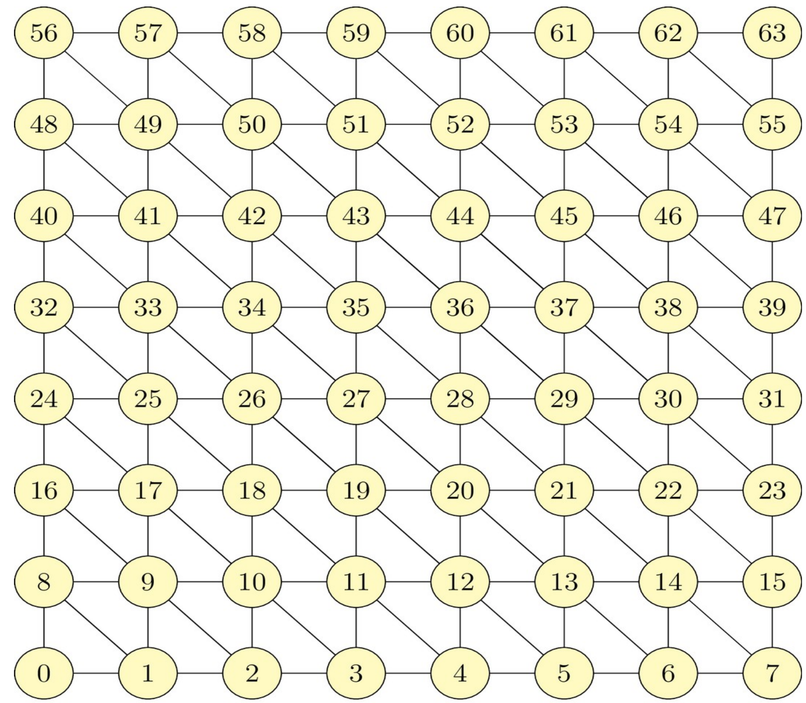
Sparse Matrix

Example of 2D-7 Point stencil

Sparse Matrix ✉ Graph

DELFT BLUE





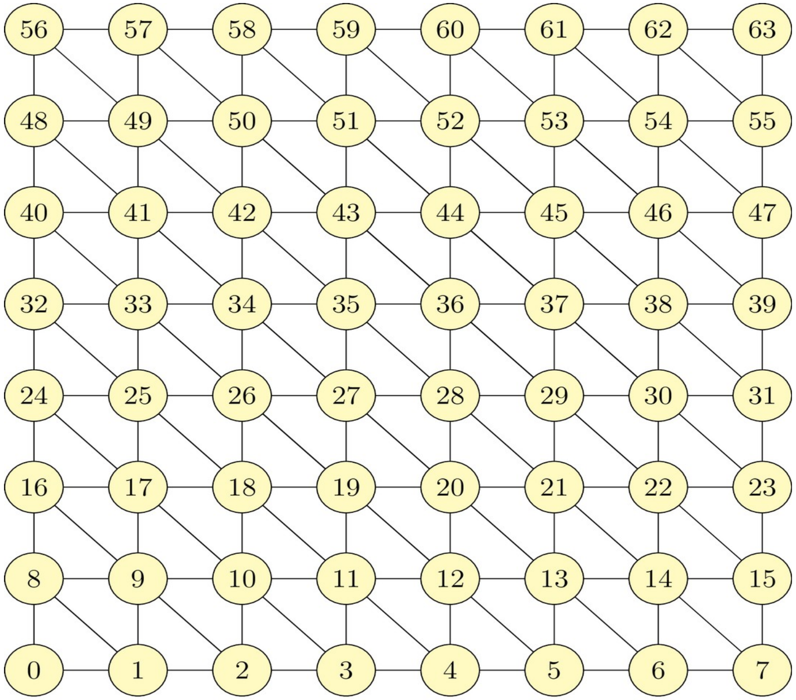
Sparse Matrix

Graph

Example of 2D-7 Point stencil

TU Delft

RACE: Recursive Algebraic Coloring



Example of 2D-7 Point stencil

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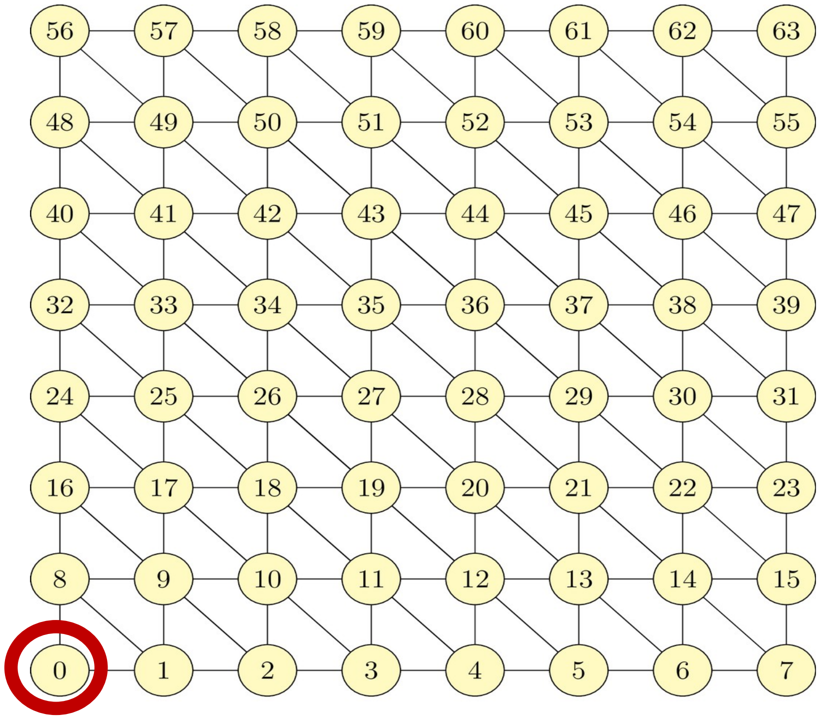

Example of 2D-7 Point stencil

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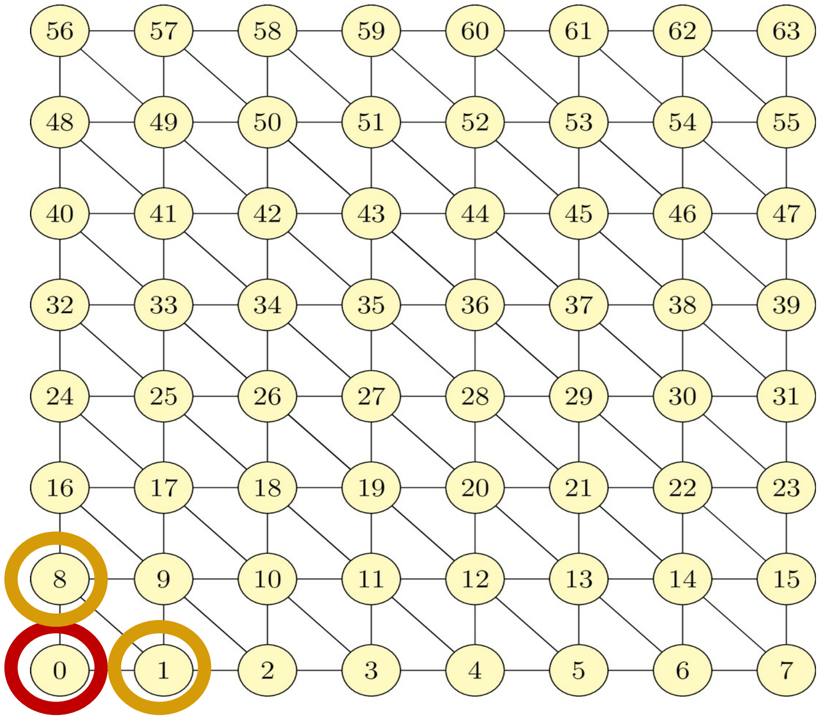
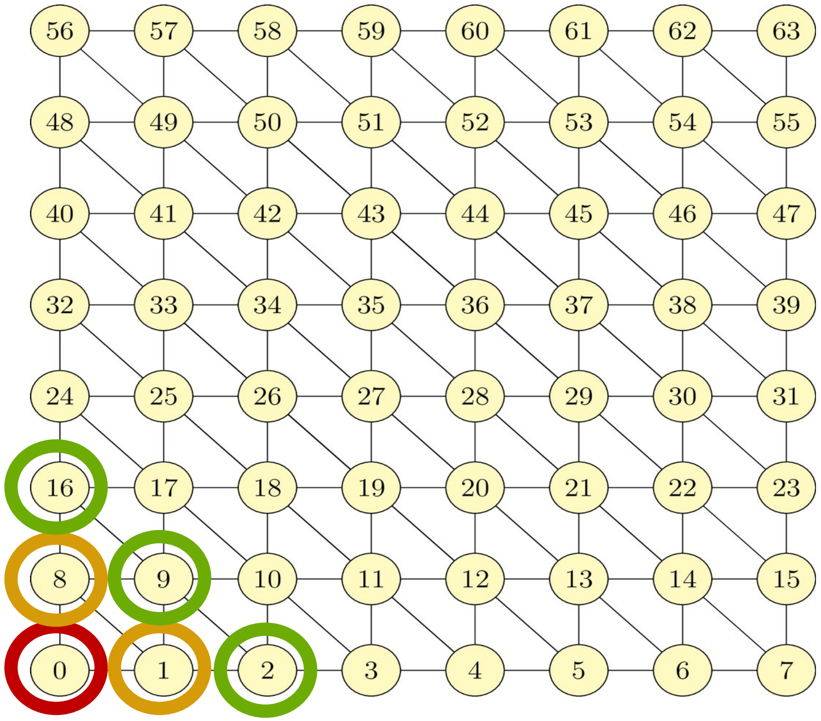


