

THE COMEDY CLUB OF HIGH-PERFORMANCE COMPUTING: LOW-RANK MATRIX APPROXIMATION TAKES THE STAGE!

Hatem Ltaief
Principal Research Scientist
Extreme Computing Research Center



NHR PerLab Online Seminar
May 16th 2023



Acknowledgments

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 - Cerebras: M. Jacquelin and L. Wilson

HPC Comedy Club



Intel #97



AMD #27



IBM/NVIDIA CPU/GPU #4



Fujitsu ARM A64FX #2

HPC Comedy Club



Intel #97



AMD #27



IBM/NVIDIA CPU/GPU #4



Fujitsu ARM A64FX #2

HPC-AI Comedy Club



Intel #97



AMD #27



IBM/NVIDIA CPU/GPU #4



Fujitsu ARM A64FX #2



جامعة الملك عبد الله
للعلوم والتقنية
King Abdullah University of
Science and Technology



SC22

Dallas, TX | hpc
accelerates.

SHAHEEN III KEY FACTS

Shaheen III supercomputer with
**25 HPE Cray EX
supercomputer cabinets**

Expected to deliver over
100 Pflops/s

20x faster than Shaheen II

4,608 CPU compute nodes, **AMD EPYC™
processors, "Genoa"**, amounting to
884,736 cores in the entire system

**2,800 NVIDIA Grace
Hopper Superchips,**
tightly coupled CPU/GPU accelerators

Cray Slingshot interconnect

Cray ClusterStor E1000 with
additional 50 PB of storage capacity

Operational by end of 2023

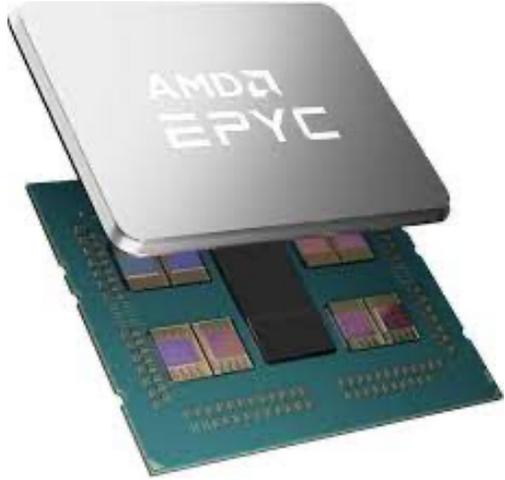
Accelerating research and developments
in **energy, environment, food,
water and healthcare**

2/3rds of KAUST faculty use
computational modeling and
simulation: **"to outcompute is
to outcompete"**



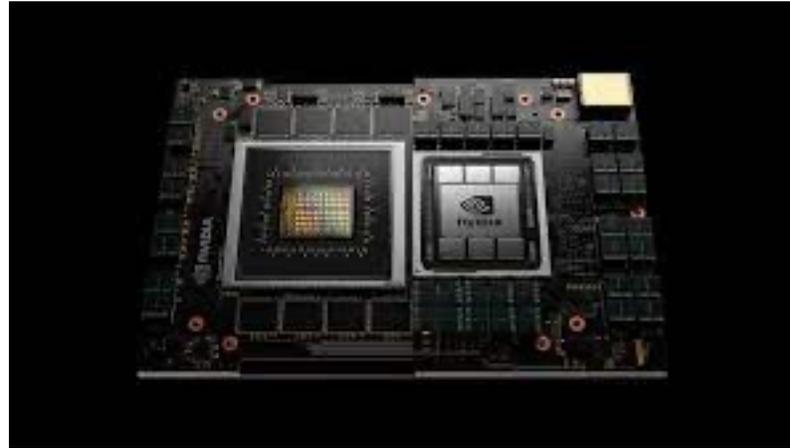
Hardware Landscape

7



AMD Epyc Genoa

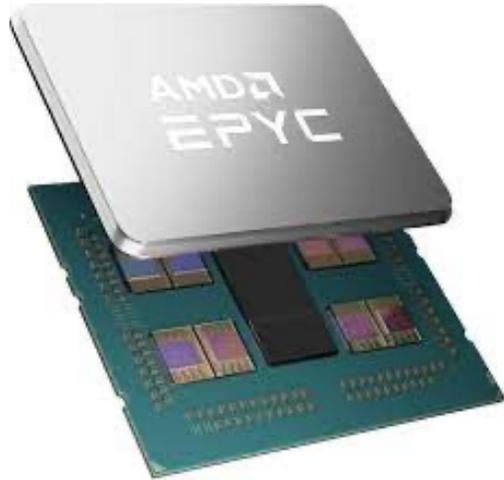
High cache capacity
High memory bandwidth
x86 programming env
Memory-bound workloads



NVIDIA Grace Hopper

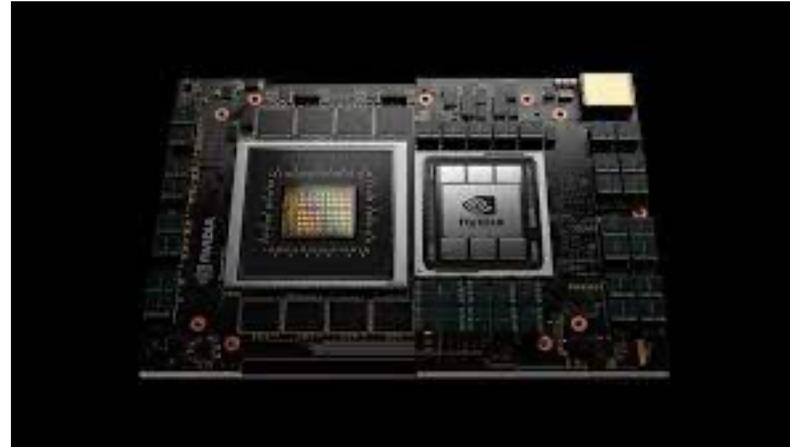
High speed CPU-GPU interconnect
Memory coherency
Support for mixed precisions
Compute-bound workloads

Hardware Landscape



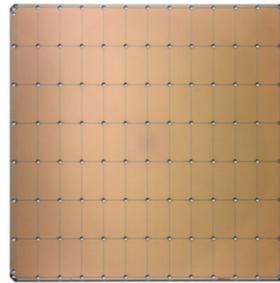
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Cerebras WSE-2
2.6 Trillion Transistors
46,225 mm² Silicon

Cerebras CS-2
Graphcore IPU

AI-focused chip
Flat memory hierarchy
High SRAM bandwidth
Inference

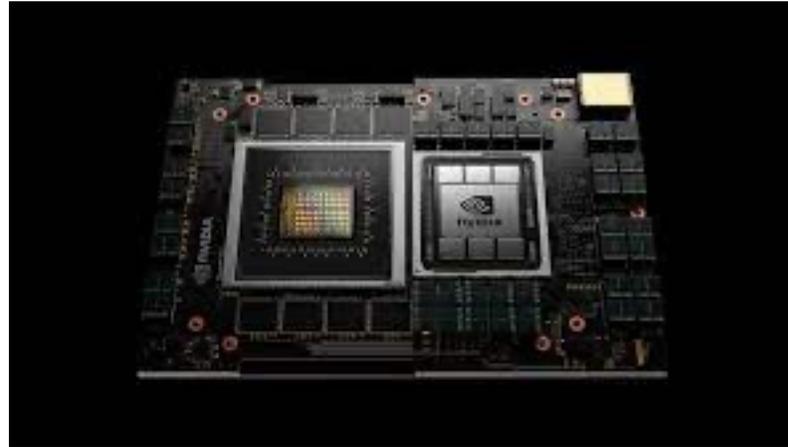
Hardware Landscape

9



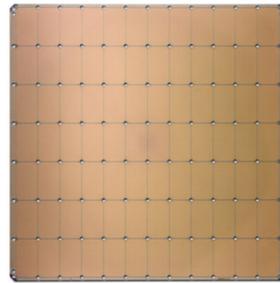
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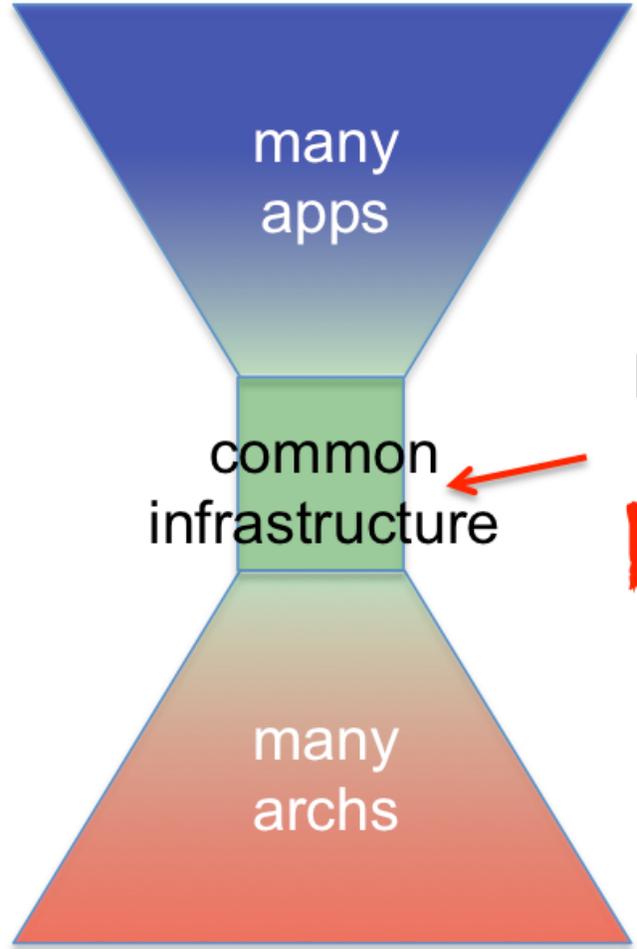
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Inference

How do we reconcile this hostile environment with HPC scientific applications?

Revisiting the Hourglass



$$A x = b$$

ECRC is right

here



@KAUST_ECRC



<https://www.facebook.com/ecrckaust>

Reshaping Linear Algebra for Massively Parallel Architectures

- Enhance user-productivity using layers of abstraction
- Expose parallelism using fine-grained computations
- Achieve scalability using asynchronous executions
- Exploit data sparsity using low-rank approximations
- Maintain code portability using standard basic blocks

Are you willing to redesign your algorithm?

One possible productive solution: **Matricization**

HPC Scientific Applications

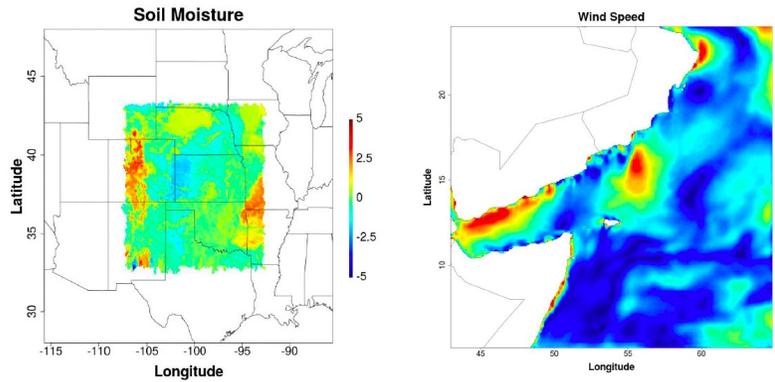
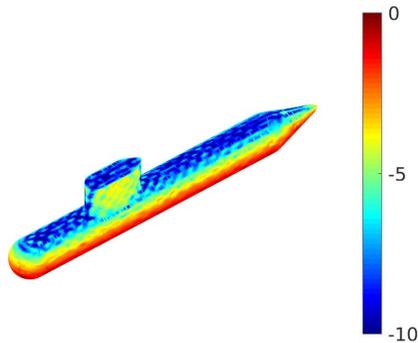
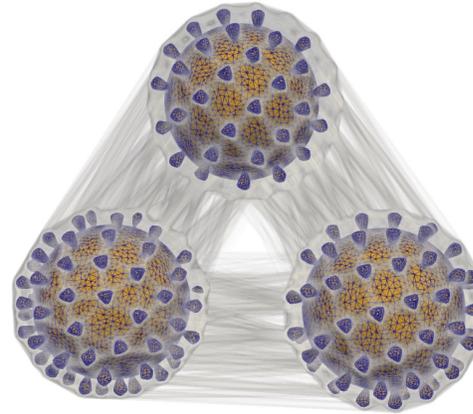


Fig. 4: **Left:** Soil moisture residuals at the topsoil of the Mississippi River basin. **Right:** Wind speed (m/s) in the Arabian Sea.

3D Geospatial Statistics



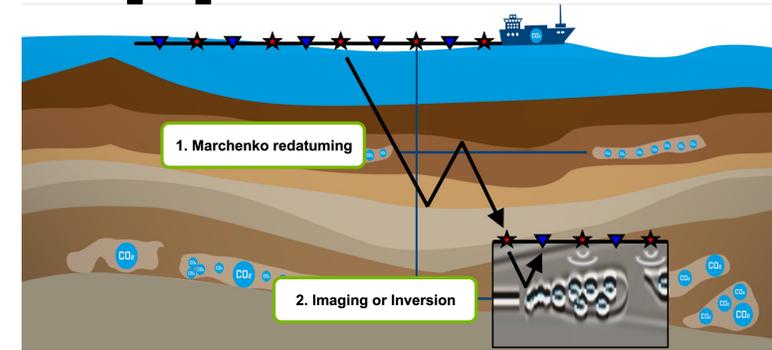
3D Computational Electromagnetics



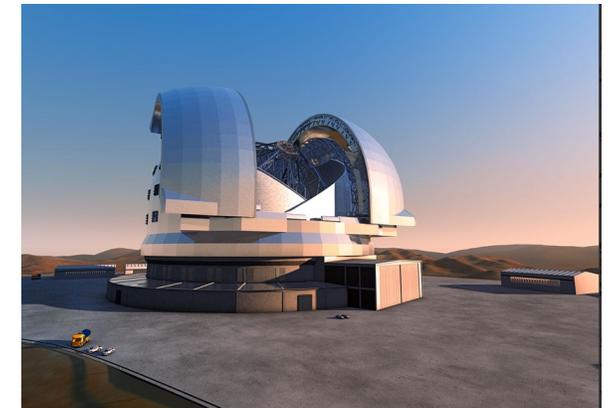
3D Mesh Deformations



Wireless Communications



Seismic Imaging



Computational Astronomy

HPC Scientific Applications

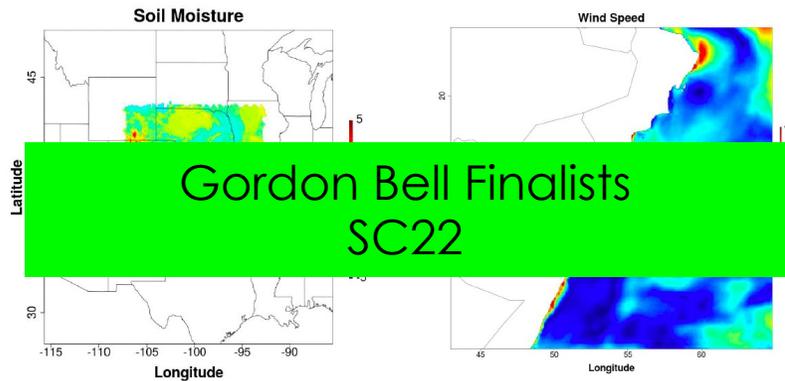
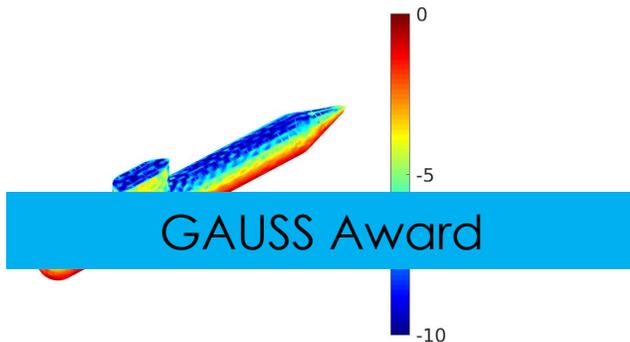
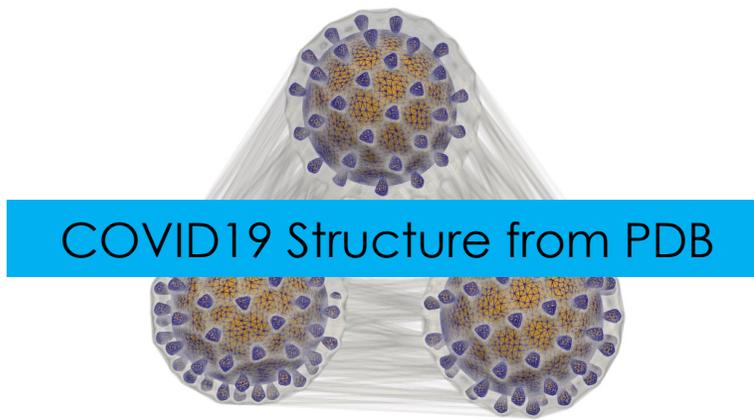


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3D Geospatial Statistics



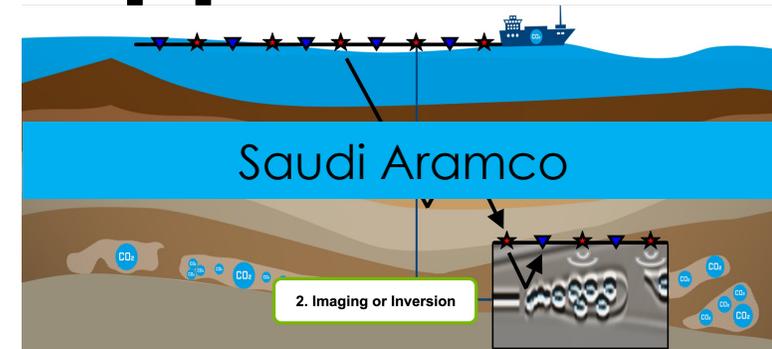
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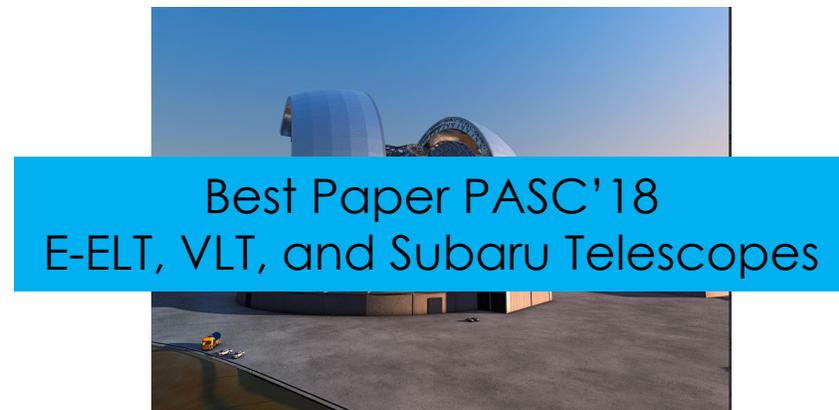
3D Mesh Deformations



Wireless Communications

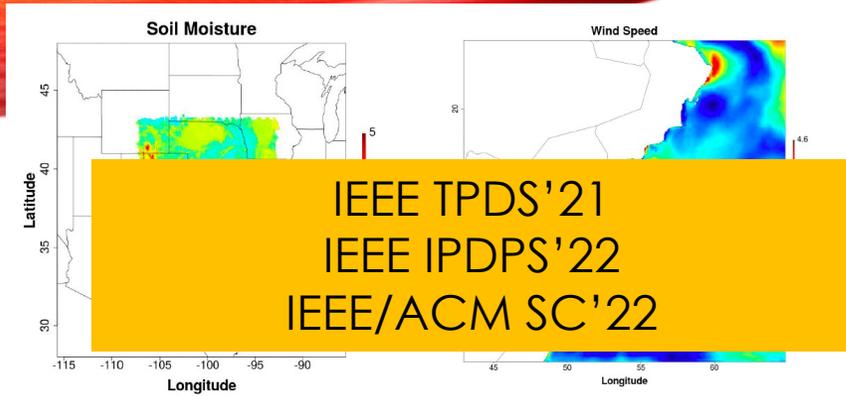


Seismic Imaging



Computational Astronomy

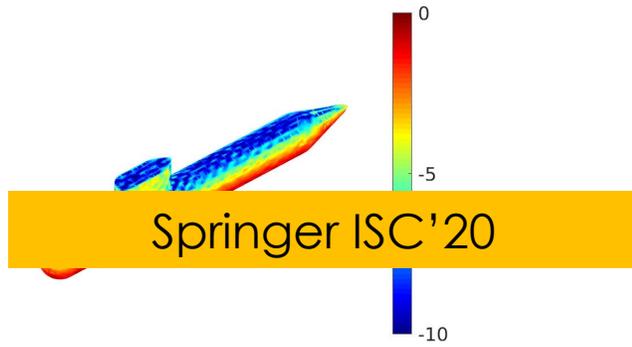
HPC Scientific Applications



IEEE TPDS'21
IEEE IPDPS'22
IEEE/ACM SC'22

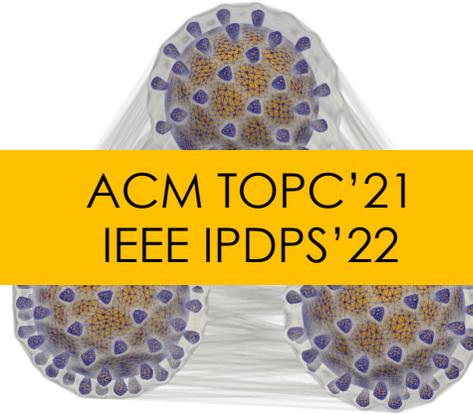
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3D Geospatial Statistics



Springer ISC'20

3D Computational Electromagnetics



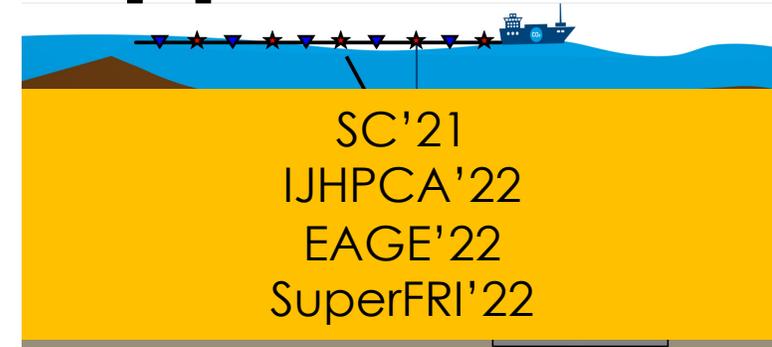
ACM TOPC'21
IEEE IPDPS'22

3D Mesh Deformations



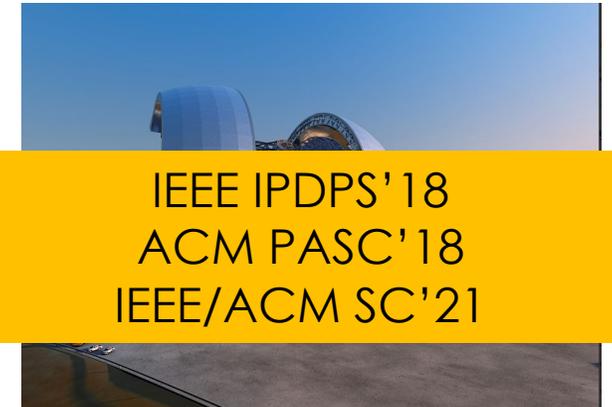
IEEE IPDPS'23
Springer ISC'23

Wireless Communications



SC'21
IJHPCA'22
EAGE'22
SuperFRI'22

Seismic Imaging



IEEE IPDPS'18
ACM PASC'18
IEEE/ACM SC'21

Computational Astronomy

HPC Scientific Applications

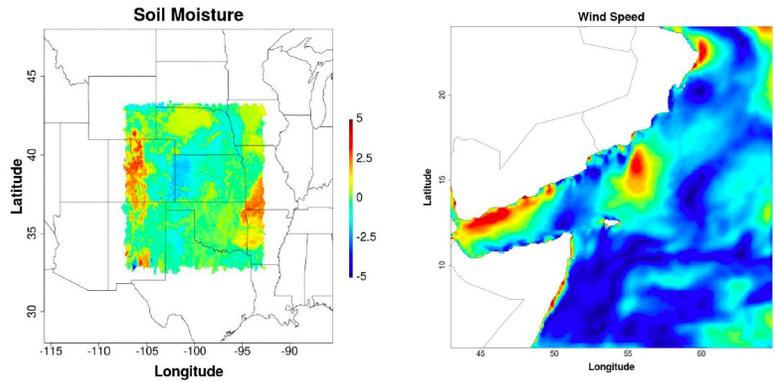
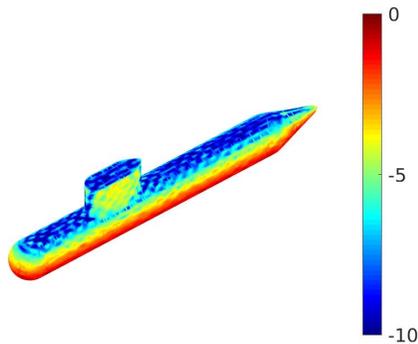
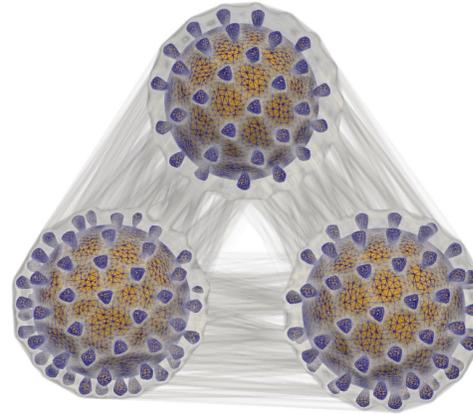


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3D Geospatial Statistics



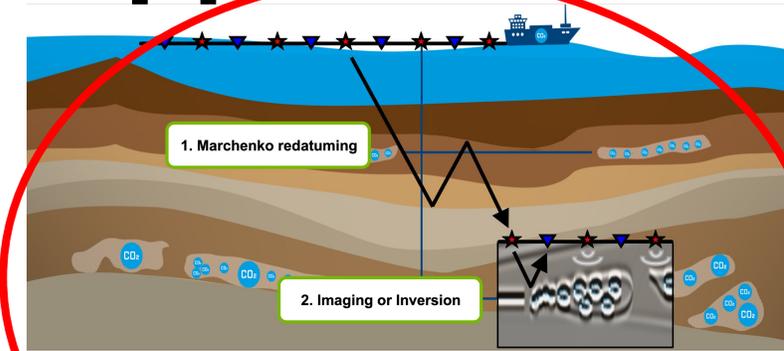
3D Computational Electromagnetics



3D Mesh Deformations



Wireless Communications



Seismic Imaging



Computational Astronomy

HPC Scientific Applications

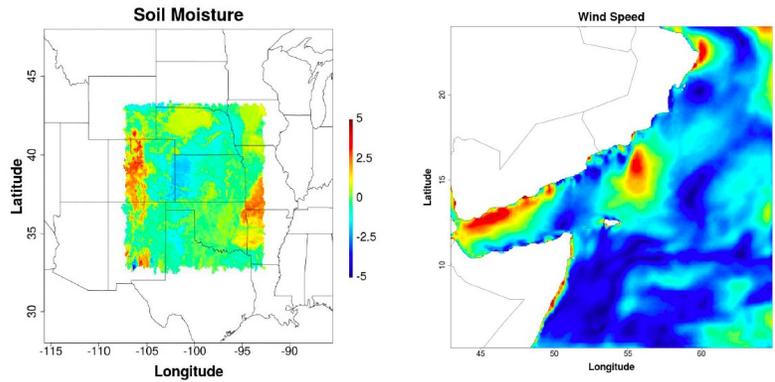
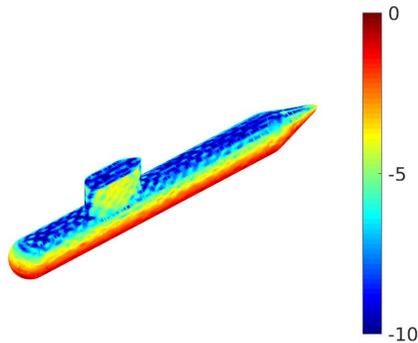
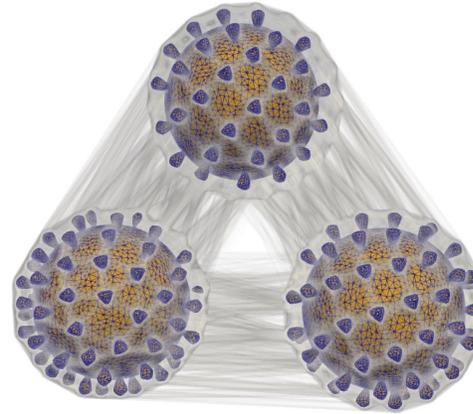


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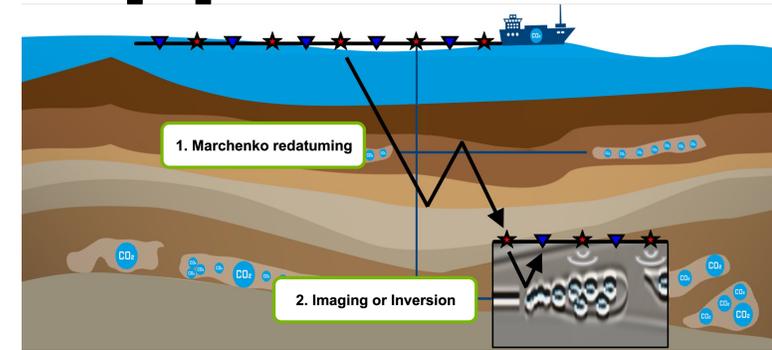
3D Computational Electromagnetics



3D Mesh Deformations



Wireless Communications



Seismic Imaging



Computational Astronomy

Supporting Several Major Ground-Based Telescopes



THE VERY LARGE TELESCOPE



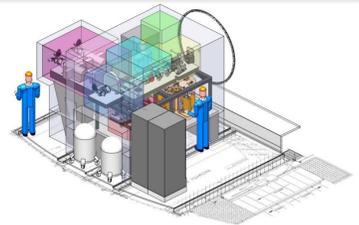
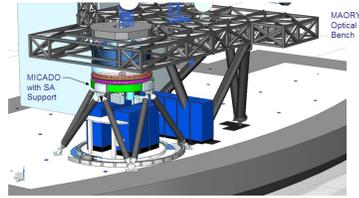
THE SUBARU TELESCOPE



THE EUROPEAN EXTREMELY LARGE TELESCOPE

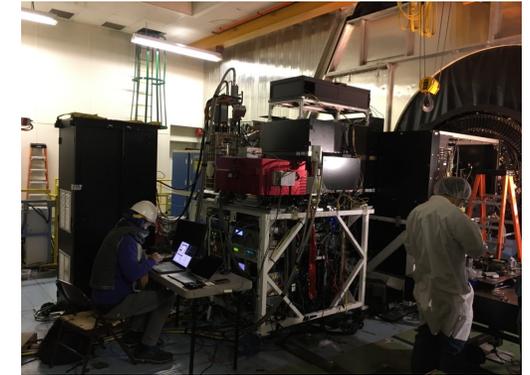
Supporting Several Major Ground-Based Telescopes

MAVIS
MCAO ASSISTED VISIBLE
IMAGER AND SPECTROGRAPH



THE VERY LARGE TELESCOPE

SCEXAO
THE SUBARU
CORONOGRAPHIC
EXTREME AO

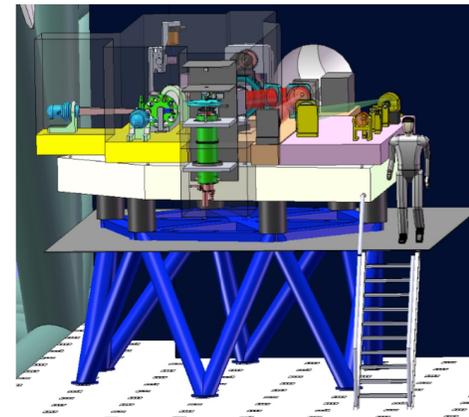


THE SUBARU TELESCOPE

EPICS
EXOPLANET IMAGING CAMERA
AND SPECTROGRAPH

MAORY
MULTI-CONJUGATE
ADAPTIVE OPTICS RELAY

MICADO
MULTI-ADAPTIVE OPTICS IMAGING
CAMERA FOR DEEP OBSERVATIONS



THE EUROPEAN EXTREMELY LARGE TELESCOPE

The Atmospheric Turbulence



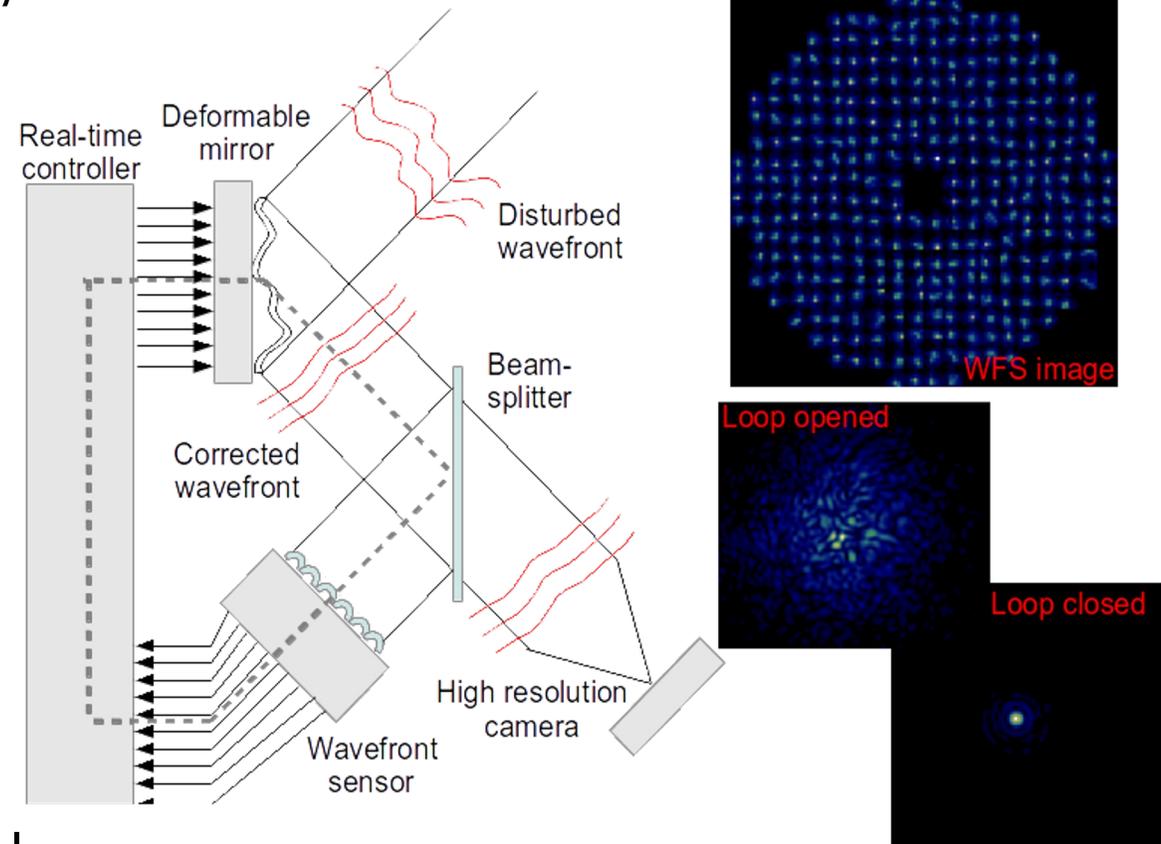
The sun observed with a compact camera

- Disturbs the trajectory of light rays
- Reduces astronomical images quality

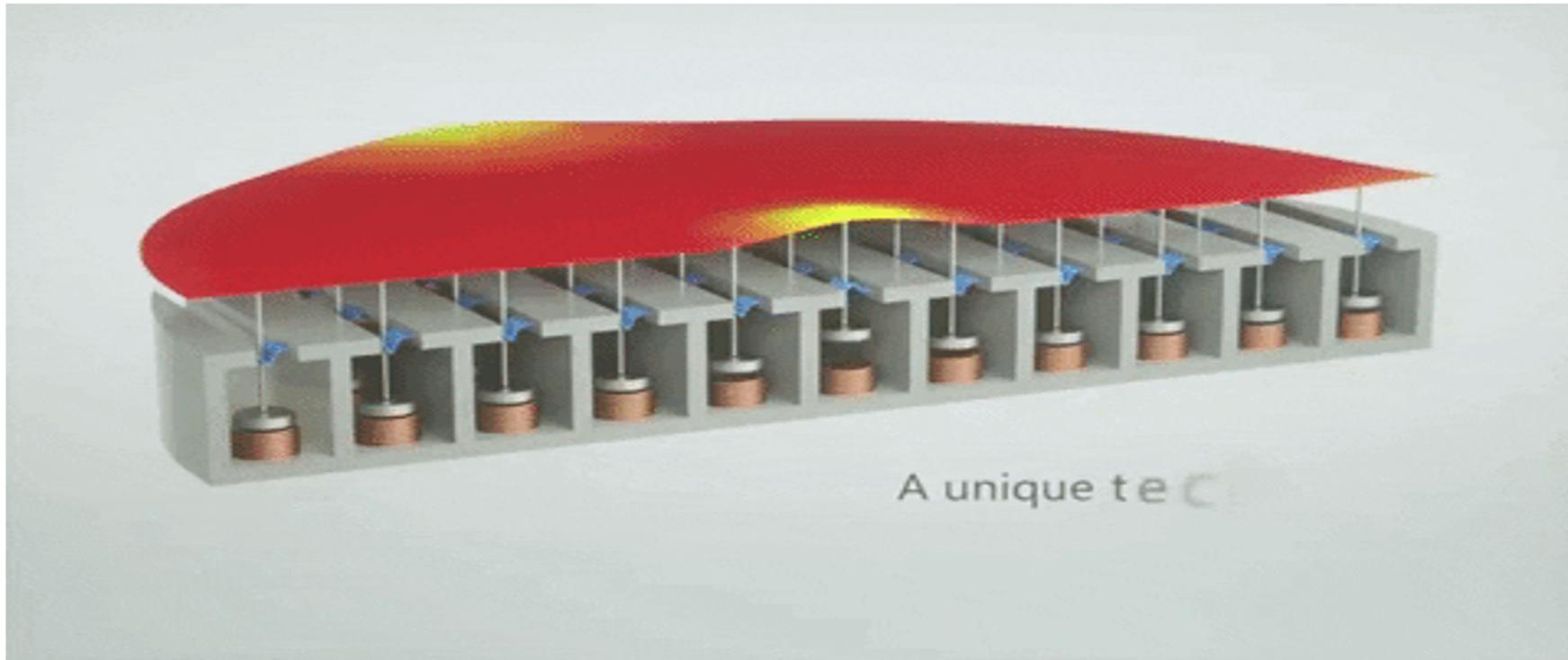
Adaptive Optics for Giant Telescopes

Control in real-time the shape of the incoming wavefront

- **Sensors are cameras** equipped with an optical device (lenslet array, pyramidal prism, etc...)
- **Deformable mirrors** to compensate for wavefront distortions
- **Typical rate of operation is 1 kHz**
- Compute **pipeline latency below 1 millisecond**
- **Stable time-to-solution** is critical to ensure stable operations (jitter of the order of 10s of μ s)
- **Matrix-Vector Multiplication (MVM)** is the most critical computational kernel