Example of 2D-7 Point stencil

RACE: Recursive Algebraic Coloring



Example of 2D-7 Point stencil

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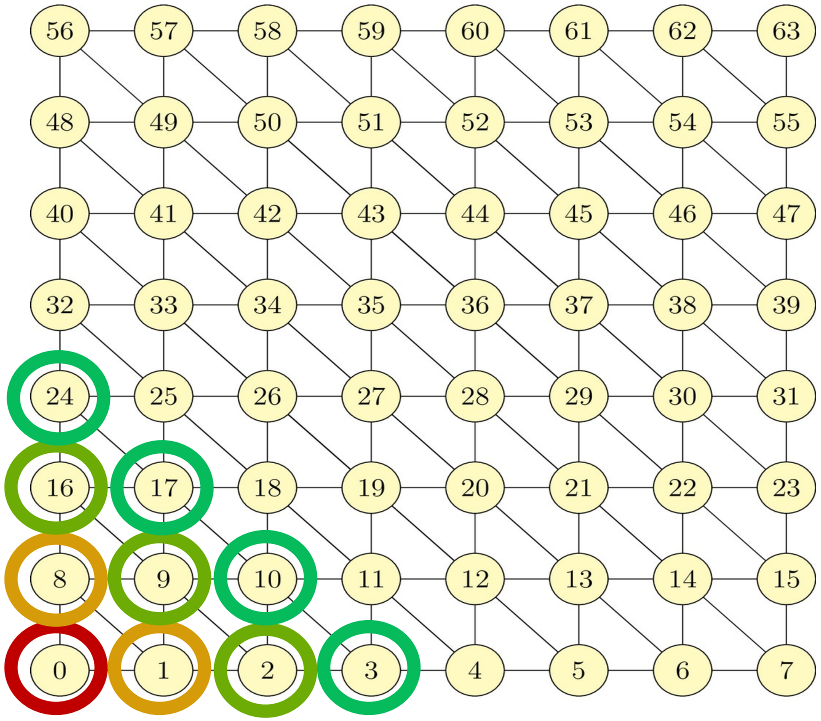
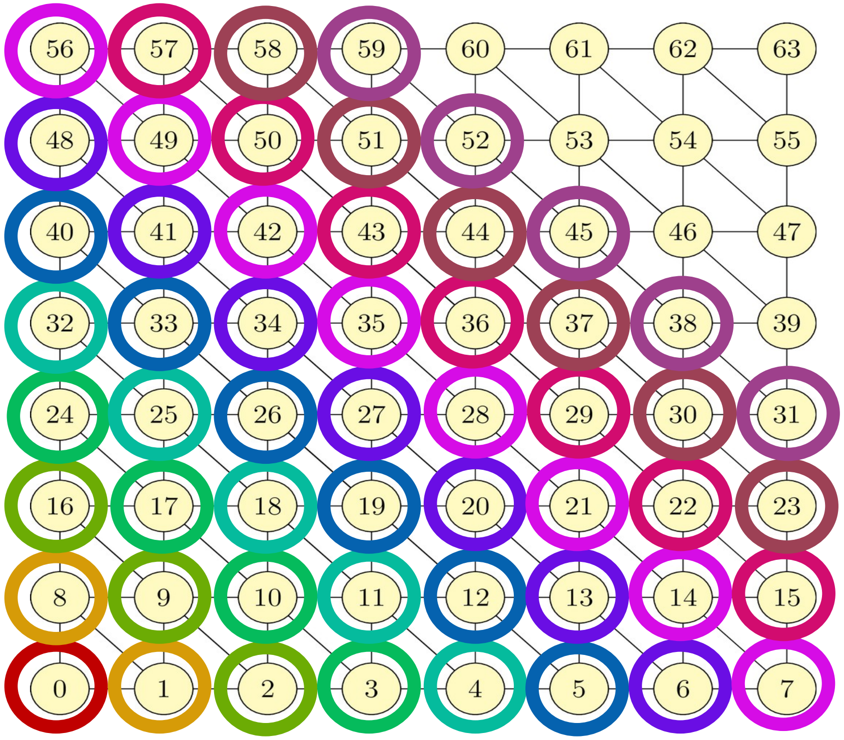


Example of 2D-7 Point stencil

RACE: Recursive Algebraic Coloring



Example of 2D-7 Point stencil

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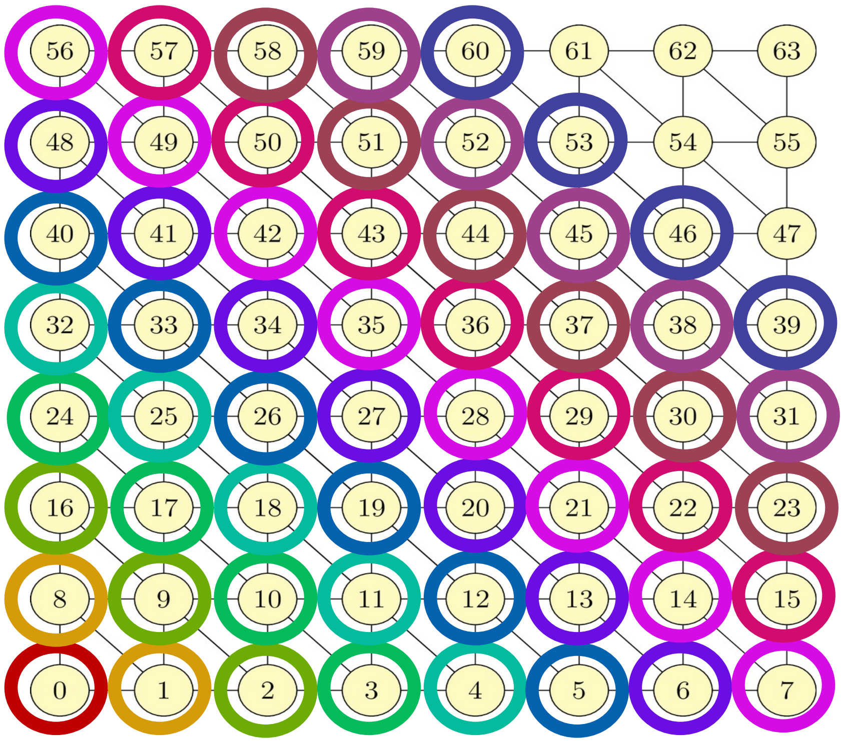
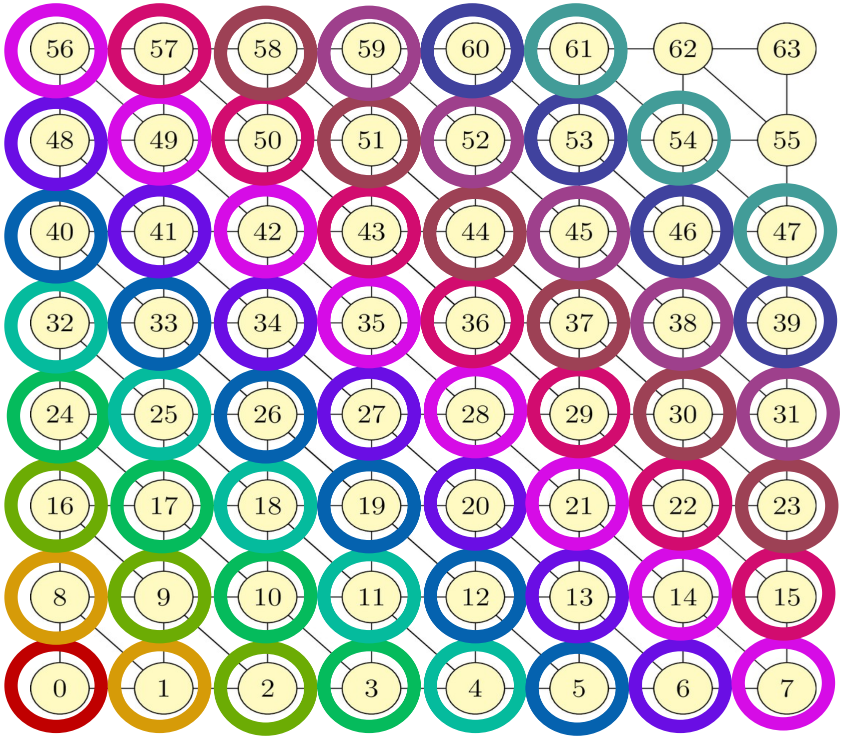