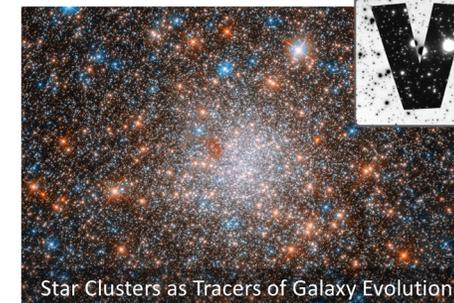
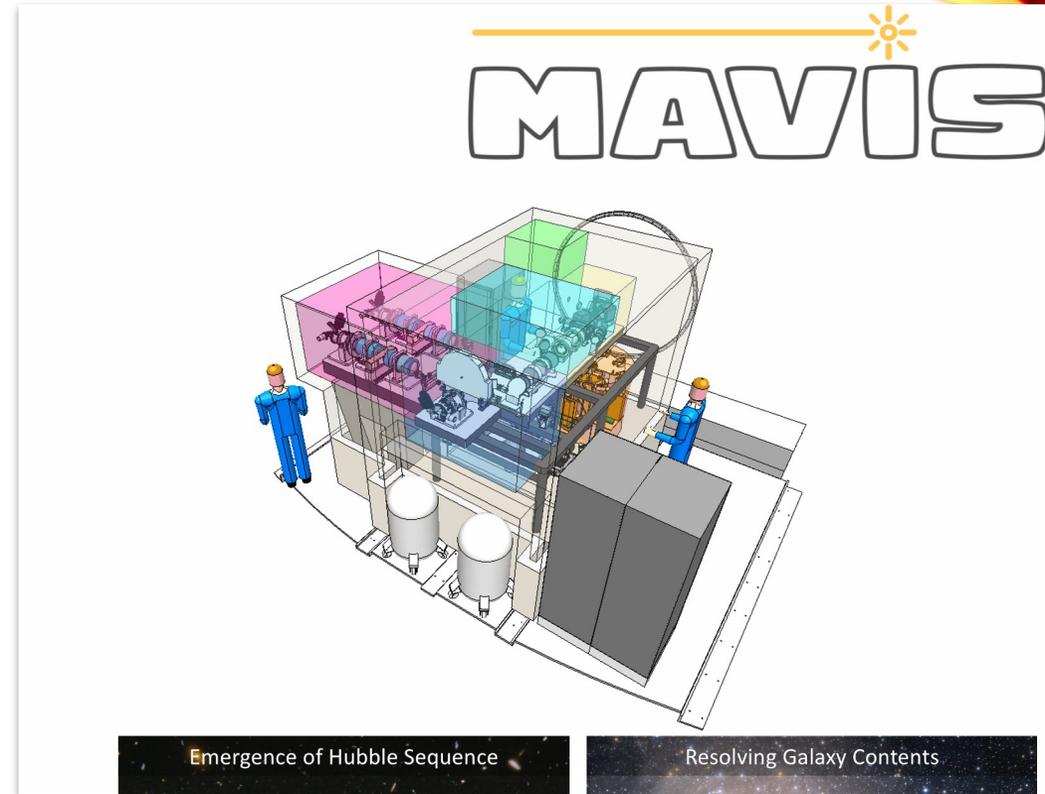
One of The Key Hardware Components: The Deformable Mirrors



MAVIS in a nutshell

Flagship 3rd-generation instrument for the Very Large Telescope

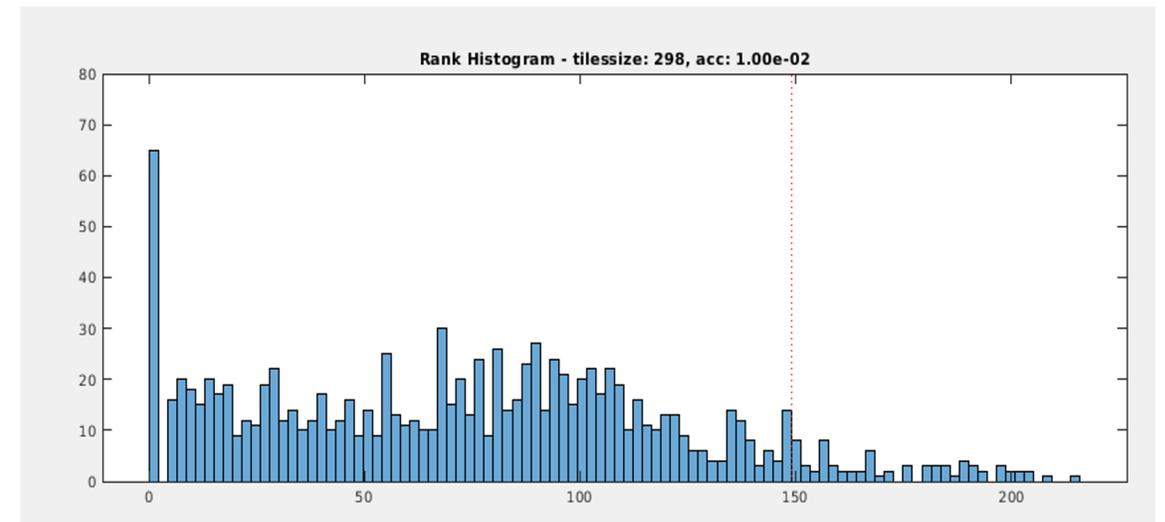
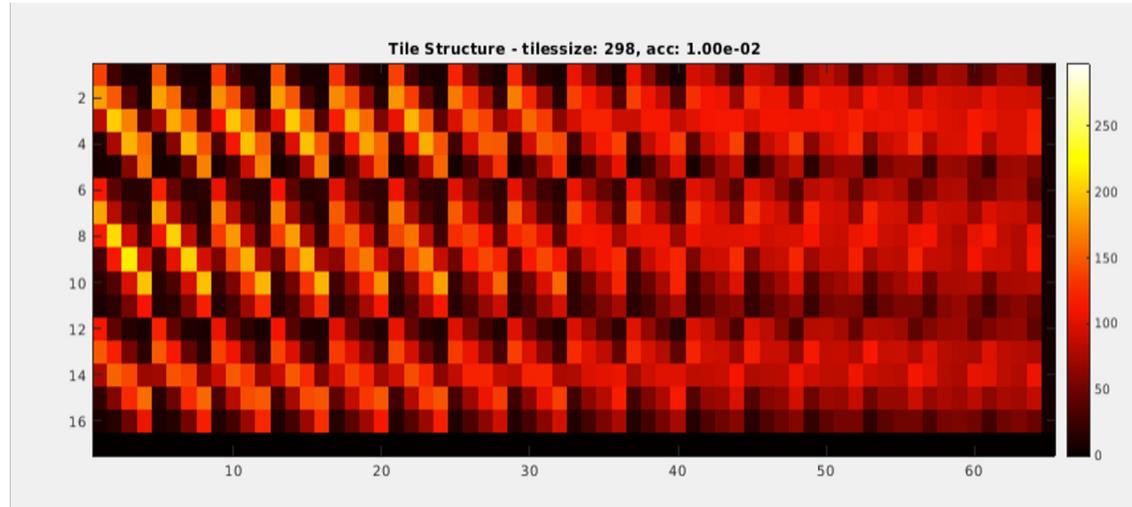
- Imager & Spectrograph fed by **Multi-Conjugate AO**
- **Scaling up** the whole AO concept:
 - More actuators
 - Faster control system
 - Exquisite calibrations
- **Fast-track** project:
 - First-light by 2026
- **Deeper & Sharper** than any space-based instrument



Rank Analysis of the Tomographic Reconstructor

Splitting the matrix into tiles and looking at ranks

- Tiles size aligned with system parameters
- Data sparse, opportunity for low-rank matrix approximations

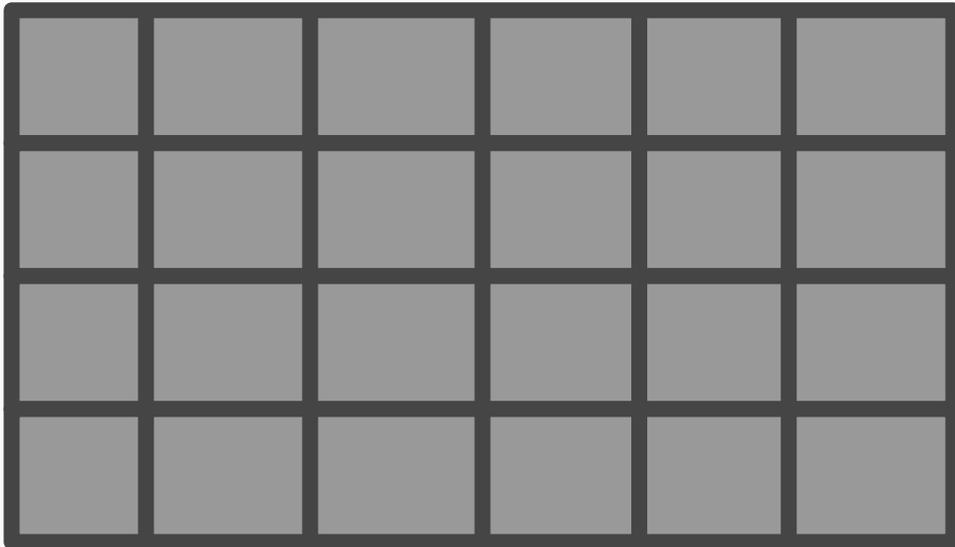


TLR-MVM

**Tile Dense
Matrix-Vector Multiplication**

4 x 6 tiles

A



x



y

TLR-MVM

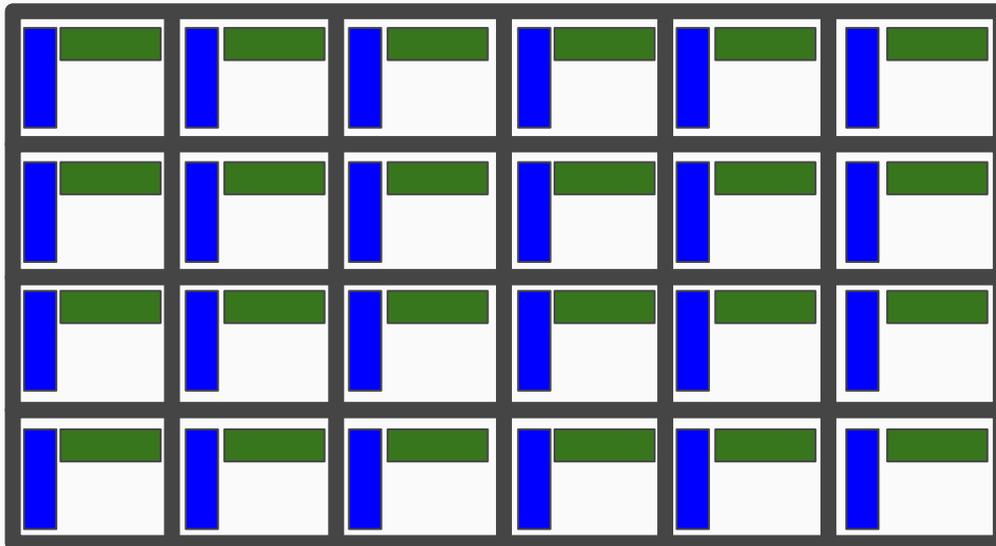
1) Compress once up-front
(SVD-like algorithms)

U bases

V bases



A



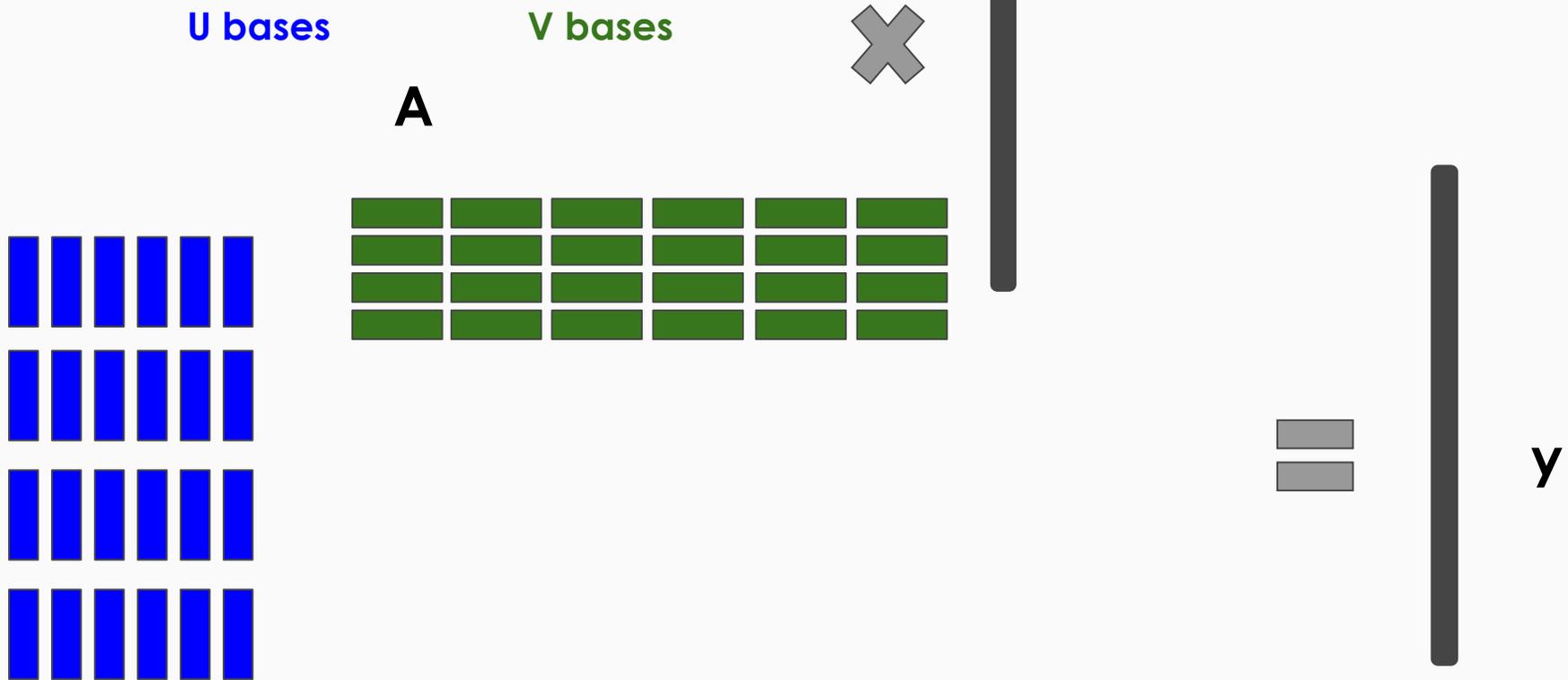
x



y

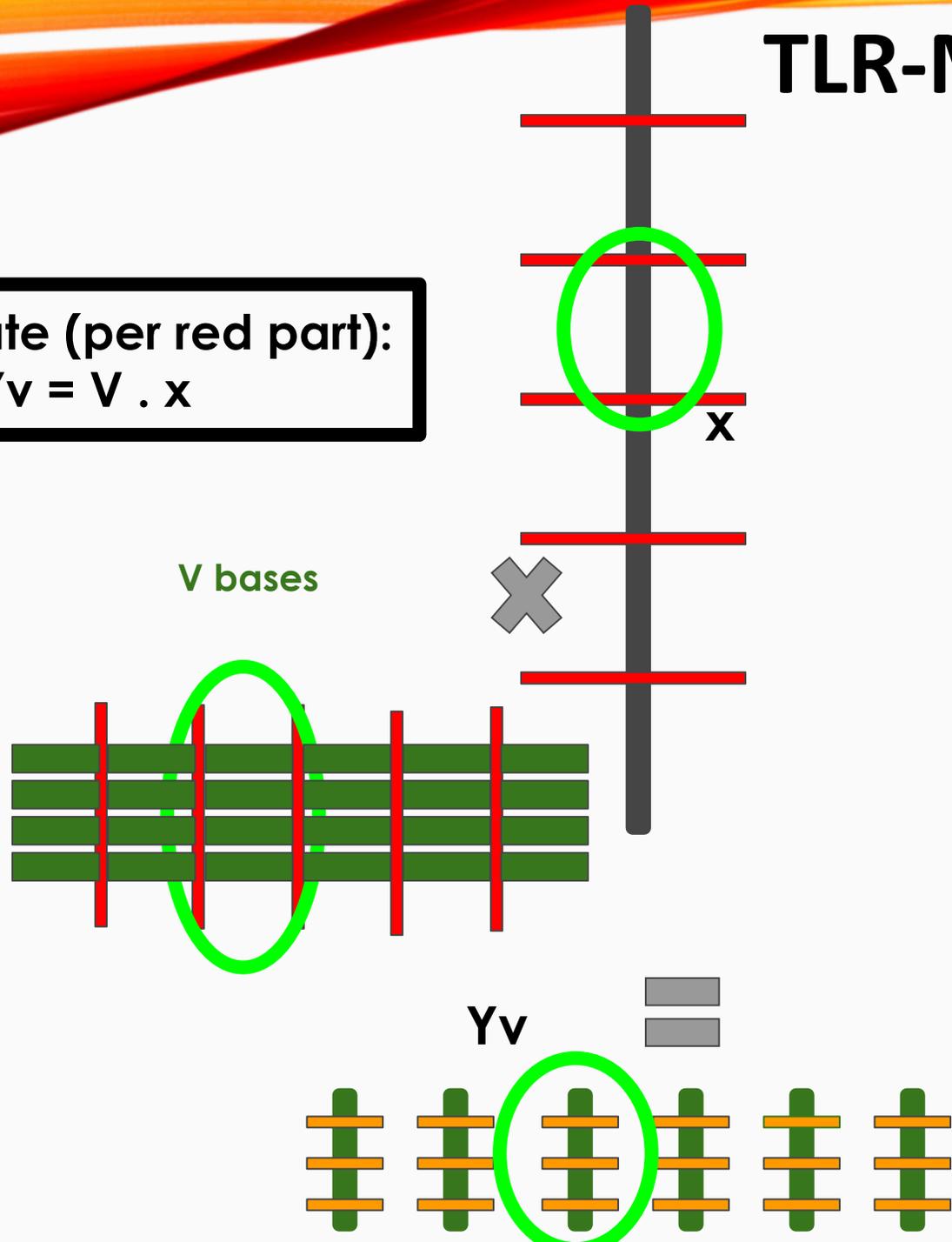
TLR-MVM

2) Stack the bases

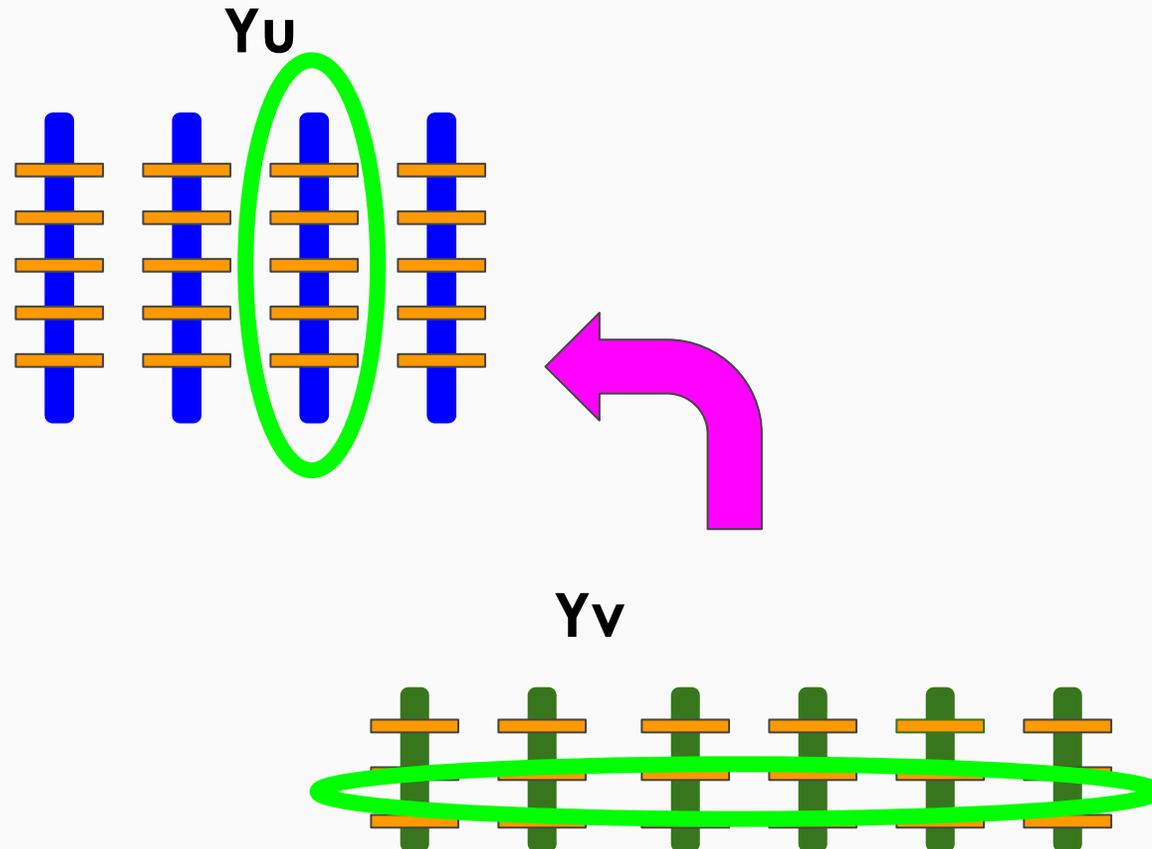


TLR-MVM

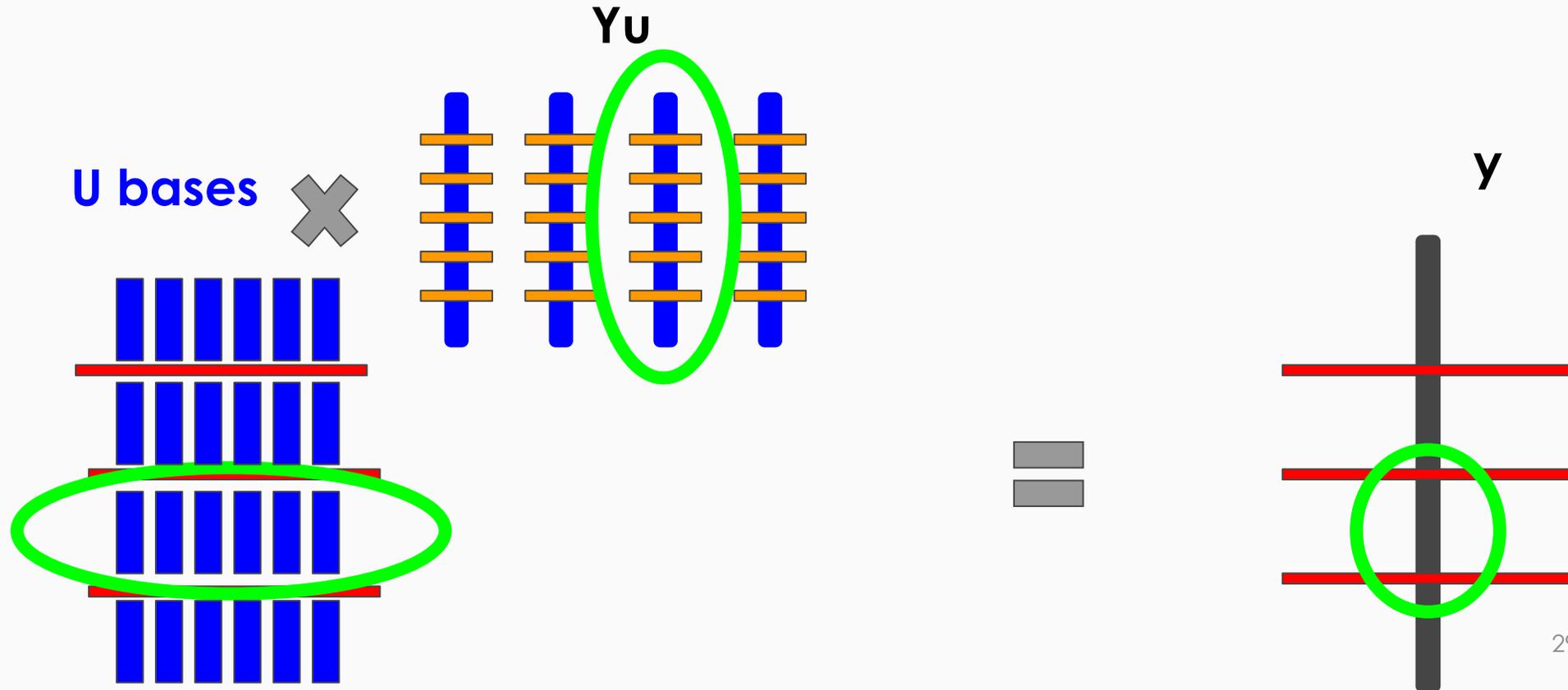
3) Calculate (per red part):
 $Y_v = V \cdot x$



4) Translate
Yv (V bases) to Yu (U bases)



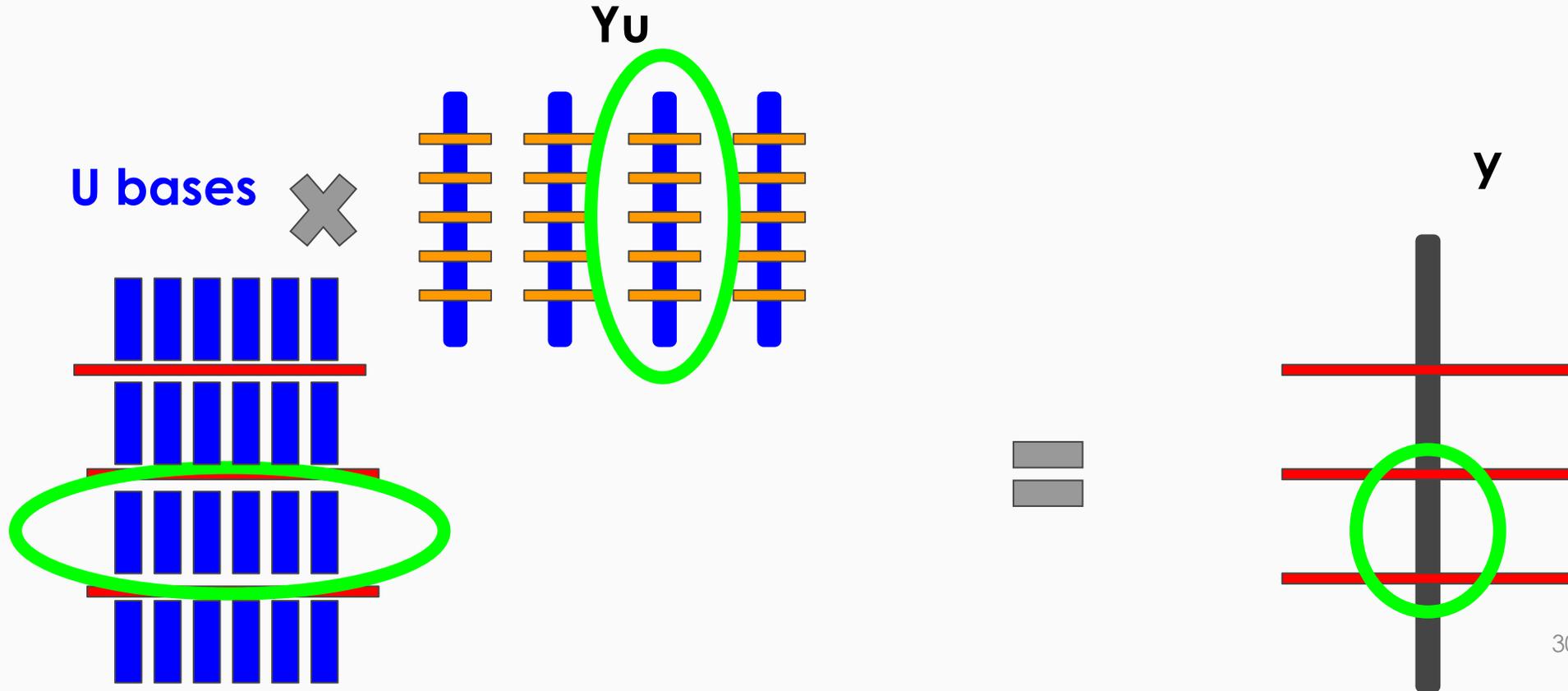
5) Calculate
 $y = U \cdot Y_u$



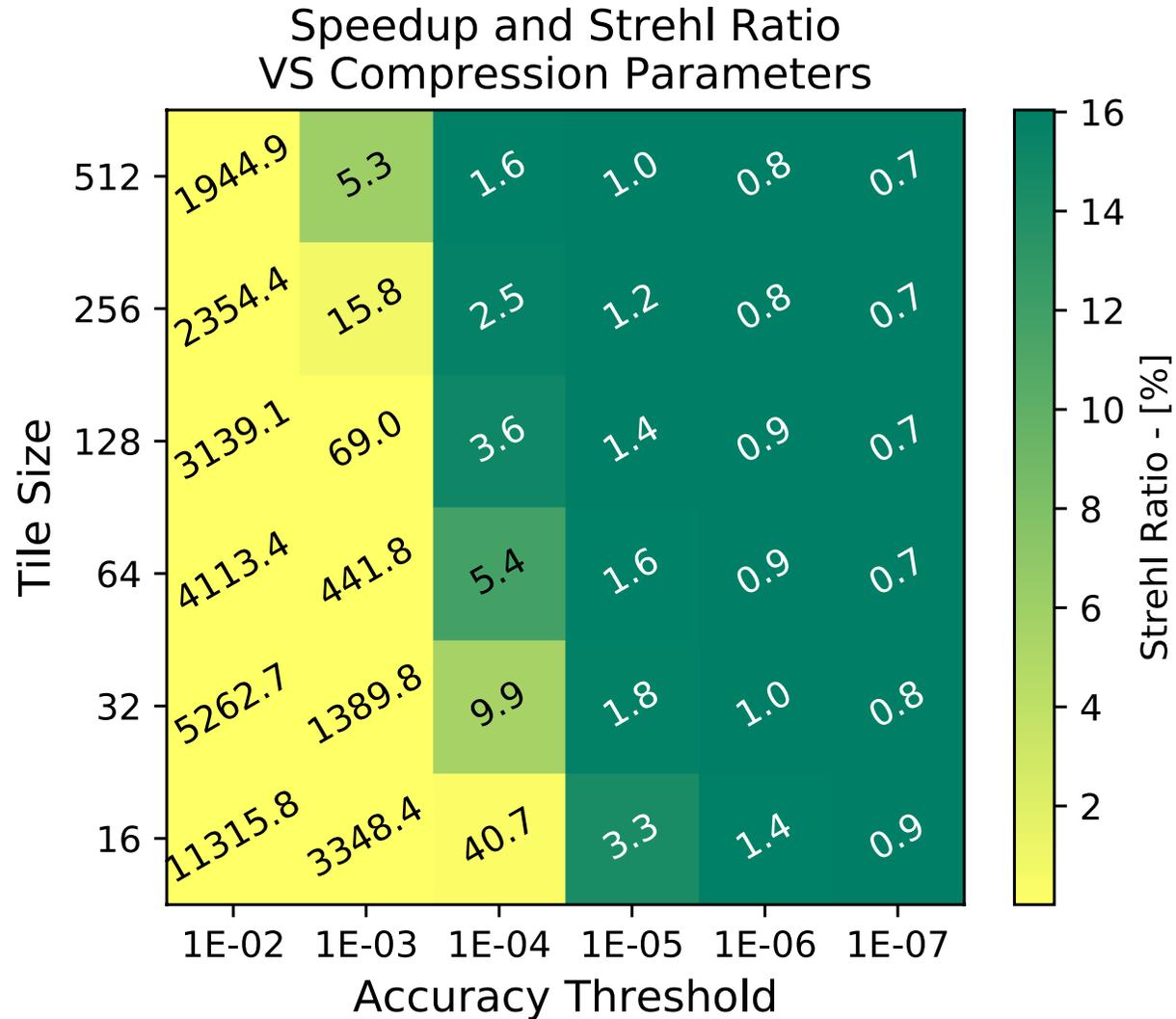
TLR-MVM

*Rely on batch GEMV calls
w/ variable sizes*

5) Calculate
 $y = U \cdot Yu$



Numerical Accuracy Assessment on MAVIS Datasets



Hardware/Software Specifications ³²

Vendor	Intel	AMD		Fujitsu	NVIDIA	NEC
Family	Cascade Lake	EPYC Rome	Instinct	Primergy A64FX	Ampere GPU	SX-Aurora TSUBASA
Model	6248	7702	MI100	FX1000	A100	B300-8
Node(s)/Card(s)	1	1	1	16	1	8
Socket(s)	2	2	N/A	4	N/A	N/A
Cores	40	128	7680	48	6912	8
GHz	2.5	2.2	1.5	2.2	2.6	1.6
Memory	384GB DDR4	512GB DDR4	32GB HBM2	32GB HBM2	40GB HBM2e	48GB HBM2
Sustained BW	232GB/s	330GB/s	1.2TB/s	800GB/s	1.5TB/s	1.5TB/s
LLC	27.5MB	512MB	8MB	32MB	40MB	16MB
Sustained BW	1.1TB/s	4TB/s	3TB/s	3.6TB/s	4.8TB/s	2.1TB/s
Compiler	Intel compiler 19.1.0	GCC compiler 8.2.0		Fujitsu compiler 4.5.0	NVCC 11.0	NEC compiler 3.1.1
BLAS library	Intel MKL 2020	BLIS 3.0.0		Fujitsu SSL II	cuBLAS 11.0	NEC NLC 2.1.0
MPI library	OpenMPI 4.0.3	OpenMPI 3.1.2		Fujitsu MPI 4.0.1	NCCL 2.0	NEC MPI 2.13.0

Hardware/Software Specifications ³³

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x86

MPI +

OpenMP

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ARM
MPI +
OpenMP

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Sustained BW	232GB/s	330GB/s	1.2TB/s	800GB/s	1.5TB/s	1.5TB/s
LLC	27.5MB	512MB	8MB	32MB	40MB	16MB
Sustained BW	1.1TB/s	4TB/s	3TB/s	3.6TB/s	4.8TB/s	2.1TB/s
Compiler	Intel compiler 19.1.0	GCC compiler 8.2.0		Fujitsu compiler 4.5.0	NVCC 11.0	NEC compiler 3.1.1
BLAS library	Intel MKL 2020	BLIS 3.0.0		Fujitsu SSL II	cuBLAS 11.0	NEC NLC 2.1.0
MPI library	OpenMPI 4.0.3	OpenMPI 3.1.2		Fujitsu MPI 4.0.1	NCCL 2.0	NEC MPI 2.13.0

Accelerators

ROCm / CUDA

Hardware/Software Specifications ³⁶

Vendor	Intel	AMD		Fujitsu	NVIDIA	NEC
Family	Cascade Lake	EPYC Rome	Instinct	Primergy A64FX	Ampere GPU	SX-Aurora TSUBASA
Model	6248	7702	MI100	FX1000	A100	B300-8
Node(s)/Card(s)	1	1	1	16	1	8
Socket(s)	2	2	N/A	4	N/A	N/A
Cores	40	128	7680	48	6912	8
GHz	2.5	2.2	1.5	2.2	2.6	1.6
Memory	384GB DDR4	512GB DDR4	32GB HBM2	32GB HBM2	40GB HBM2e	48GB HBM2
Sustained BW	232GB/s	330GB/s	1.2TB/s	800GB/s	1.5TB/s	1.5TB/s
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MPI library	OpenMPI 4.0.3	OpenMPI 3.1.2		Fujitsu MPI 4.0.1	NCCL 2.0	NEC MPI 2.13.0

Vector
MPI +
OpenMP

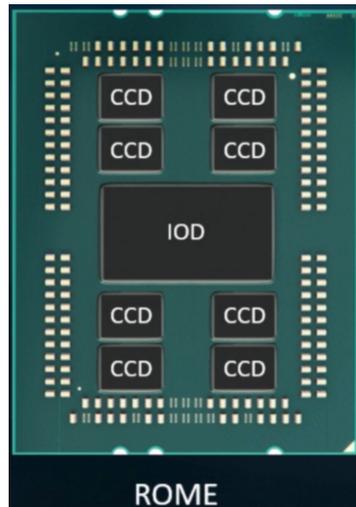
Hardware/Software Specifications ³⁷

Vendor	Intel	AMD	Fujitsu	NVIDIA	NEC	
Family	Cascade Lake	EPYC Rome	Instinct	Primergy A64FX	Ampere GPU	SX-Aurora TSUBASA
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HBM