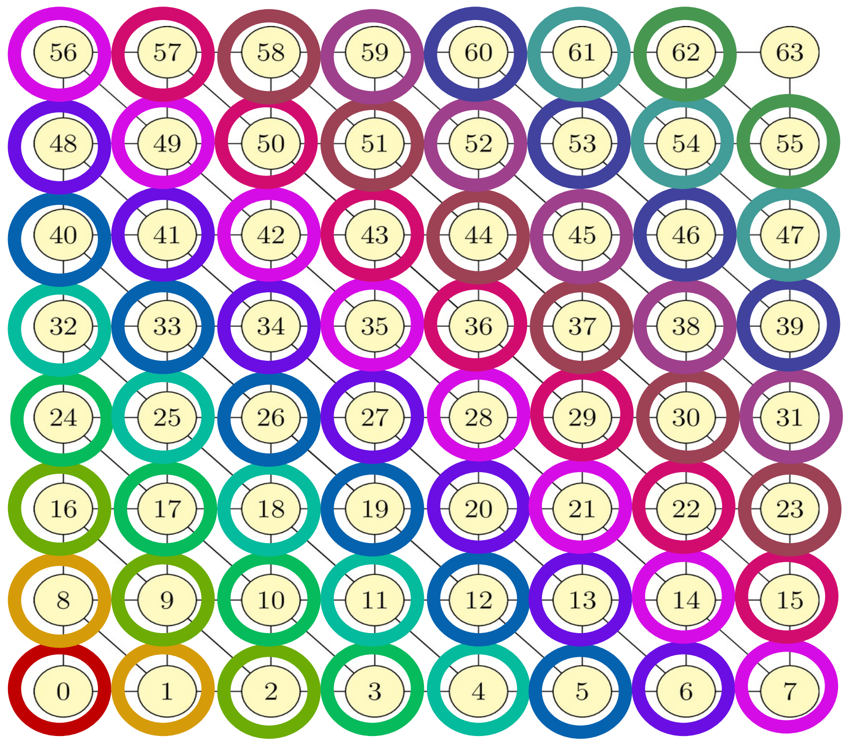
Example of 2D-7 Point stencil

RACE: Recursive Algebraic Coloring



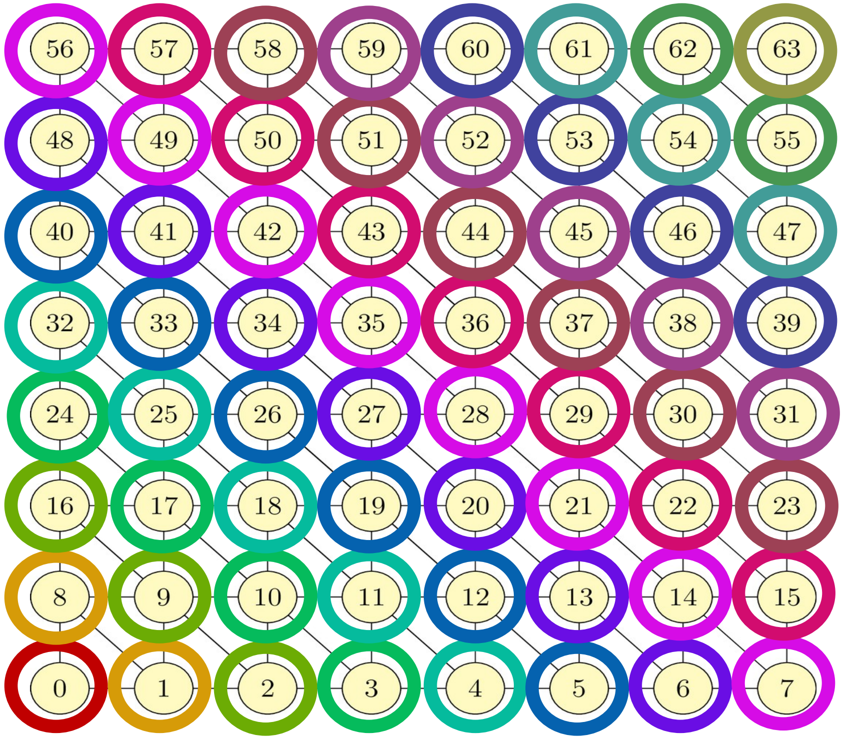
Example of 2D-7 Point stencil

RACE: Recursive Algebraic Coloring



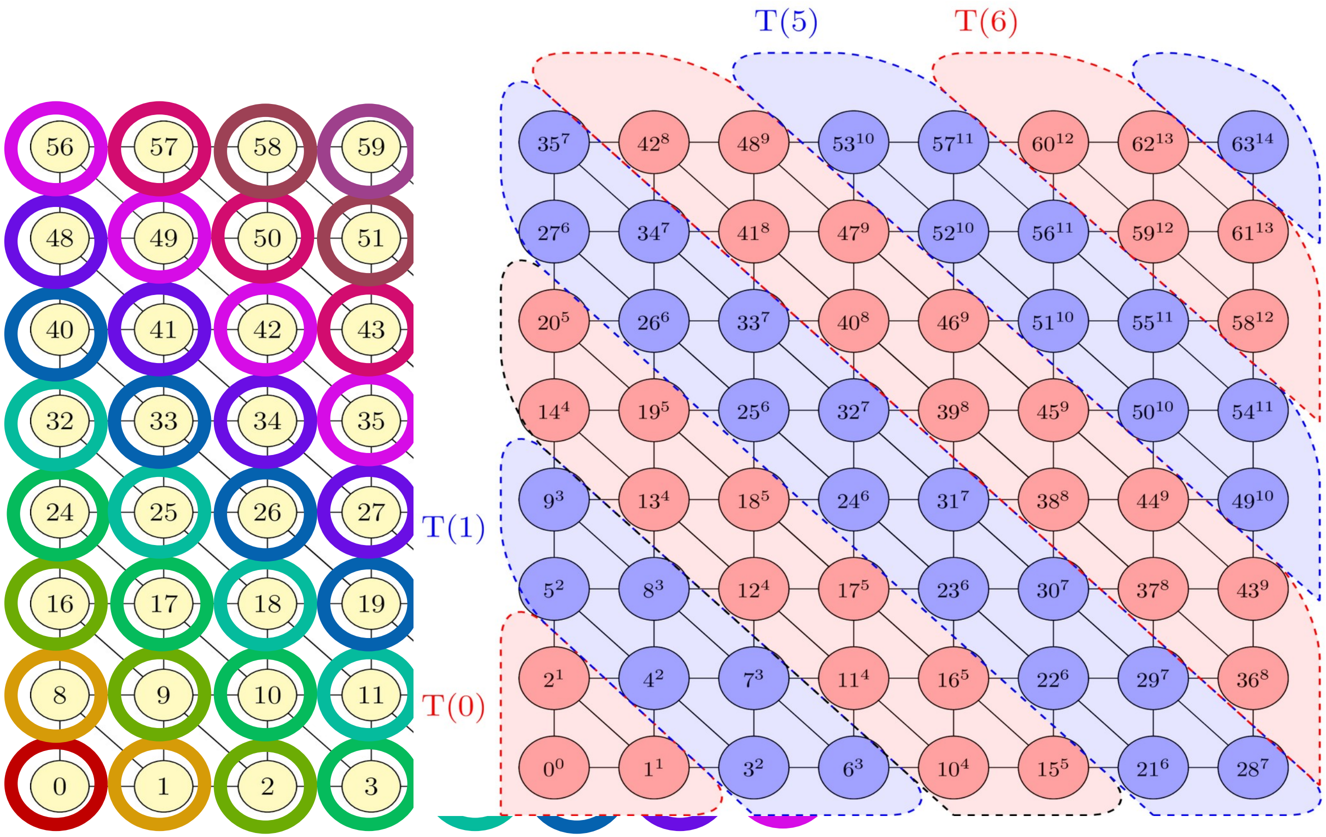
Example of 2D-7 Point stencil

RACE: Recursive Algebraic Coloring



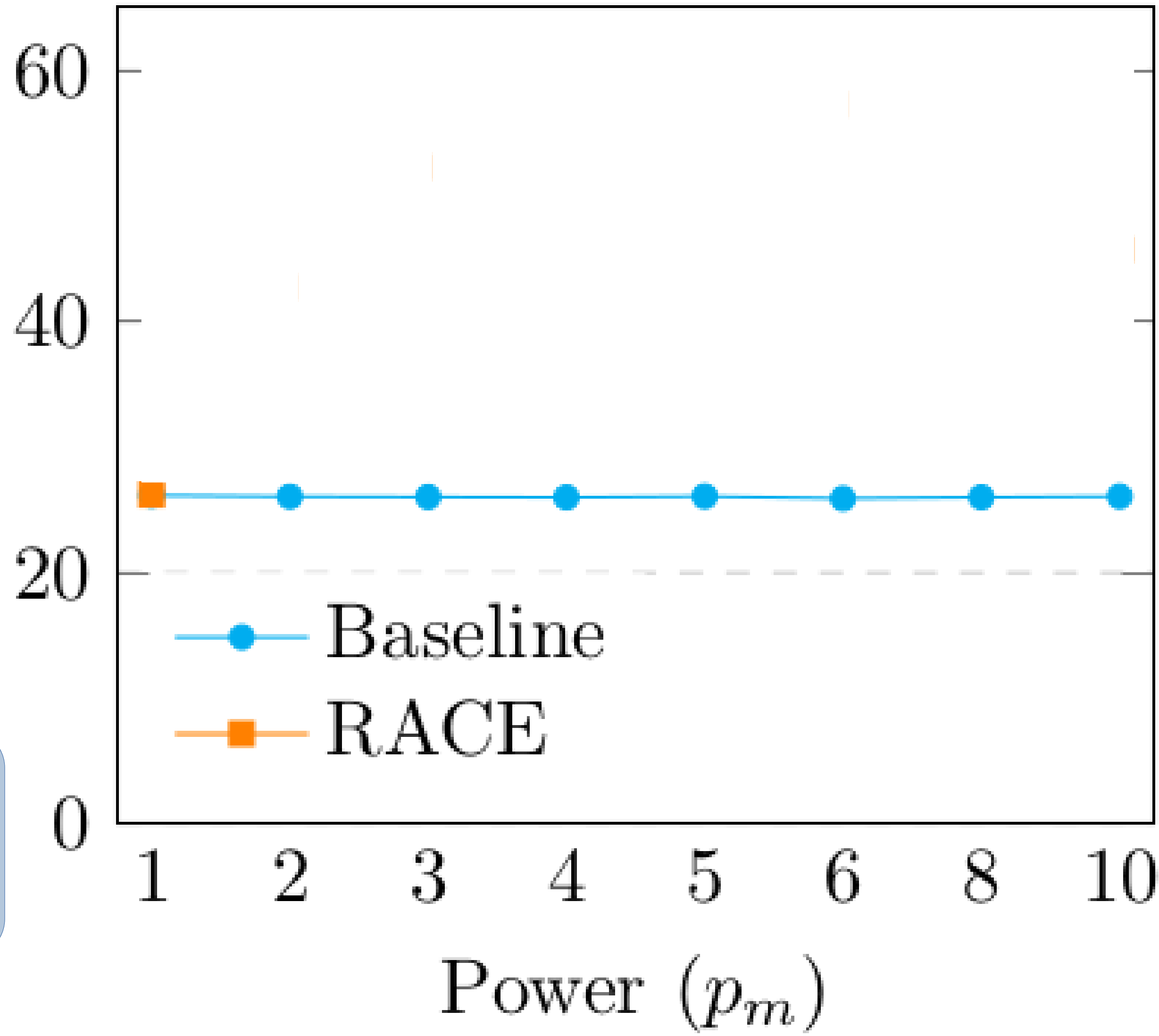
Example of 2D-7 Point stencil

RACE: Recursive Algebraic Coloring



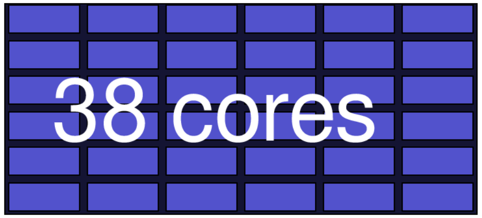