Hardware/Software Specifications ³⁸

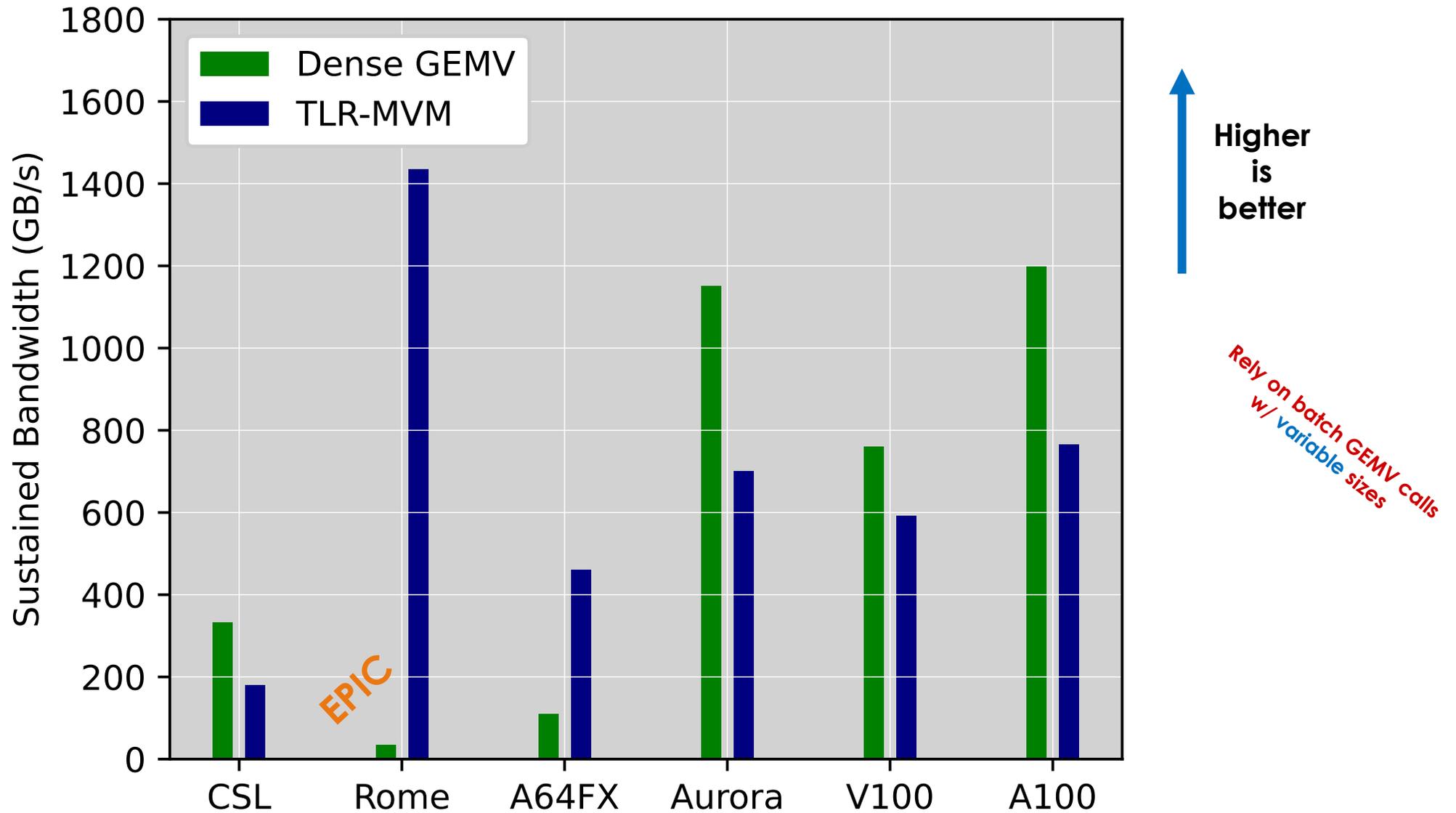
Vendor	Intel	AMD	Fujitsu	NVIDIA	NEC	
Family	Cascade Lake	EPYC Rome	Instinct	Primergy A64FX	Ampere GPU	SX-Aurora TSUBASA
Model	6248	7702	MI100	FX1000	A100	B300-8
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Cores	40	128	7680	48	6912	8
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Sustained BW	1.1TB/s	4TB/s	3TB/s	3.6TB/s	4.8TB/s	2.1TB/s
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MPI library	OpenMPI 4.0.3	OpenMPI 3.1.2	Fujitsu MPI 4.0.1	NCCL 2.0	NEC MPI 2.13.0	



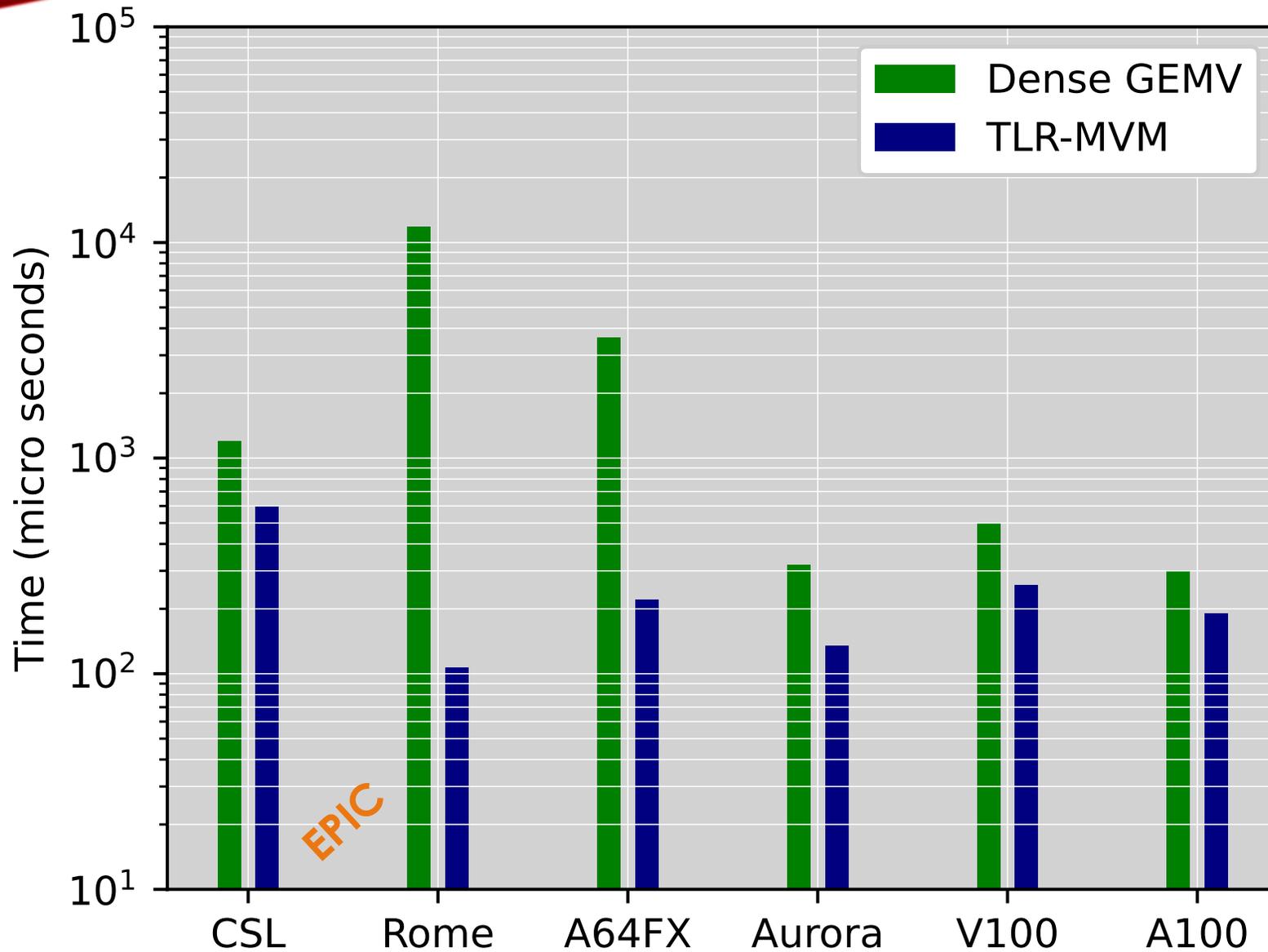
- IOD = "I/O Die" doing all the memory/PCI/other socket traffic
- CCD = "Core Compute Die", a chiplet having compute cores only
- CCX = "Core Compute Complex", a set of cores sharing a L3 cache



Sustained Bandwidth on Synthetic Datasets



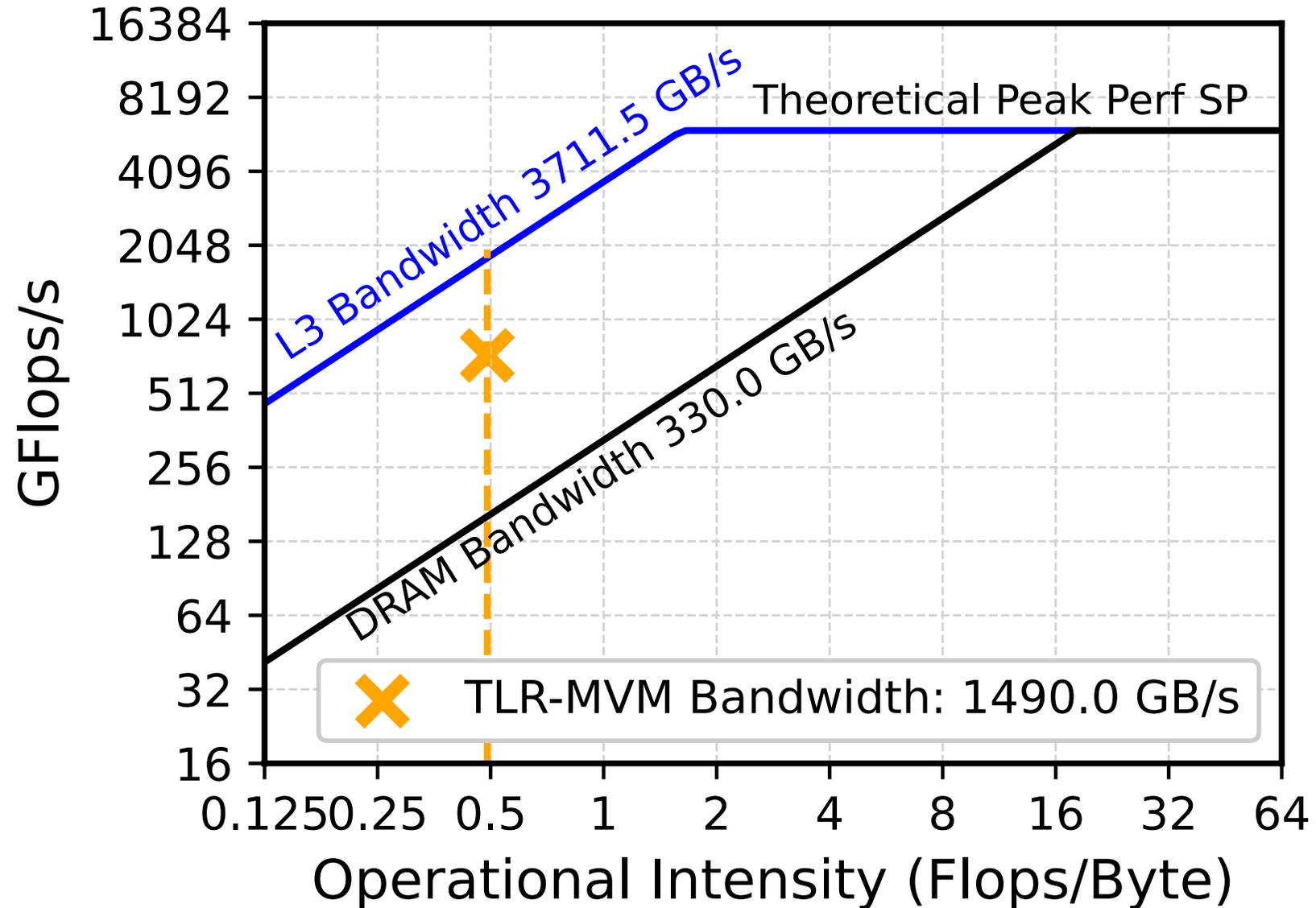
Time to Solution on Synthetic Datasets



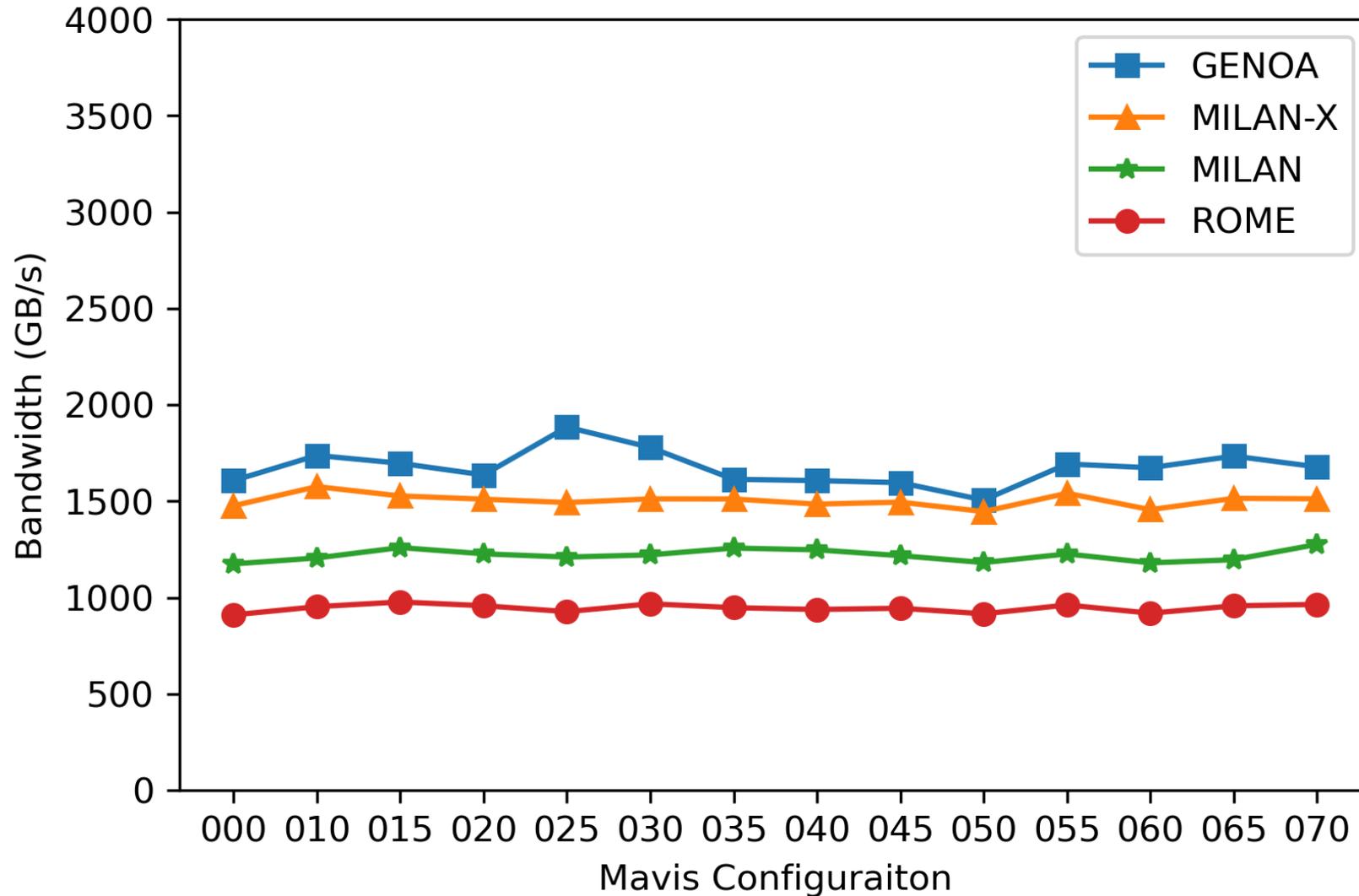
Lower
is
better

*Rely on batch GEMV calls
w/ variable sizes*

Roofline Performance Model



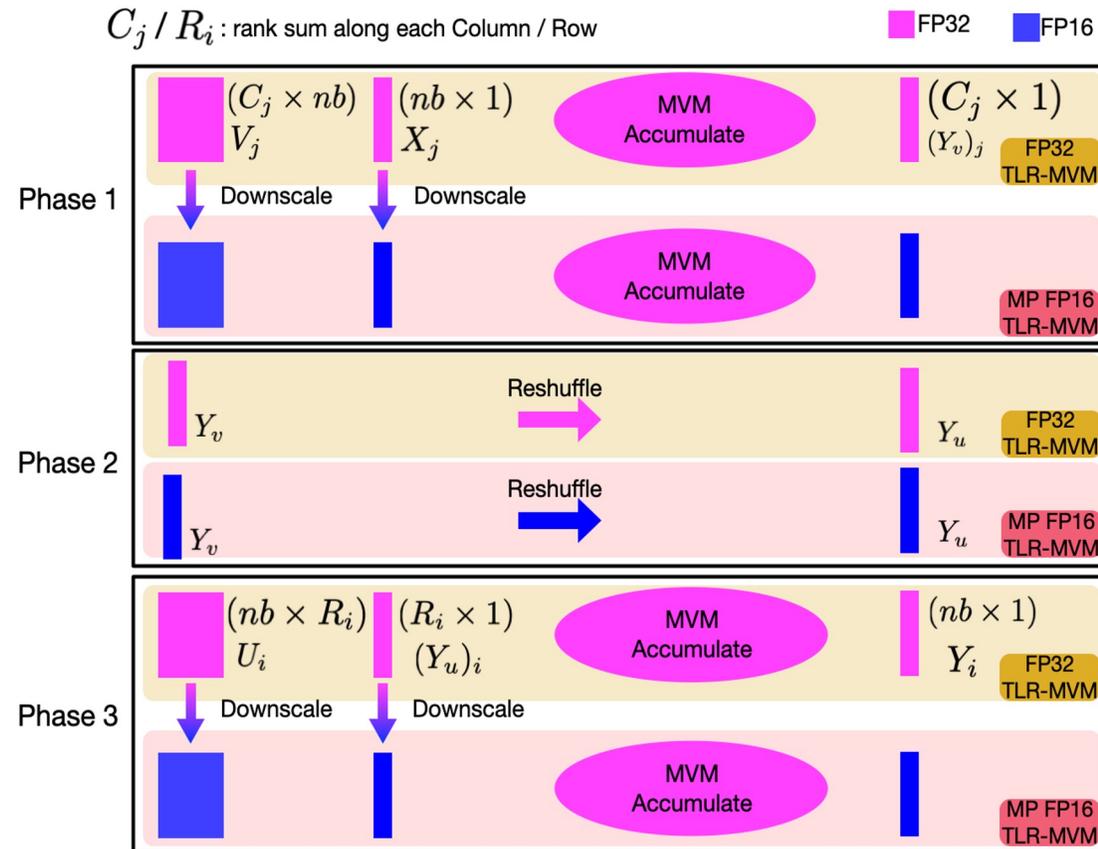
Performance Across AMD x86 Generations



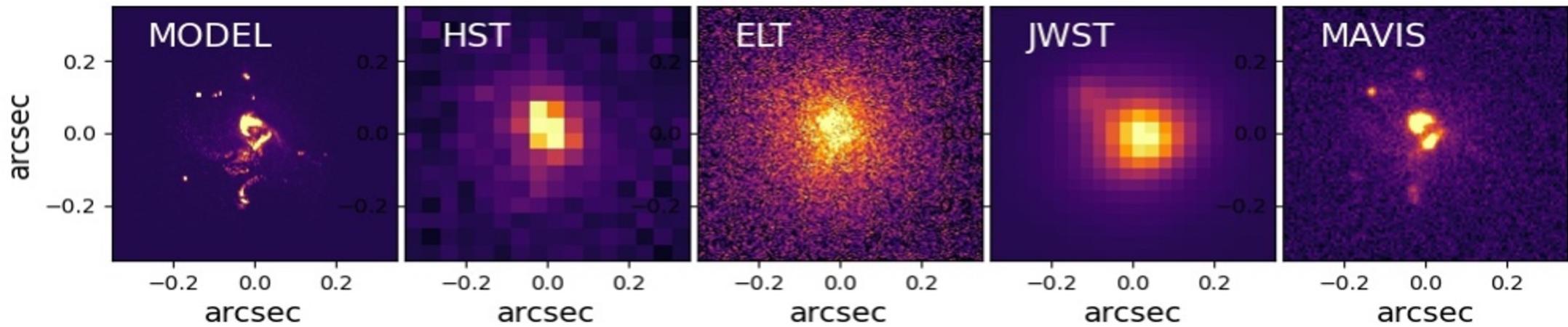
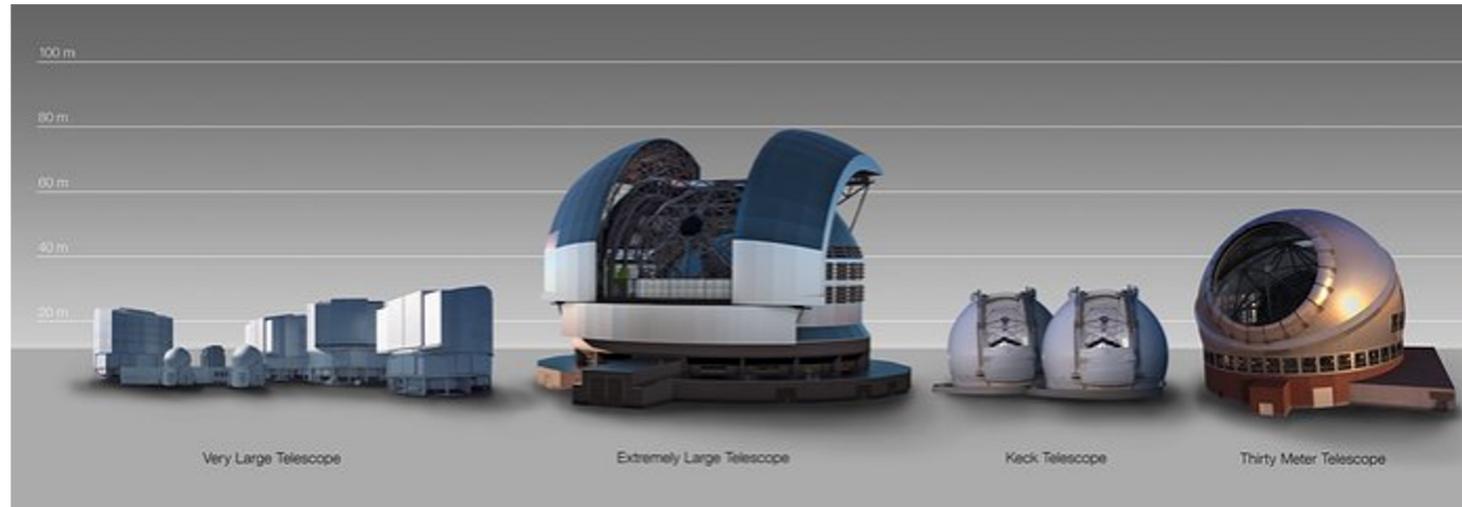
The Case for Mixed Precisions