Example of 2D-7 Point stencil

RACE MPK Performance



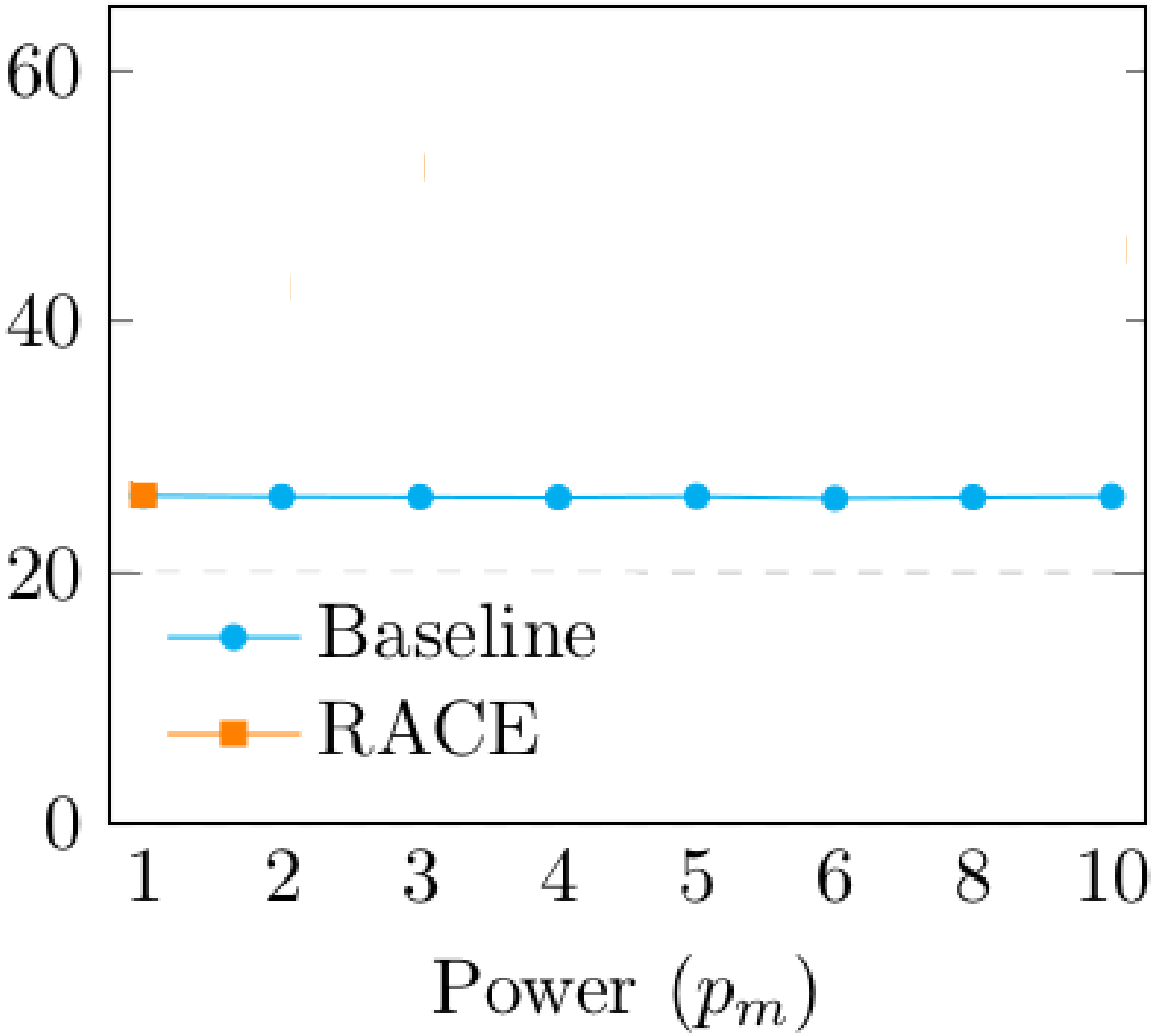
256 GB RAM
(146 GB/s)

RACE MPK Performance

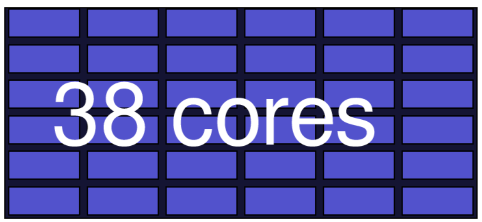


57MB L3 Cache
(420 GB/s)

256 GB RAM
(146 GB/s)



RACE MPK Performance



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256 GB RAM
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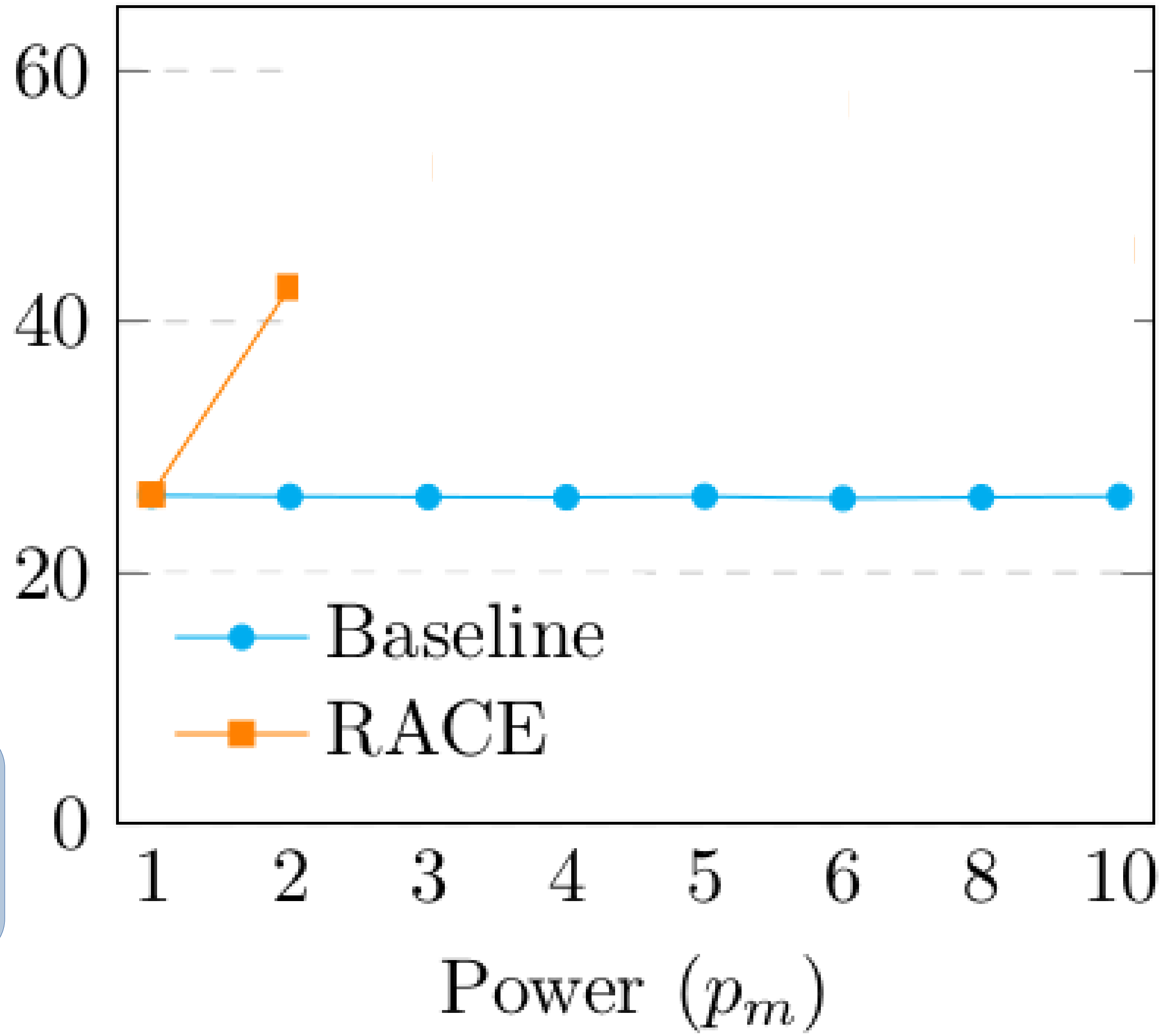
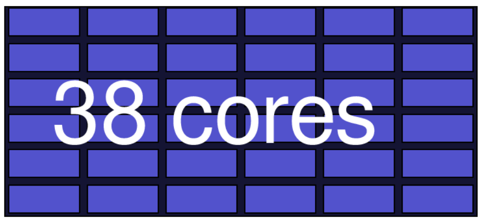