Data transactions with AO hardware rely on UINT16

- WFS cameras provide 12-16 bits data stream as input
- Deformable mirror actuators are controlled through a set of UINT16 commands



MAVIS Instrument



HPC Scientific Applications

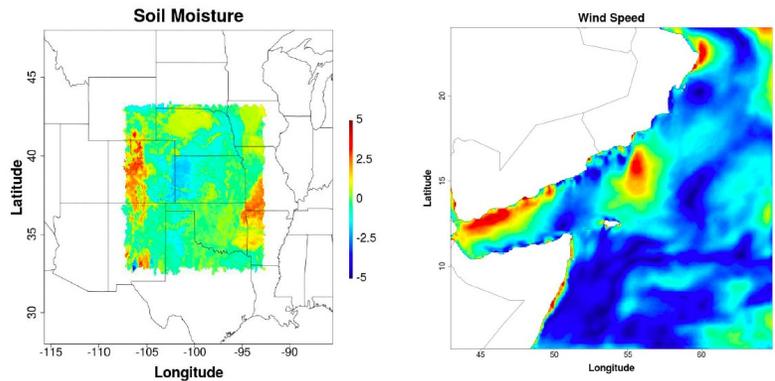
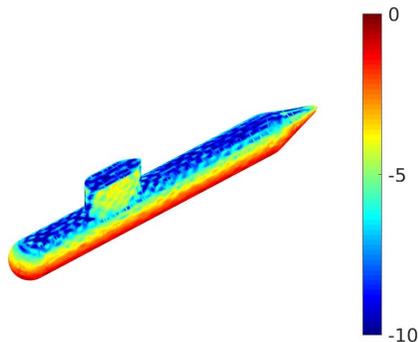
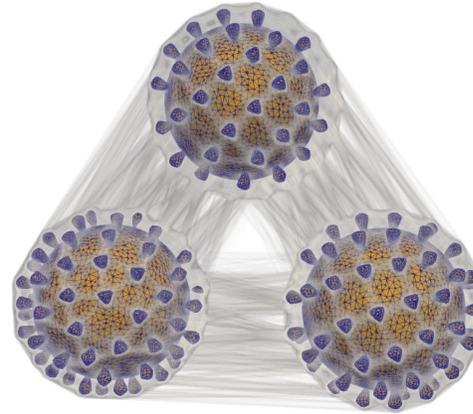


Fig. 4: **Left:** Soil moisture residuals at the topsoil of the Mississippi River basin. **Right:** Wind speed (m/s) in the Arabian Sea.

3D Geospatial Statistics



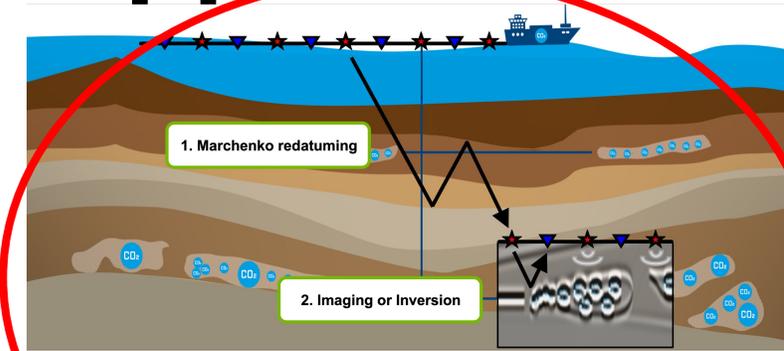
3D Computational Electromagnetics



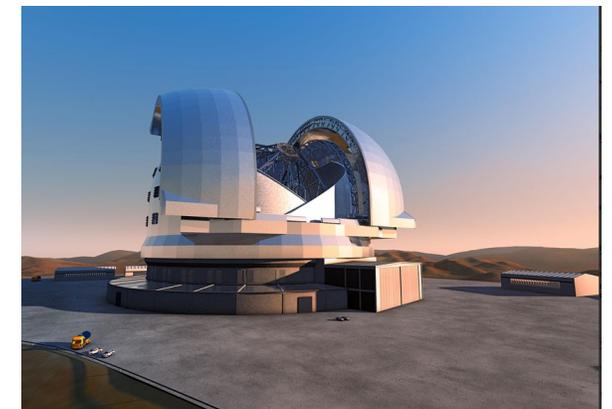
3D Mesh Deformations



Wireless Communications



Seismic Imaging



Computational Astronomy

Powering Seismic Redatuming w/ TLR-MVM

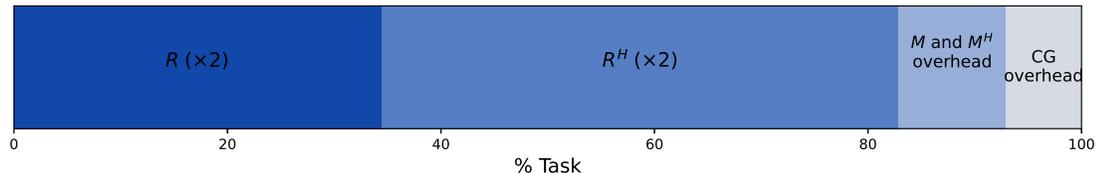
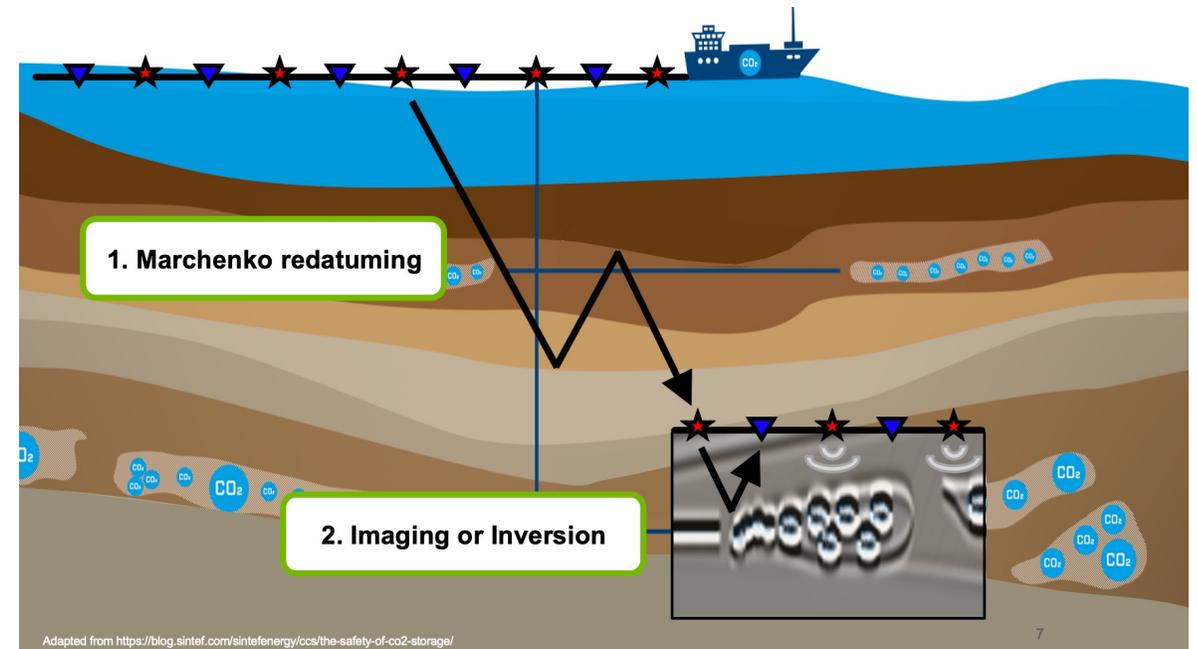
Seismic redatuming is an important technique to get insights from the Earth's subsurface.

This requires solving an inverse problem. Traditionally, due to computational challenges, only the adjoint is applied.

Some latest research show an alternative method to improve the solution of inverse problems by using an iterative solver, e.g., conjugate gradient iterative solver. This comes at the cost of evaluating multiple expensive MVM operations, as shown in the following equations:

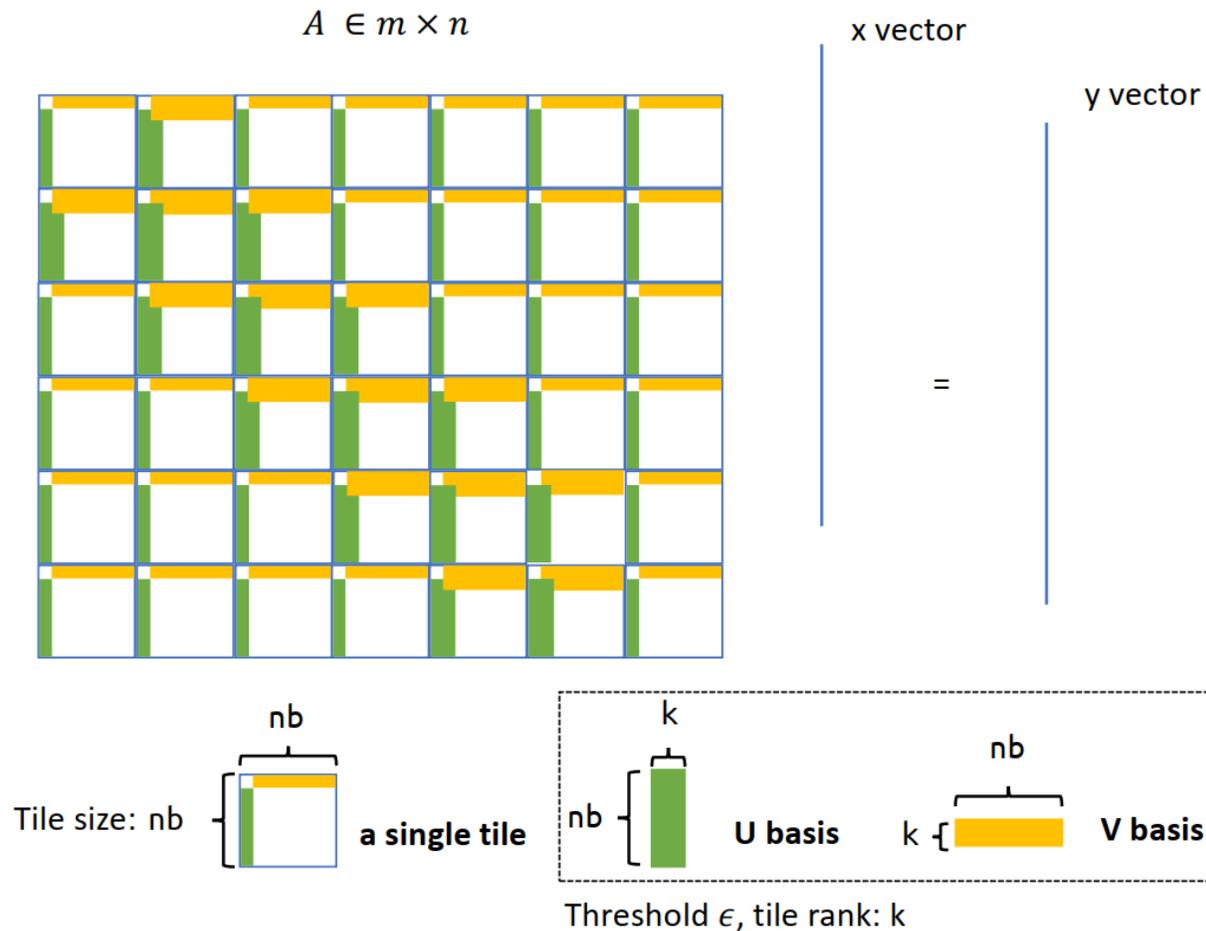
$$\mathbf{x} = \mathbf{R}^H \mathbf{y} : \quad x(t, \mathbf{x}_R, \mathbf{x}_A) = \mathcal{F}_{\omega_{max}}^{-1} \left(\int_{\delta\mathbb{D}} R^*(\omega, \mathbf{x}_B, \mathbf{x}_R) \mathcal{F}_{\omega_{max}}(y(t, \mathbf{x}_B, \mathbf{x}_A)) d\mathbf{x}_B \right),$$

$$\mathbf{y} = \mathbf{R}\mathbf{x} : \quad y(t, \mathbf{x}_B, \mathbf{x}_A) = \mathcal{F}_{\omega_{max}} \left(\int_{\delta\mathbb{D}} R(\omega, \mathbf{x}_B, \mathbf{x}_R) \mathcal{F}_{\omega_{max}}^{-1}(x(t, \mathbf{x}_R, \mathbf{x}_A)) d\mathbf{x}_R \right).$$

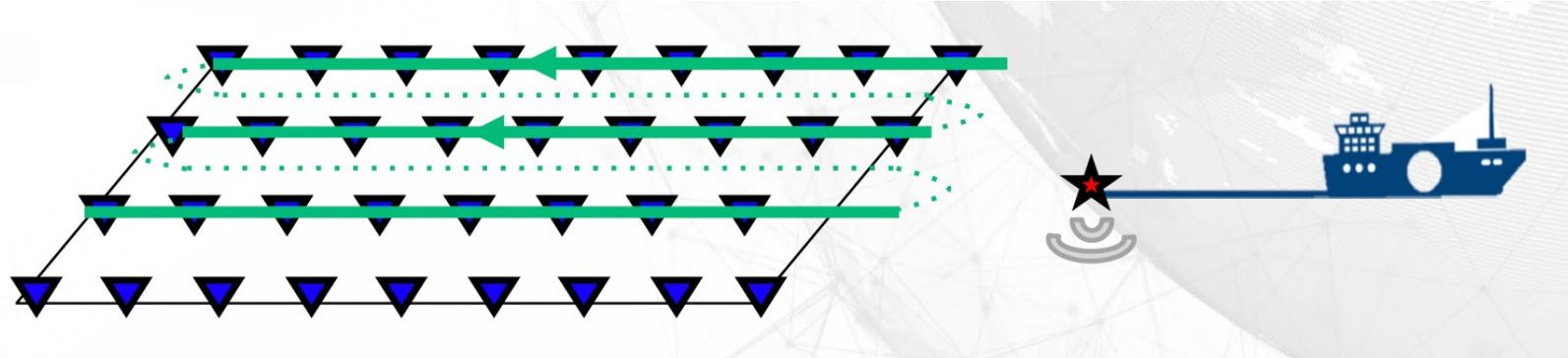


Powering Seismic Redatuming w/ TLR-MVM

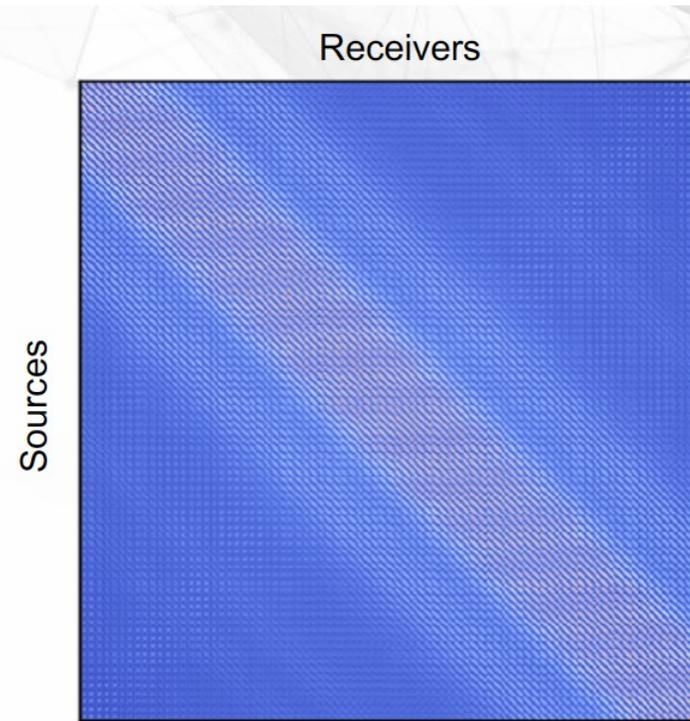
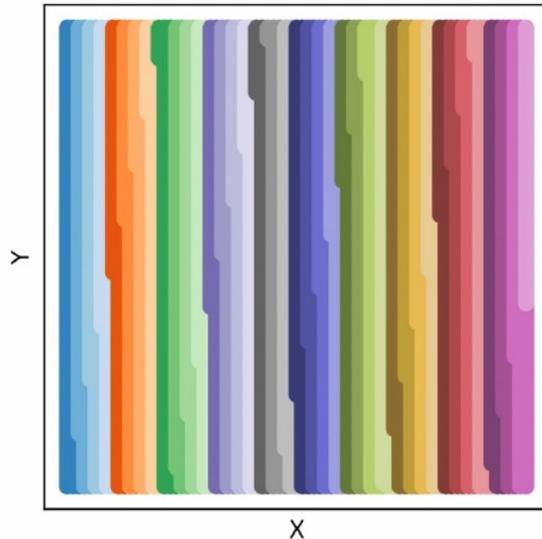
We use tile low-rank matrix-vector multiplication (TLR-MVM) to address the complexity bottleneck.