RACE MPK Performance



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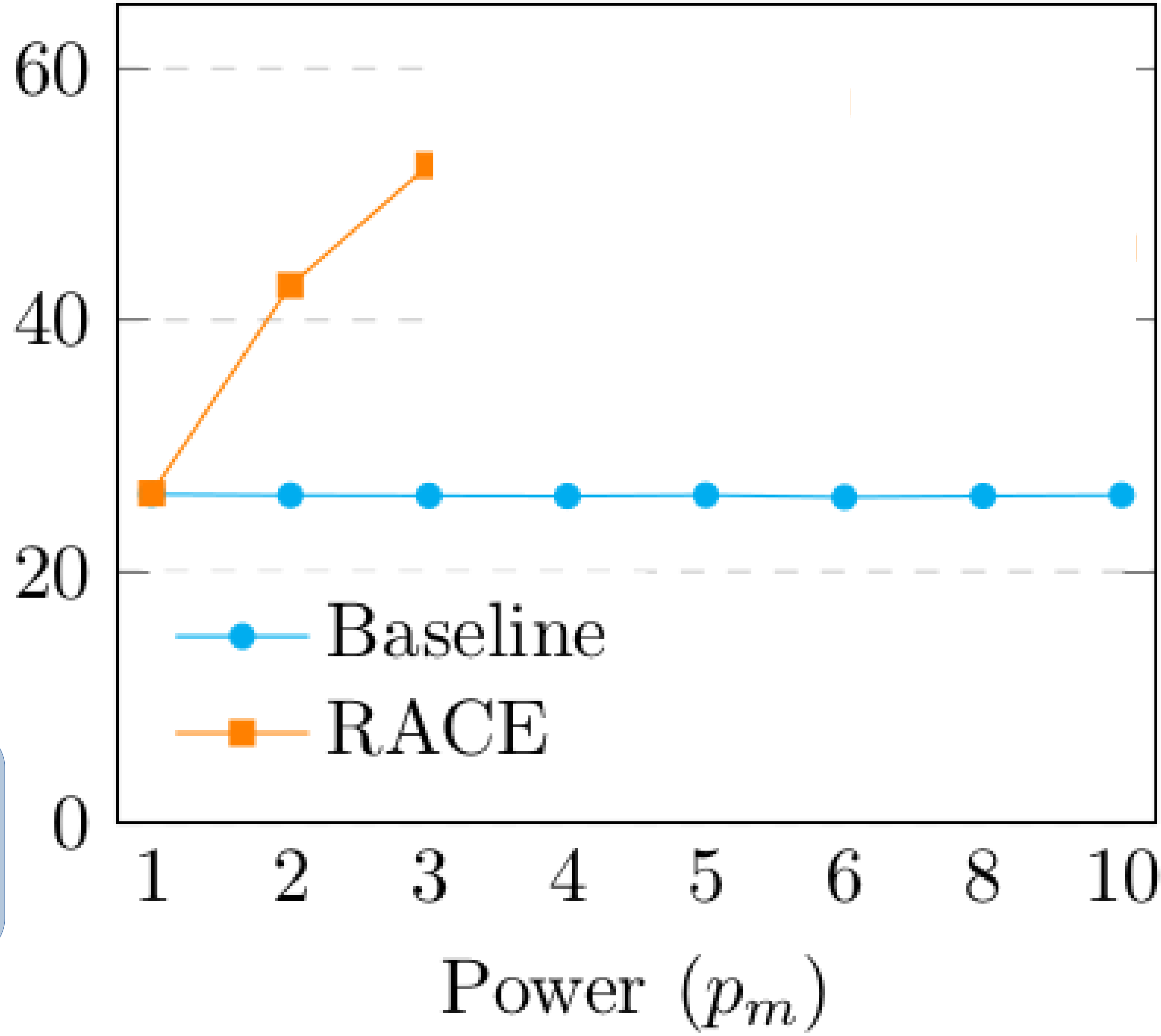
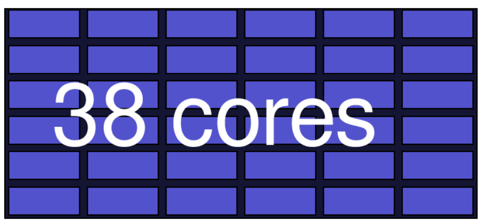
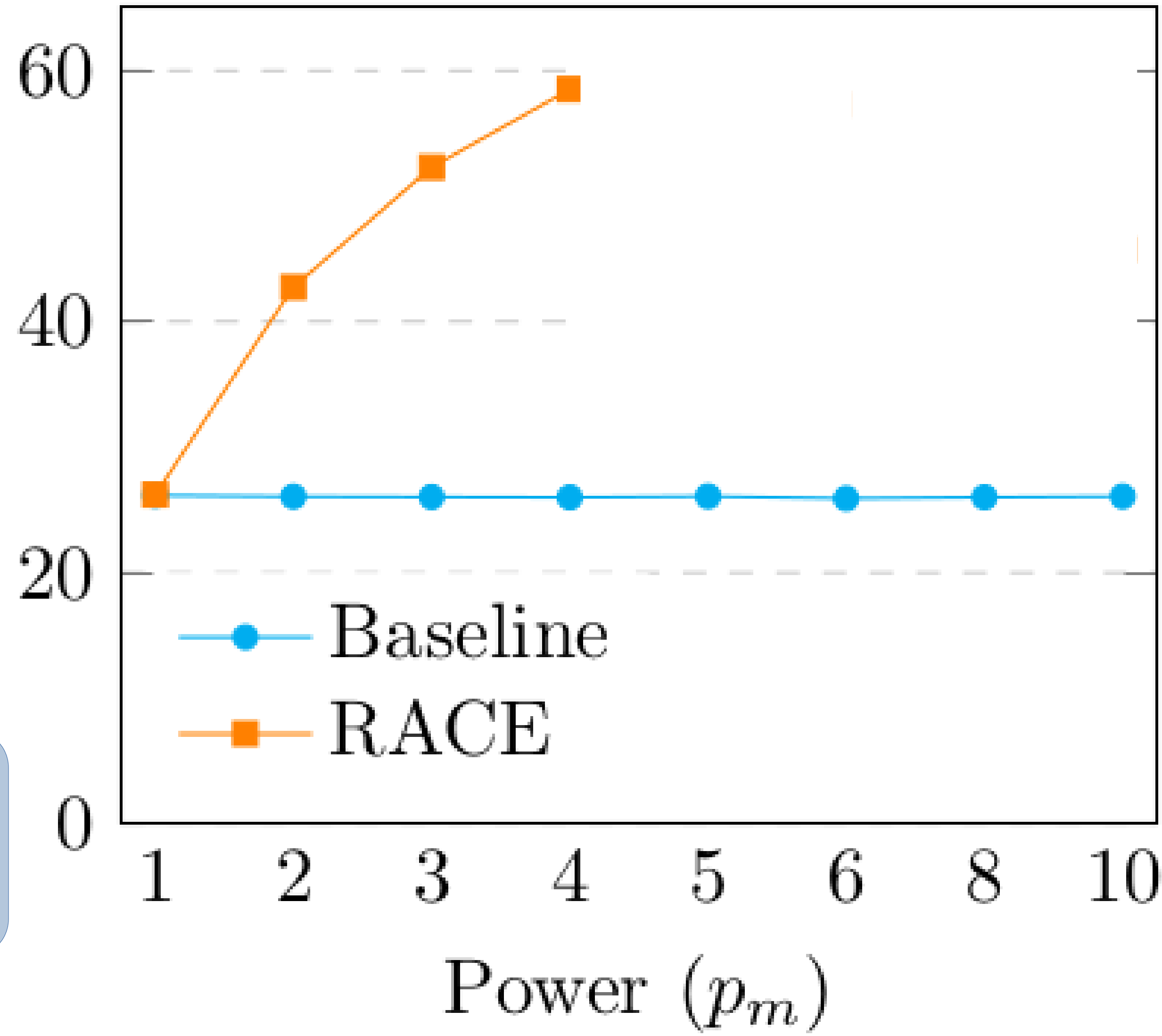


RACE MPK Performance

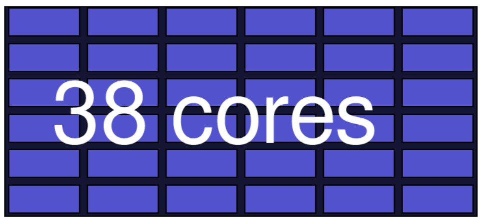


57MB L3 Cache
(420 GB/s)