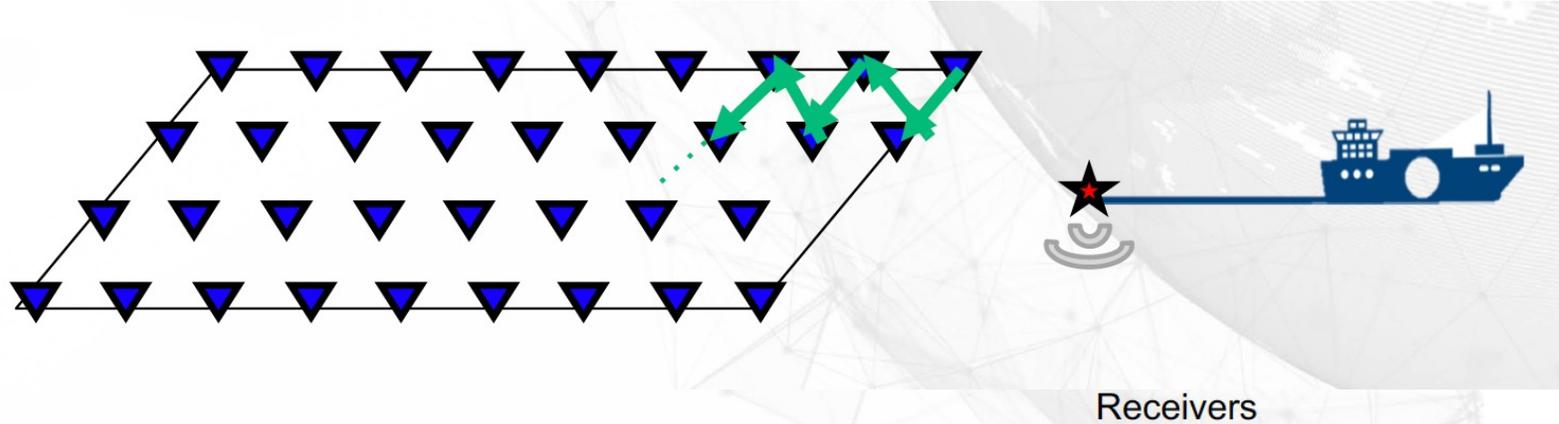
Distance-Aware Reordering



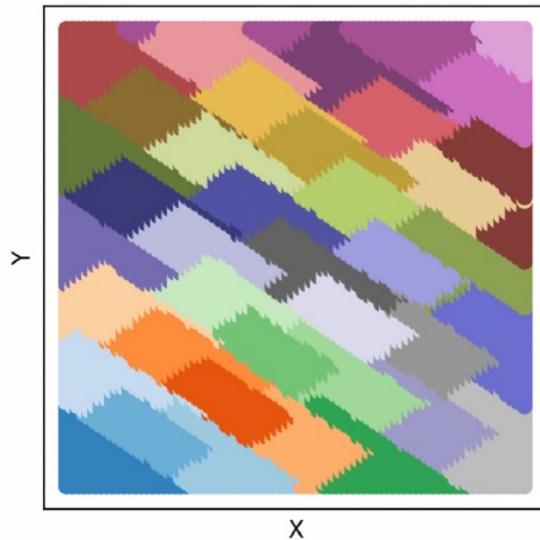
'Conventional' ordering



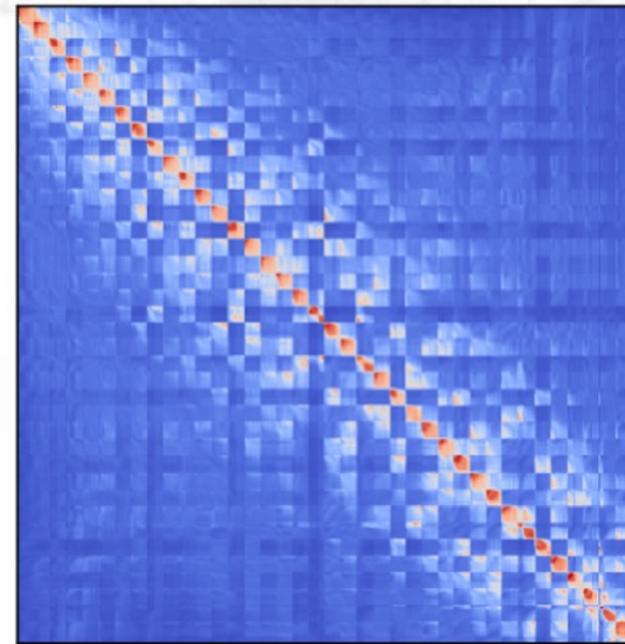
Distance-Aware Reordering



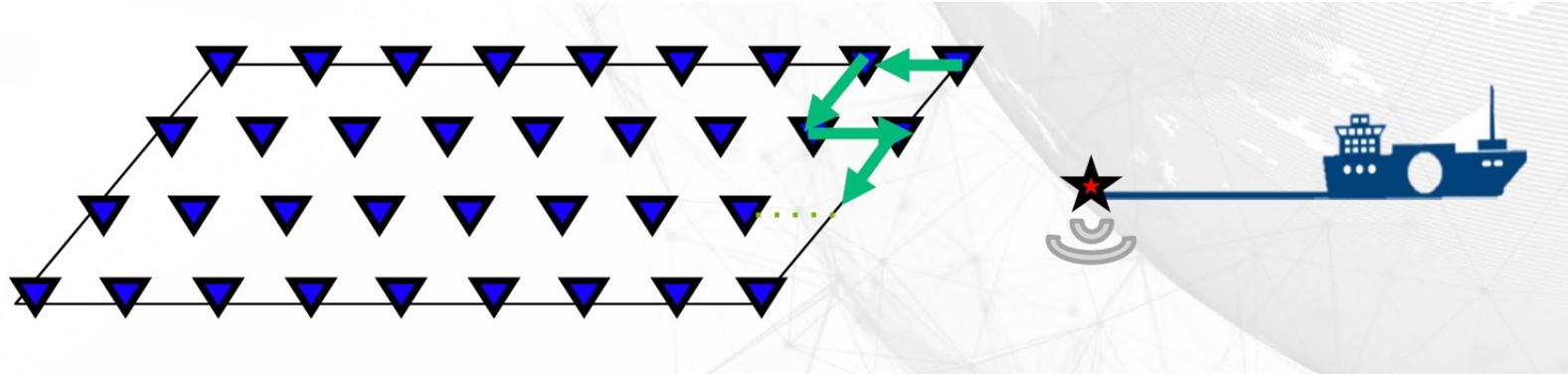
L1 ordering



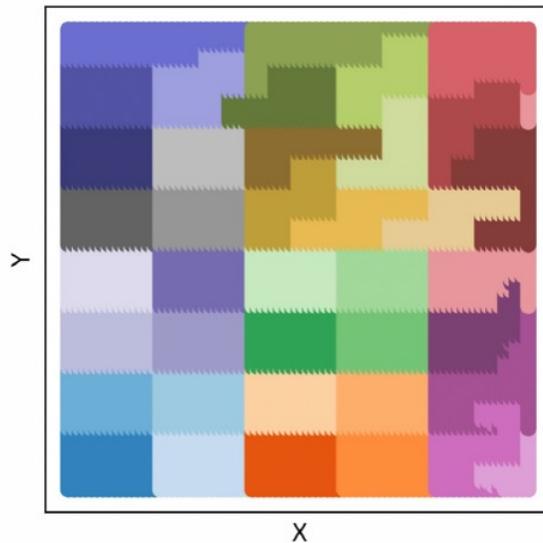
Sources



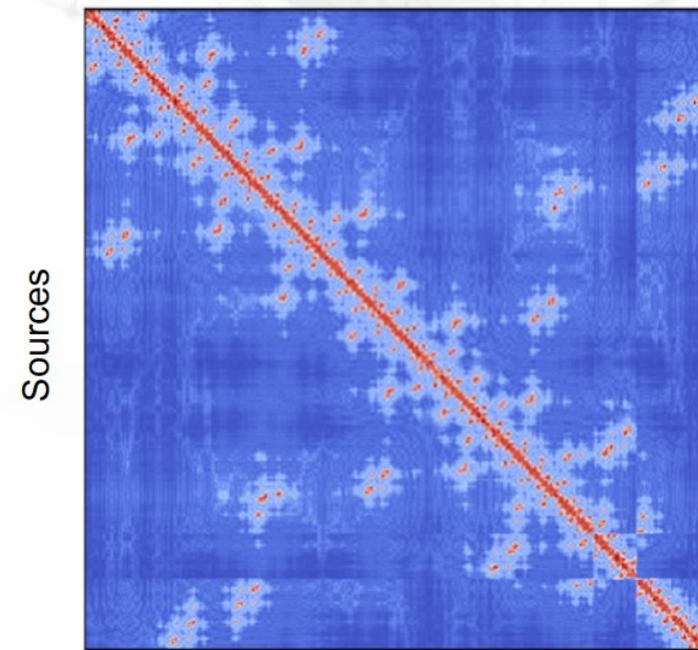
Distance-Aware Reordering



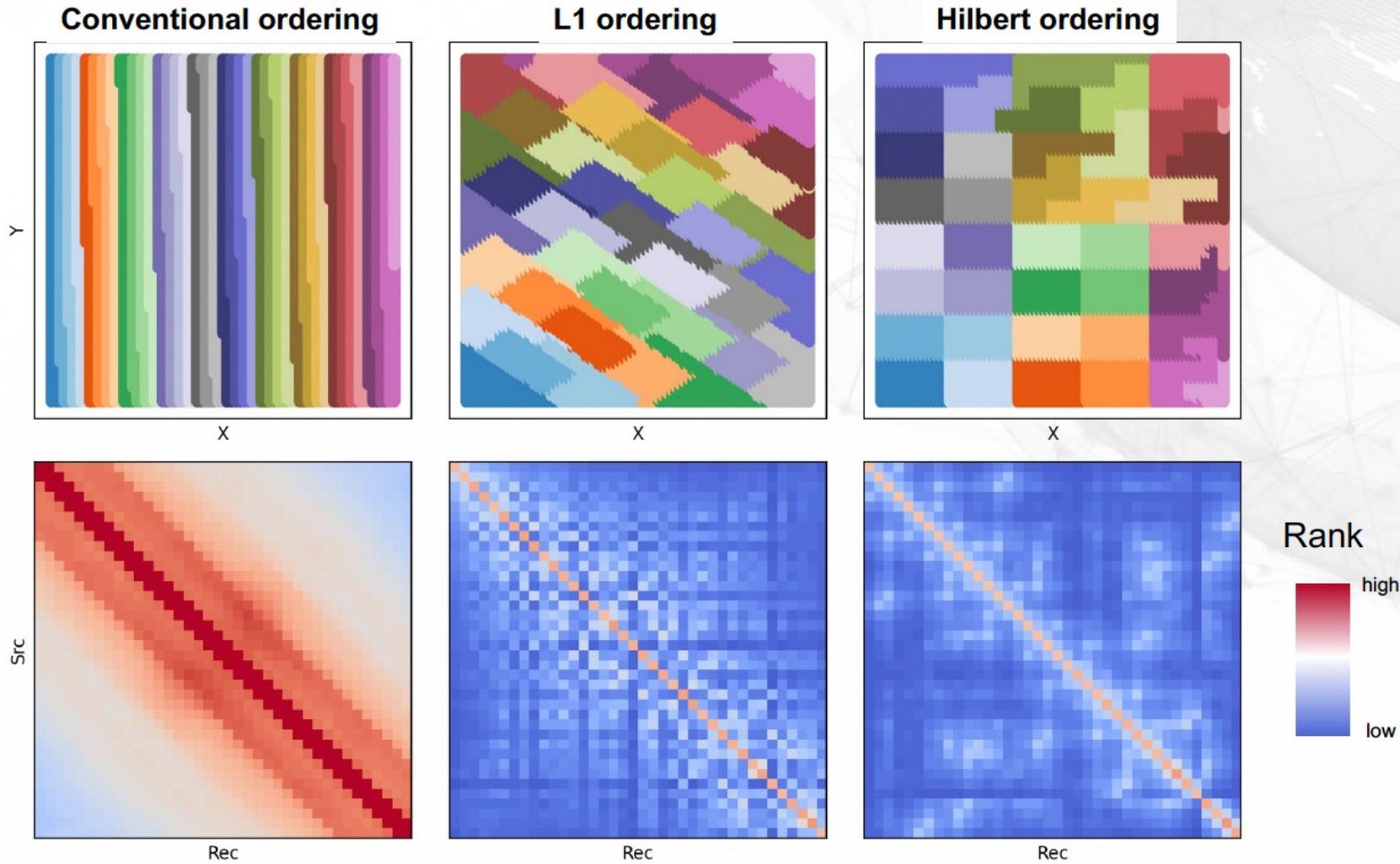
Hilbert ordering



Receivers



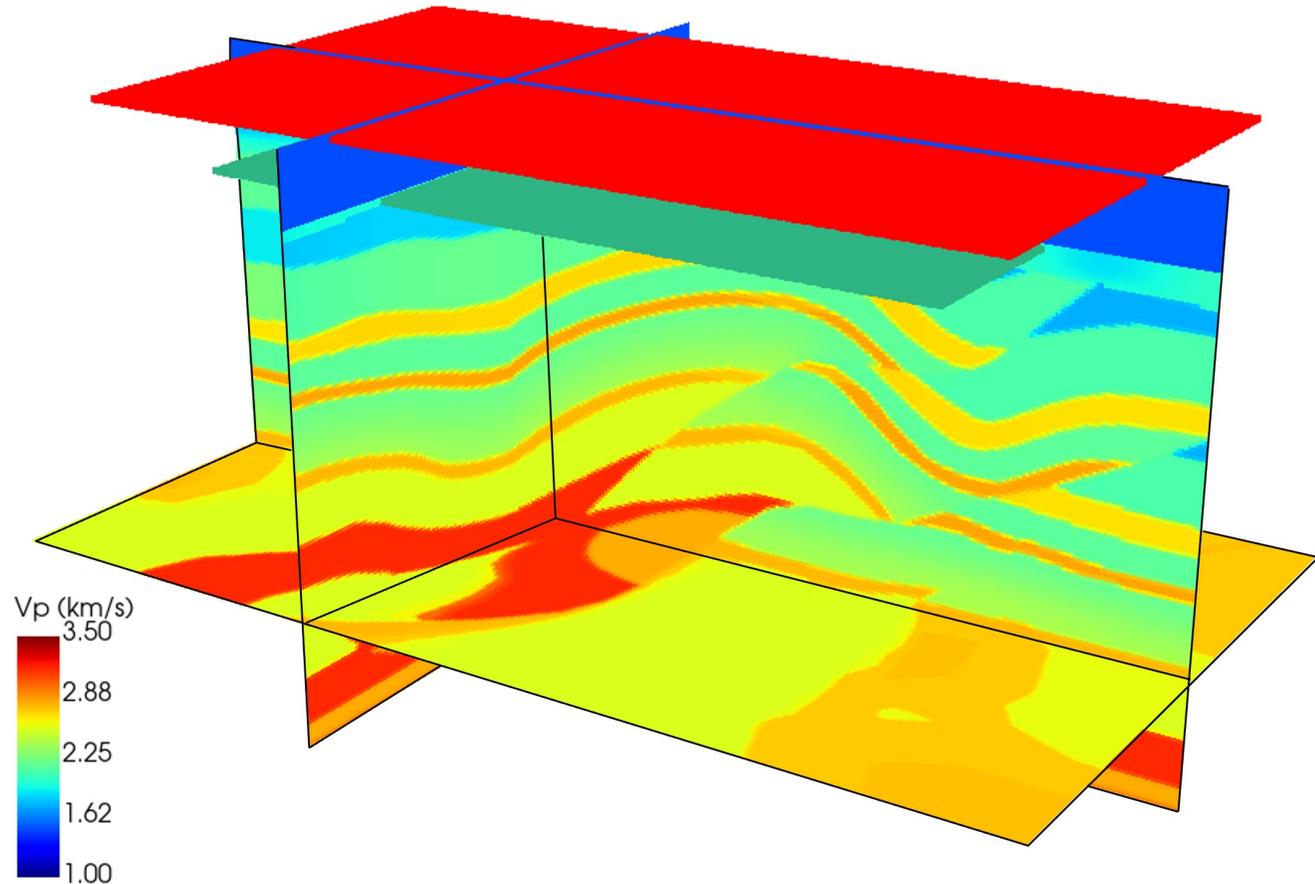
Distance-Aware Reordering



SEG/EAGE Overthrust Model

Jointly developed between the Society of Exploration Geophysicists (SEG) and the European Association of Geo-scientists and Engineers (EAGE)

- 3D Geological open model
- $3 \times 5 \times 2.3 \text{ km}^3$
- 217×120 sources
- 177×90 receivers
- 230 complex-valued frequency matrices of size 26040×15930