256 GB RAM
(146 GB/s)

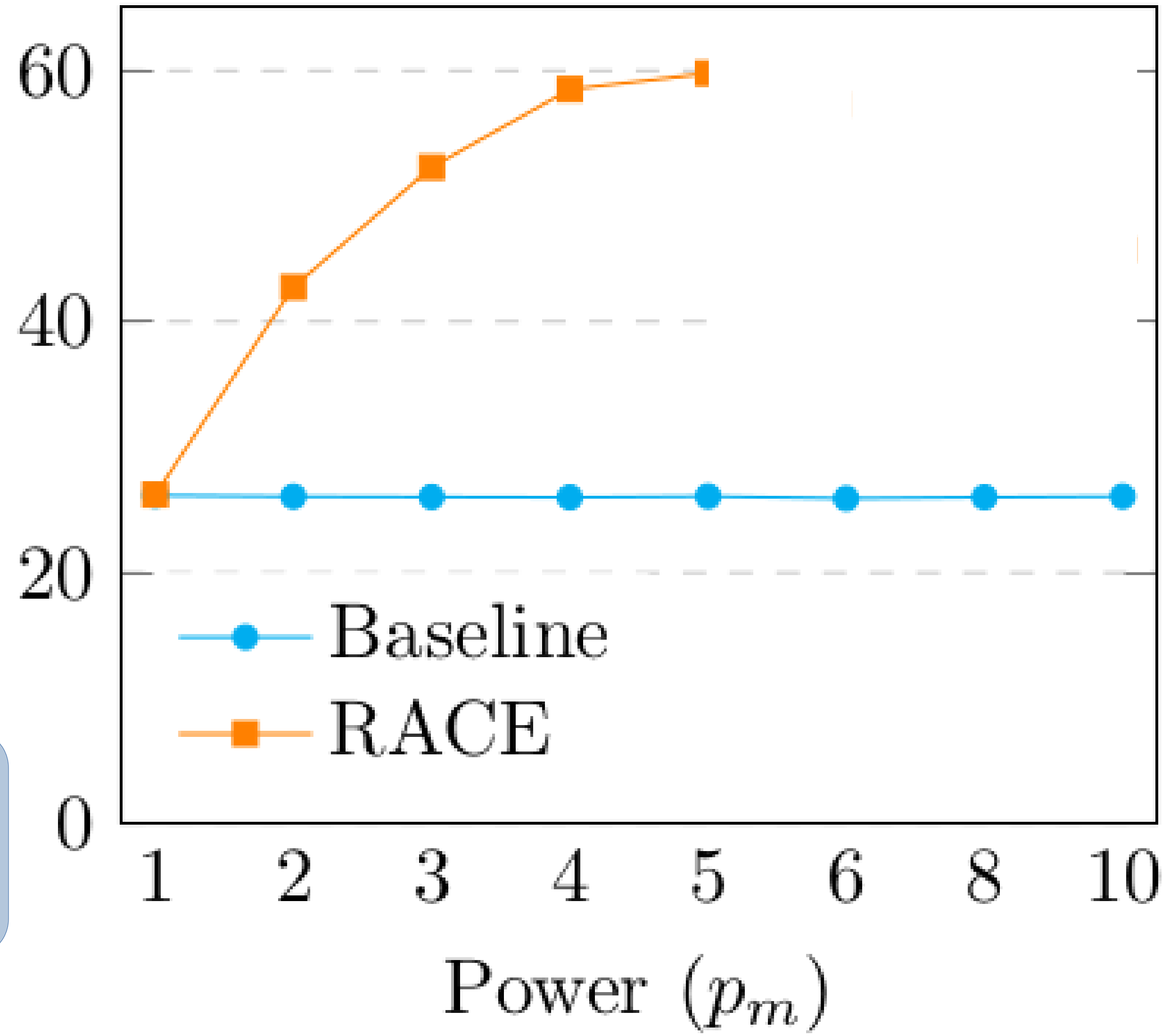


RACE MPK Performance



57MB L3 Cache
(420 GB/s)

256 GB RAM
(146 GB/s)

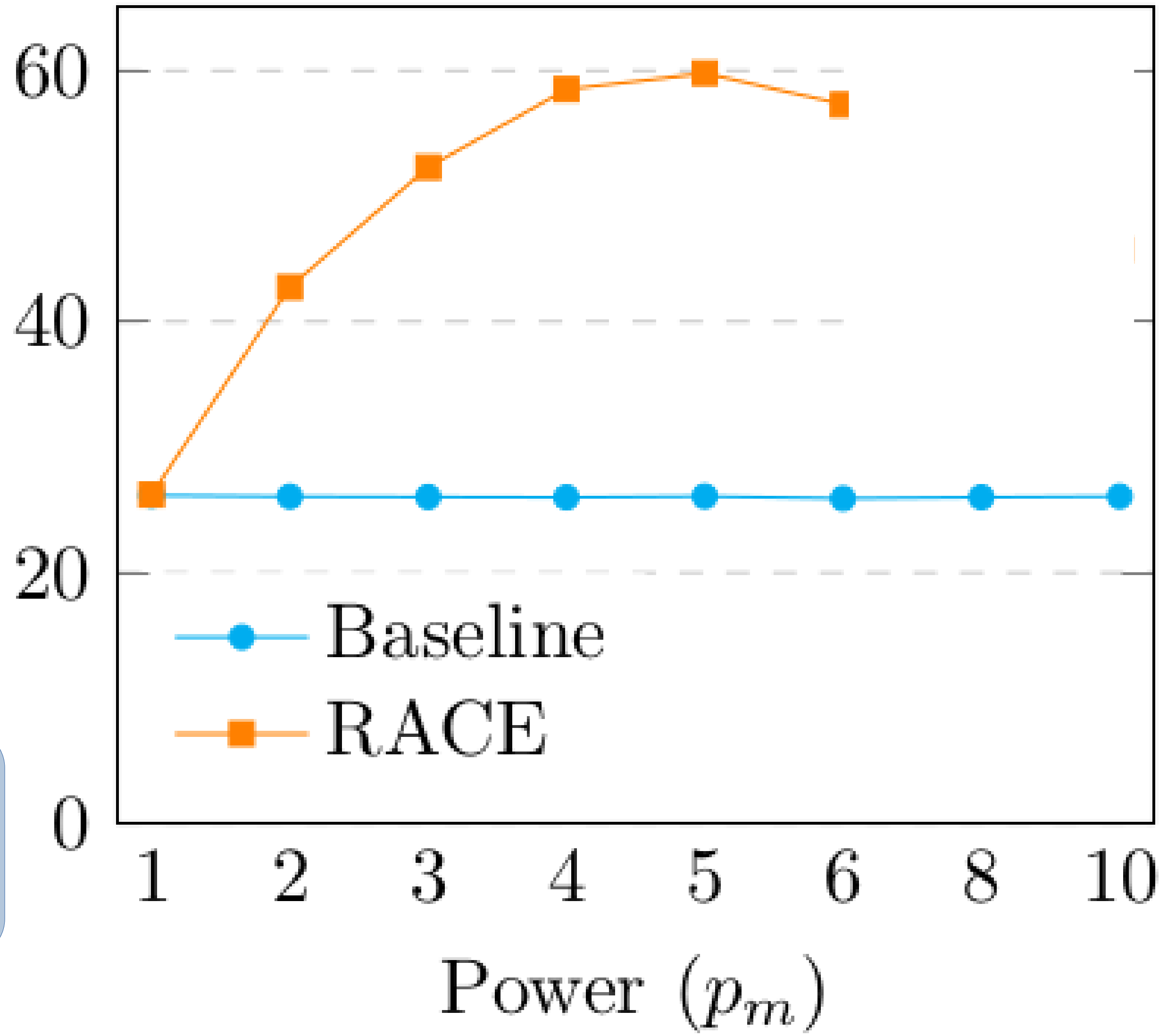


RACE MPK Performance

38 cores

57MB L3 Cache
(420 GB/s)