Numerical Accuracy

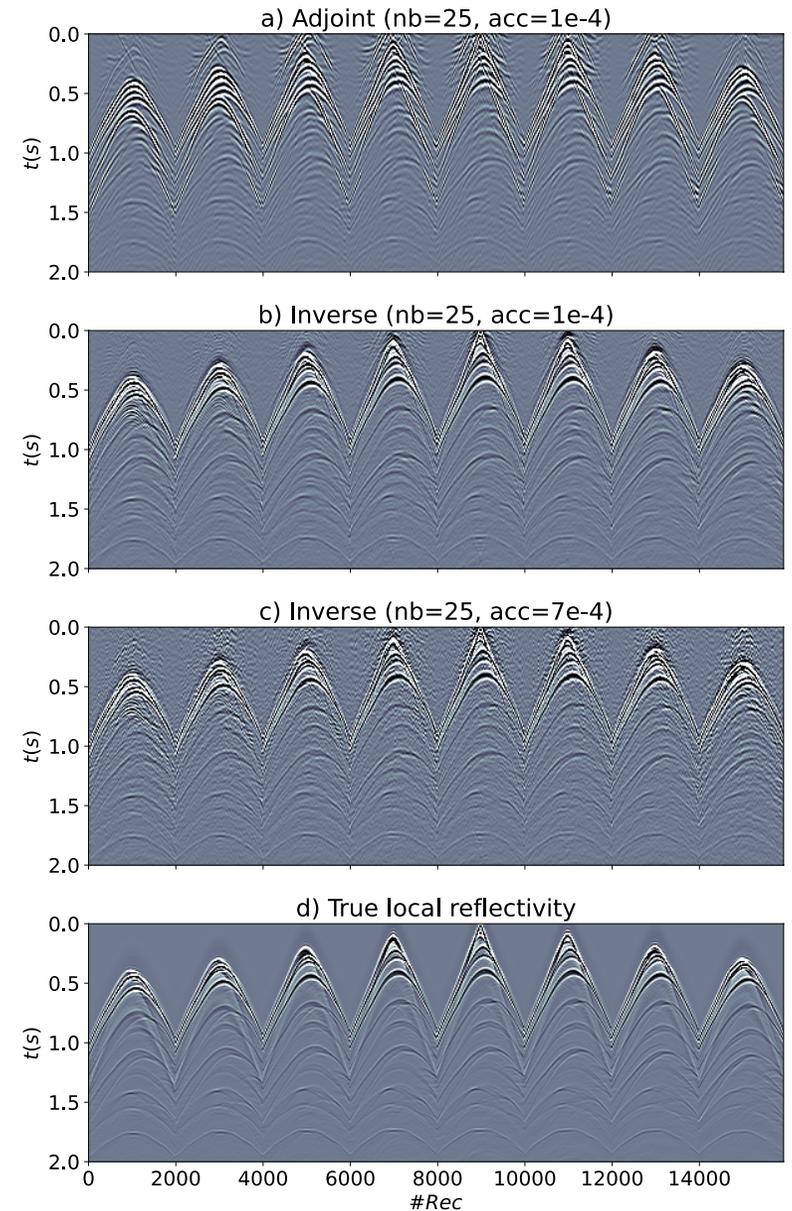
Checking the traces of 8 receivers

Accuracy Threshold: $1e-4$

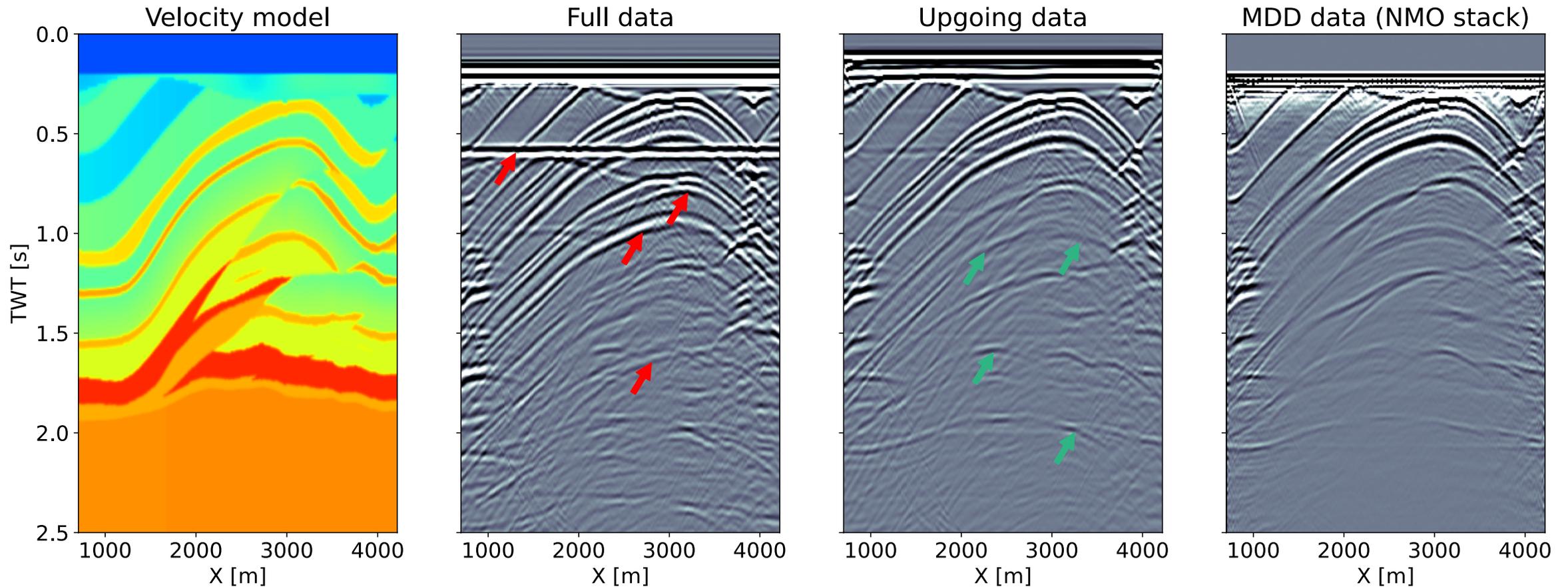
Good

Bad

Ground Truth

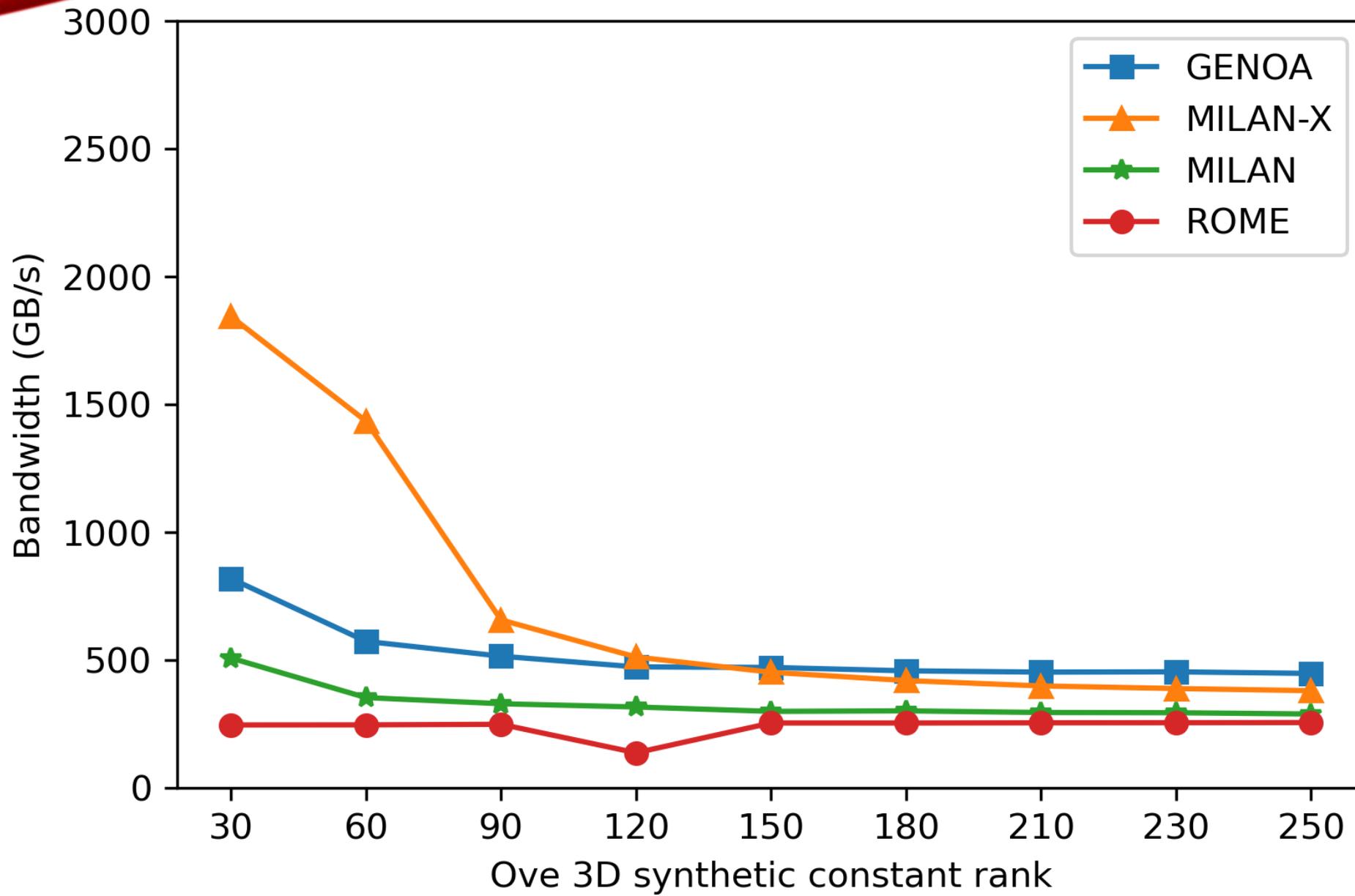


Numerical Accuracy

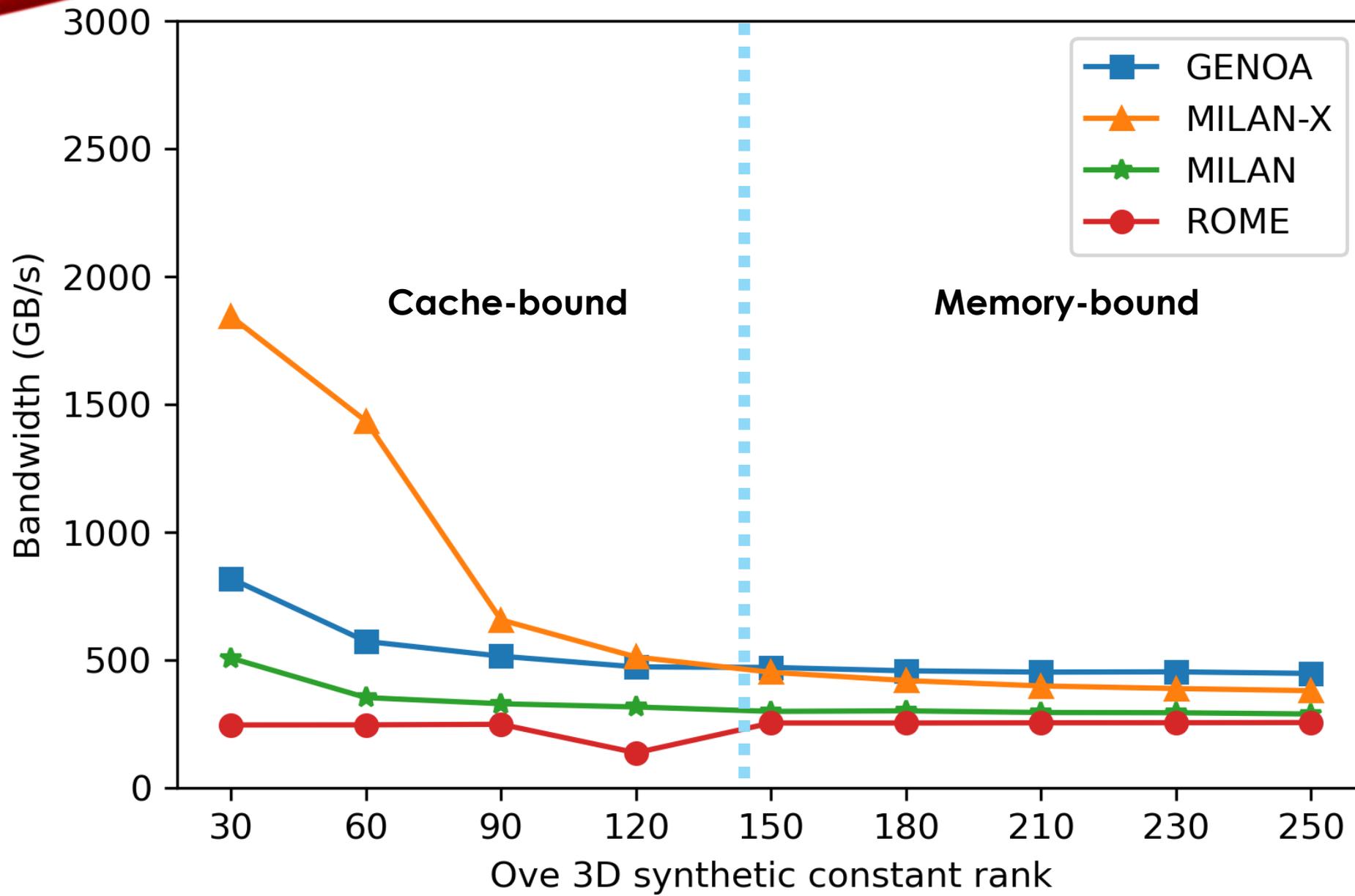


**Post-acquisition processing powered by TLR-MVM
to remove free-surface related effects**

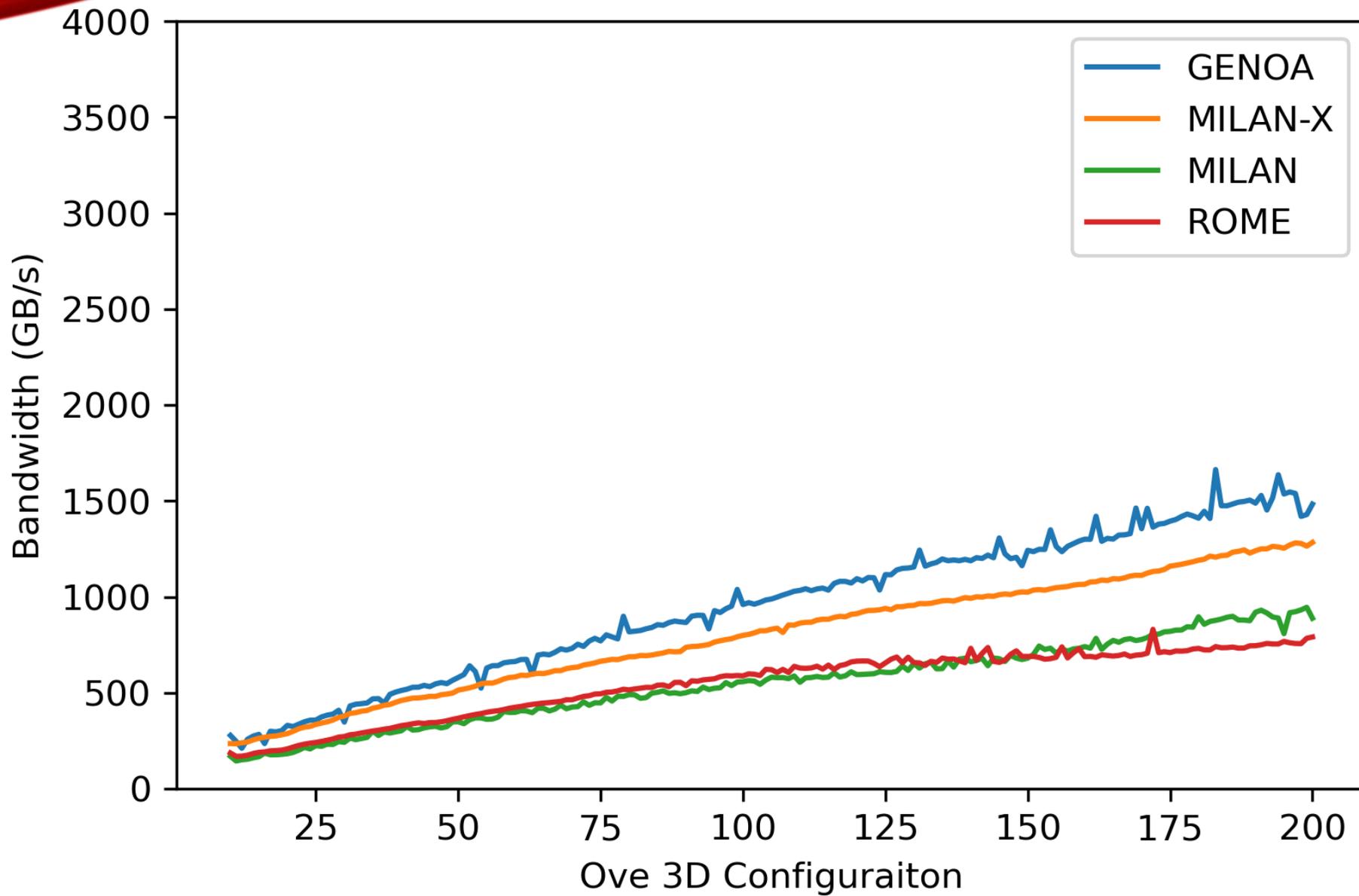
Performance Results



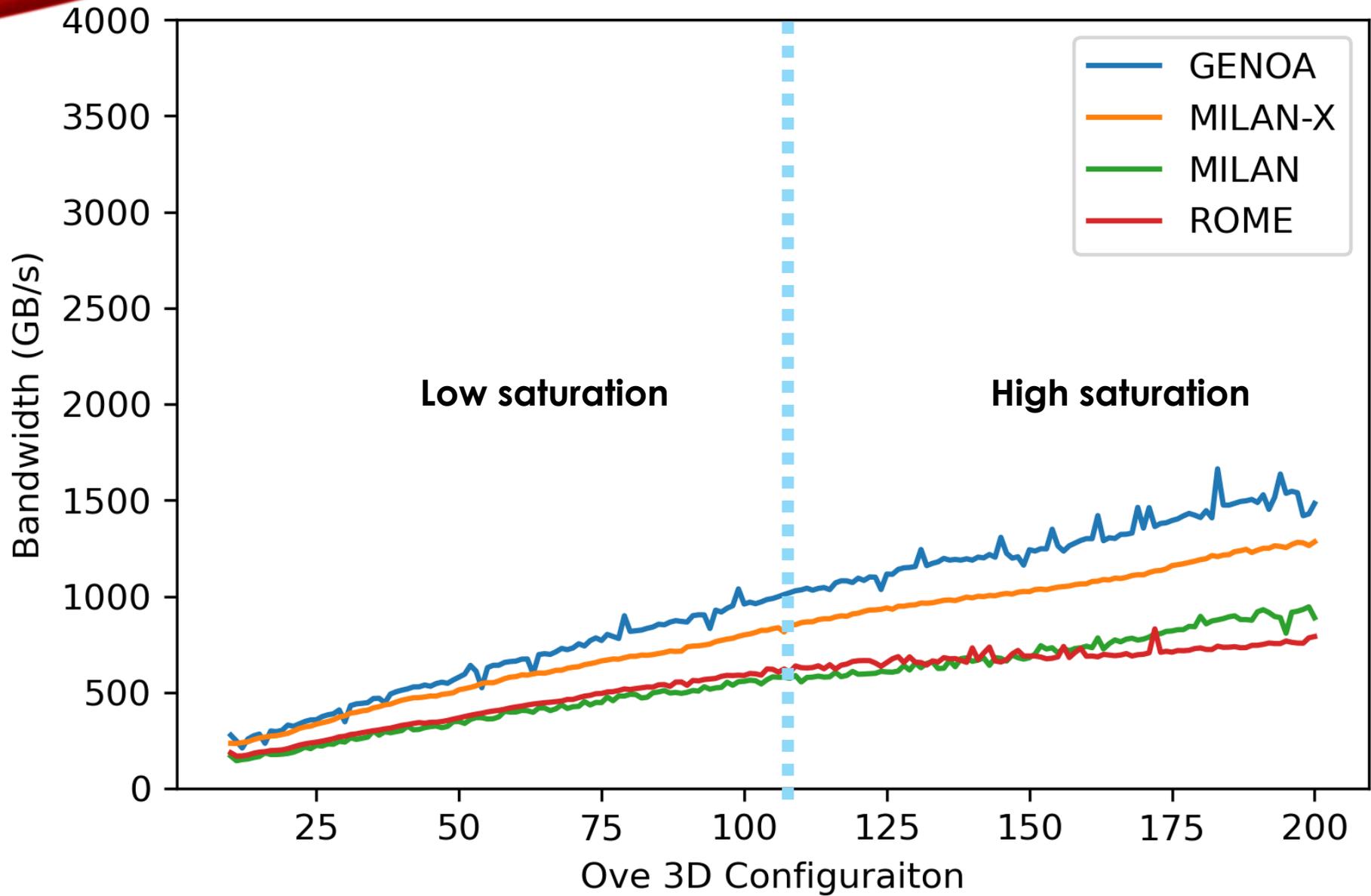
Performance Results



Performance Results



Performance Results



Summary

- Algorithms first!
- Low-rank matrix approximations are key for solving challenging scientific problems at scale
- Reconciling HPC workloads with the hostile hardware landscape
- Steering AI-focused hardware for HPC scientific applications is worth exploring (*ISC23 paper presentation*)
- Exploiting cache size and leveraging its high bandwidth

We are recruiting!



THANK YOU!

@HatemLtaief

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NHR PerLab Online Seminar
May 16th 2023