256 GB RAM
(146 GB/s)

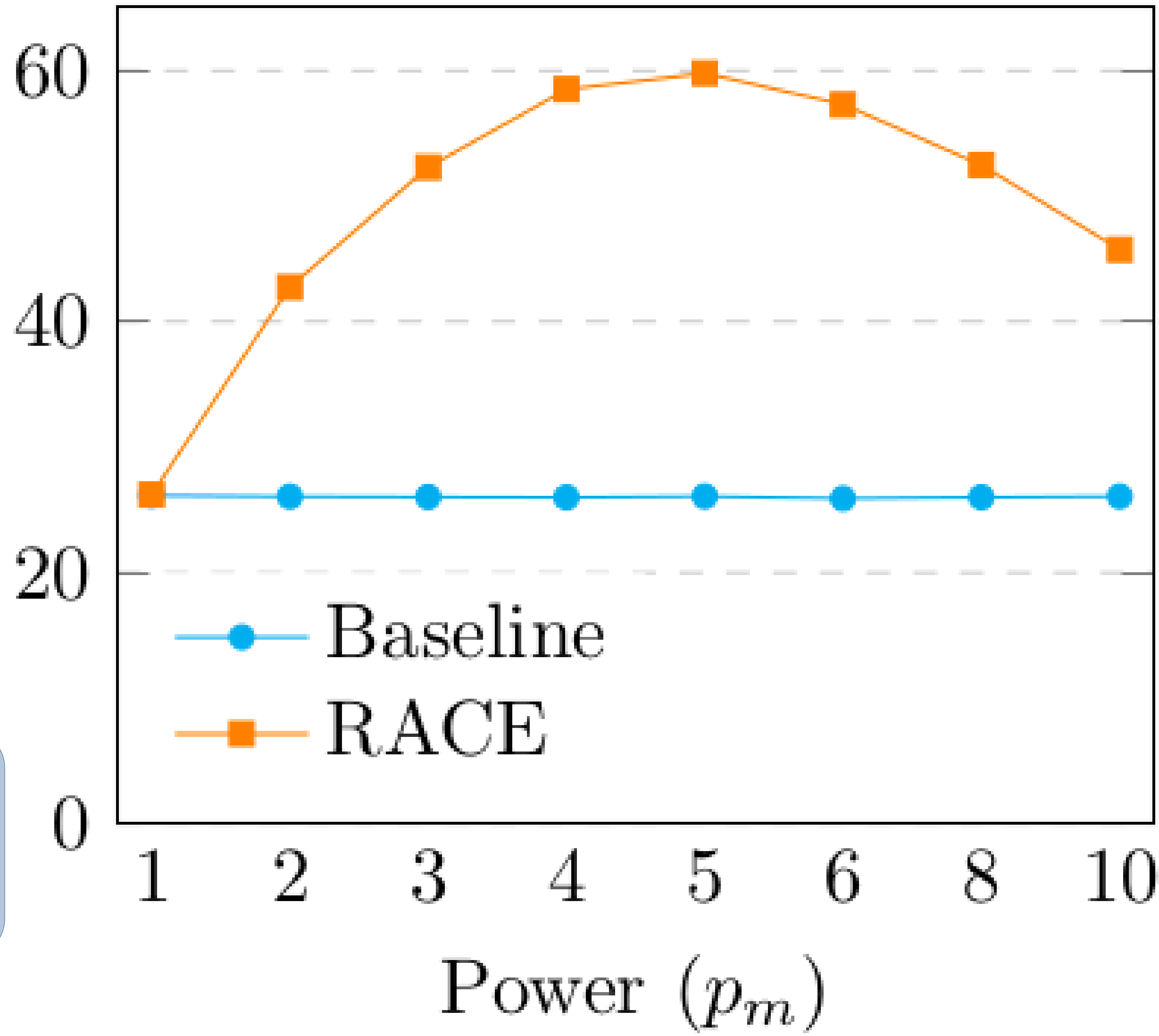


RACE MPK Performance

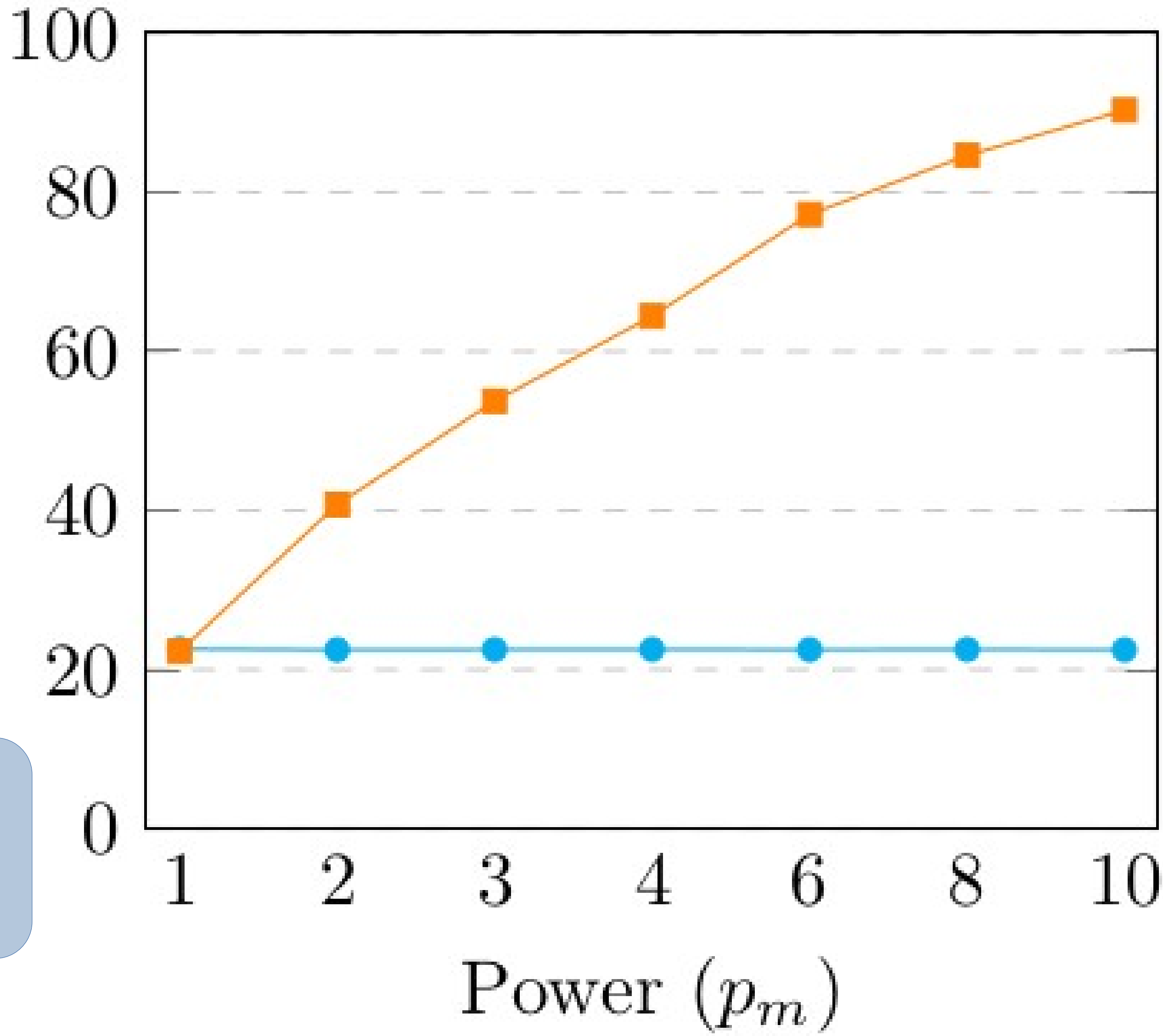
38 cores

57MB L3 Cache
(420 GB/s)

256 GB RAM
(146 GB/s)



RACE MPK Performance



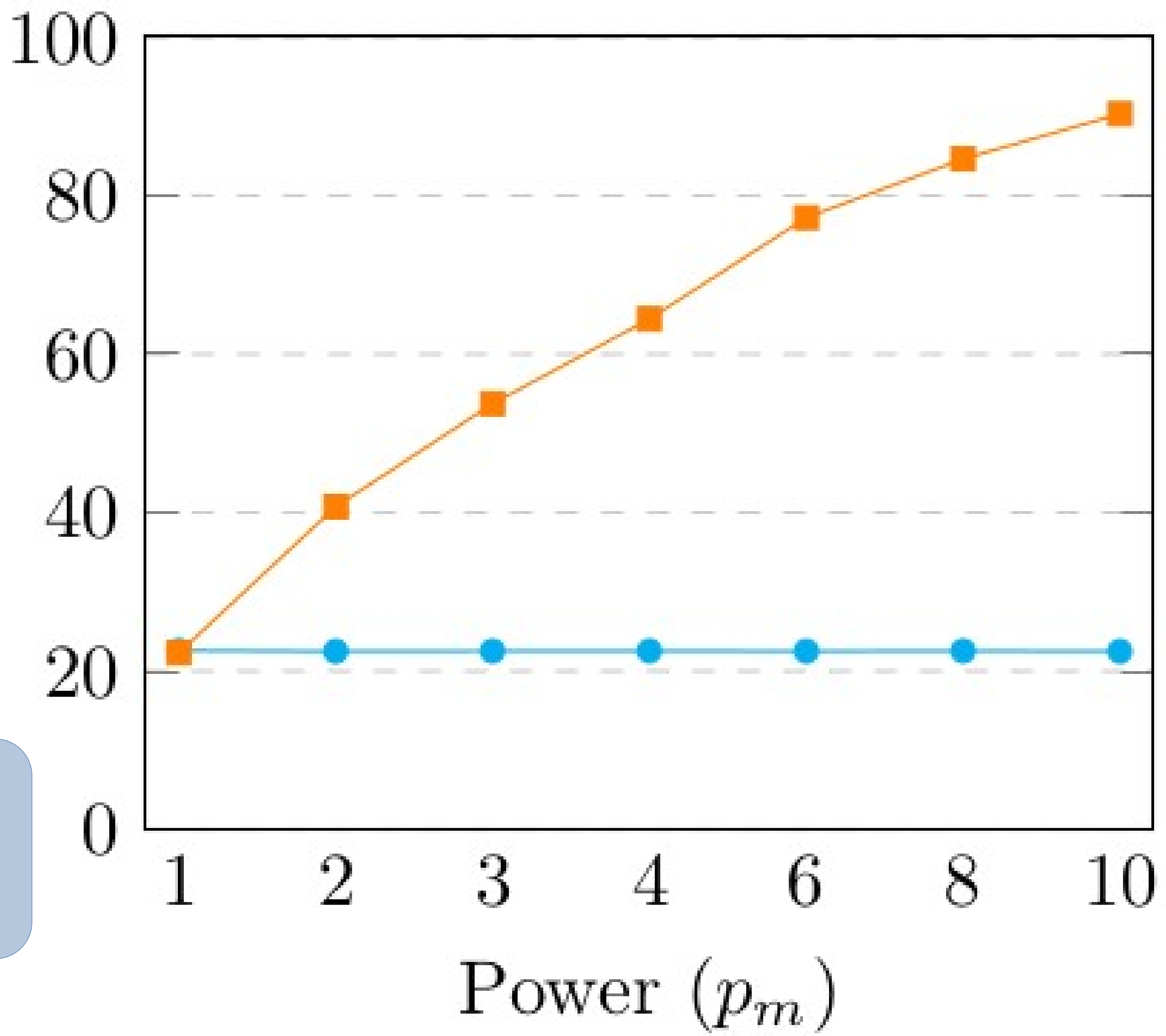
256 GB RAM
(146 GB/s)

RACE MPK Performance

64 cores

256 MB L3 Cache
(2600 G B/s)

256 GB RAM
(146 GB/s)



Example: Nalu-Wind Model

Preconditioner	Iter.	#effective SpMVs	Solve time (s)	Time (s)

Example: Nalu-Wind Model

Preconditioner	Iter.	#effective SpMVs	Solve time (s)	Time (s)
None	43	43	3.72	3.83

Example: Nalu-Wind Model

Preconditioner	Iter.	#effective SpMVs	Solve time (s)	Time (s)
None	43	43	3.72	3.83
Jacobi	24	24	1.73	1.83

Example: Nalu-Wind Model

Preconditioner	Iter.	#effective SpMVs	Solve time (s)	Time (s)
None	43	43	3.72	3.83
Jacobi	24	24	1.73	1.83
GS	13	26	1.73	1.83

Example: Nalu-Wind Model

Preconditioner	Iter.	#effective SpMVs	Solve time (s)	Time (s)
None	43	43	3.72	3.83
Jacobi	24	24	1.73	1.83
GS	13	26	1.73	1.83
Poly(5)	6	30	1.76	2.24

Example: Nalu-Wind Model

Preconditioner	Iter.	#effective SpMVs	Solve time (s)	Time (s)
None	43	43	3.72	3.83
Jacobi	24	24	1.73	1.83
GS	13	26	1.73	1.83
Poly(5)	6	30	1.76	2.24
RACE + Poly(5)	6	30	1.16	1.64

DELFT BLUE

Example: Nalu-Wind Model

Preconditioner	Iter.	#effective SpMVs	Solve time (s)	Time (s)
None	43	43	3.72	3.83
Jacobi	24	24	1.73	1.83
GS	13	26	1.73	1.83
Poly(5)	6	30	1.76	2.24
RACE + Poly(5)	6	30	1.16	1.64
Jacobi(5)	5	25	1.29	1.40

TU Delft

Example: Nalu-Wind Model

Preconditioner	Iter.	#effective SpMVs	Solve time (s)	Time (s)
None	43	43	3.72	3.83
Jacobi	24	24	1.73	1.83
GS	13	26	1.73	1.83
Poly(5)	6	30	1.76	2.24
RACE + Poly(5)	6	30	1.16	1.64
Jacobi(5)	5	25	1.29	1.40
RACE + Jacobi(5)	5	25	0.60	0.70

What else can we do with RACE?

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s-step
Krylov

What else can we do with RACE?

s-step Krylov

Approx. Triangu-lar solves

What else can we do with RACE?

s-step Krylov

Approx. Triangu-lar solves

Fancier Polynomial Precon-ditioners

What else can we do with RACE?

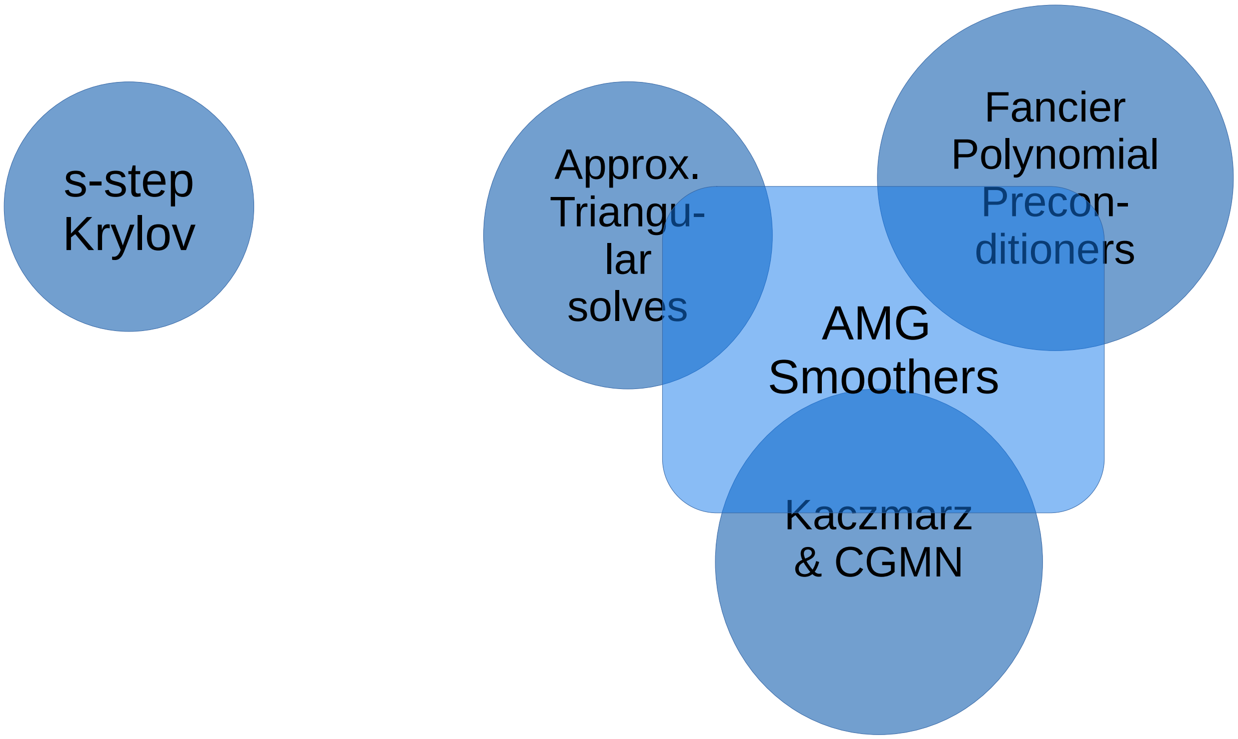
s-step Krylov

Approx. Triangu-lar solves

Fancier Polynomial Precon-ditioners

Kaczmarz & CGMN

What else can we do with RACE?



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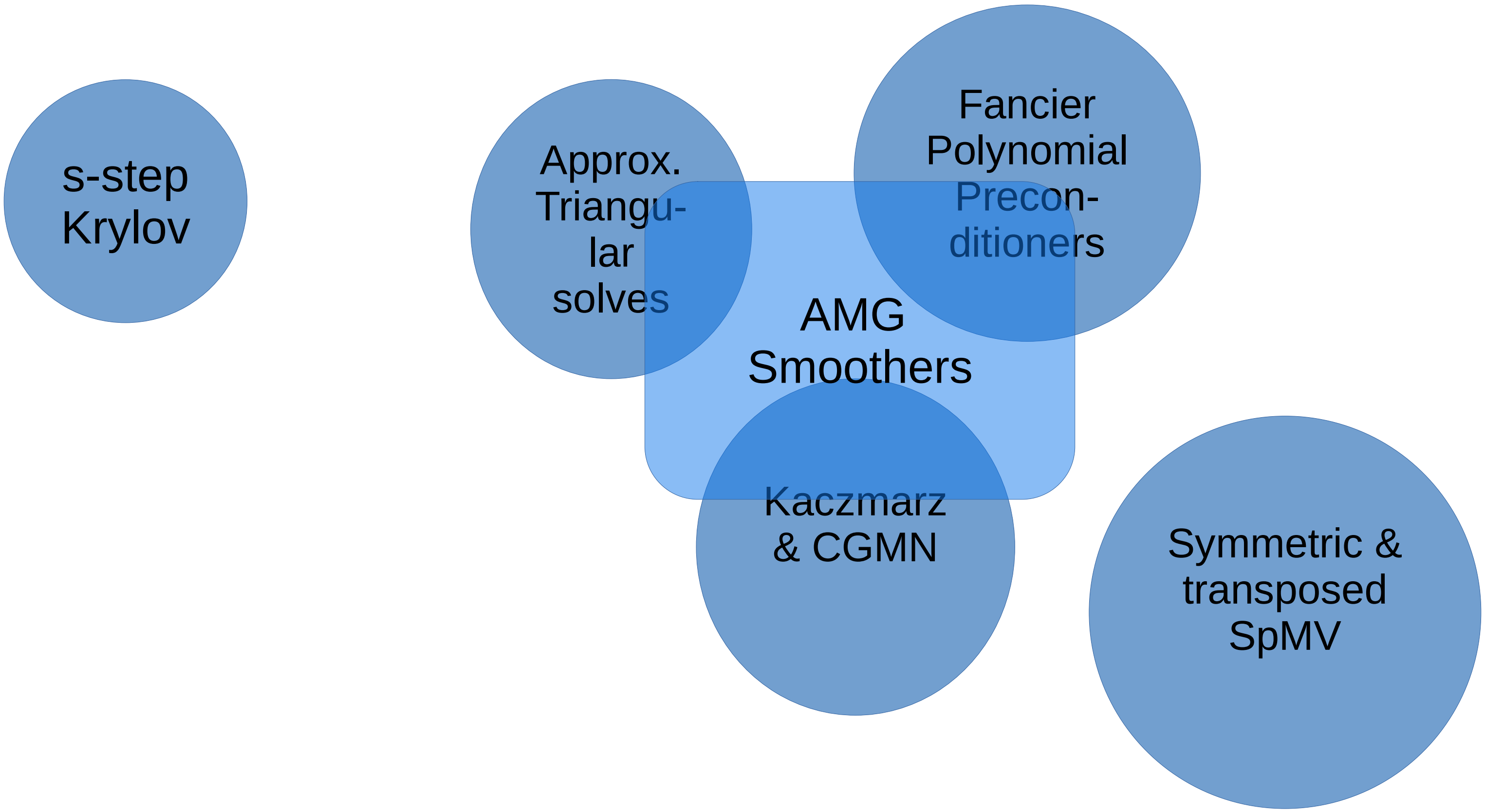
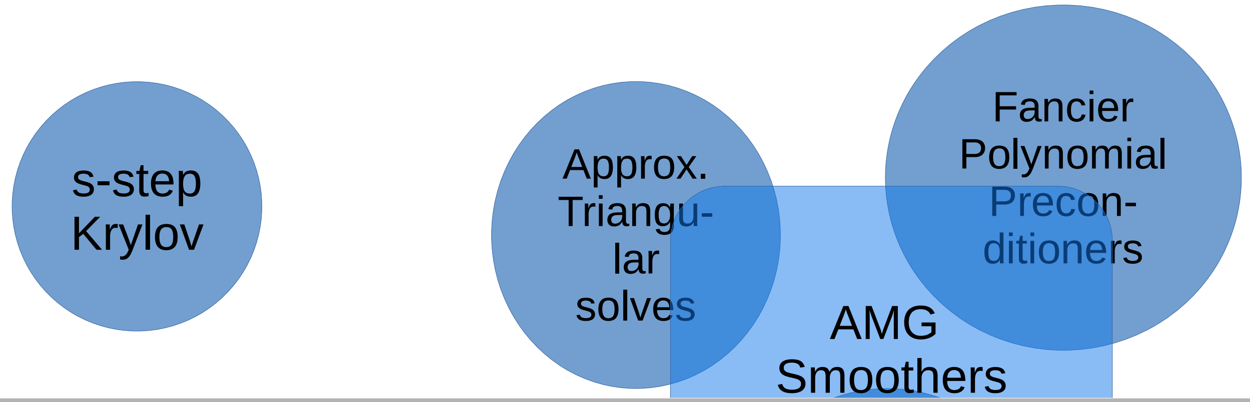


What else can we do with RACE?



Alappat et al.: A Recursive Algebraic Coloring Technique for Hardware-efficient Symmetric Sparse Matrix-vector Multiplication, ACM TOPC 7 (3), 2020

Alappat et al.: Level-based blocking for Sparse Matrices: Sparse Matrix-Power-Vector Multiplication. IEEE TPDS 34(2), 2023

Alappat et al.: Algebraic Temporal Blocking for Iterative Solvers on Multi-Core CPUs. To be submitted, will be on arXiv soon.

DCSE Summerschool next week:

Linear Algebra on High Performance Computers

Paolo Bientinesi
(Umeå University)

Gerhard Wellein
(U. Erlangen)

Laura Grigori
(EPFL)

Few places available:
https://www.aanmelder.nl/143287