

Right Precision, Right Place: Rethinking HPC Applications with Adaptive Mixed Precisions

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Workshop on Mixed- and Adaptive-Precision Numerics
for Scientific Computing (MxP4S)

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Acknowledgments

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UTK: Q. Cao (now at SLU), G. Bosilca (now at NVIDIA), and J. Dongarra

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Cerebras: M. Jacquelin and L. Wilson
AMD: M. Gontier and M. Jaghoub

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Shaheen-2/3 and Ibex @ KAUST Supercomputing Lab, Saudi Arabia
HAWK @ HLRS, Germany (M. Resch)
Frontier @ ORNL, USA (US DOE)
Summit @ ORNL, USA (US DOE)
Fugaku @ Riken, Japan (S. Matsuoka)
Leonardo @ CINECA, Italy (G. Scipione)
Fromage @ NVIDIA, UK (F. Spiga)

AlgoDoers Team:

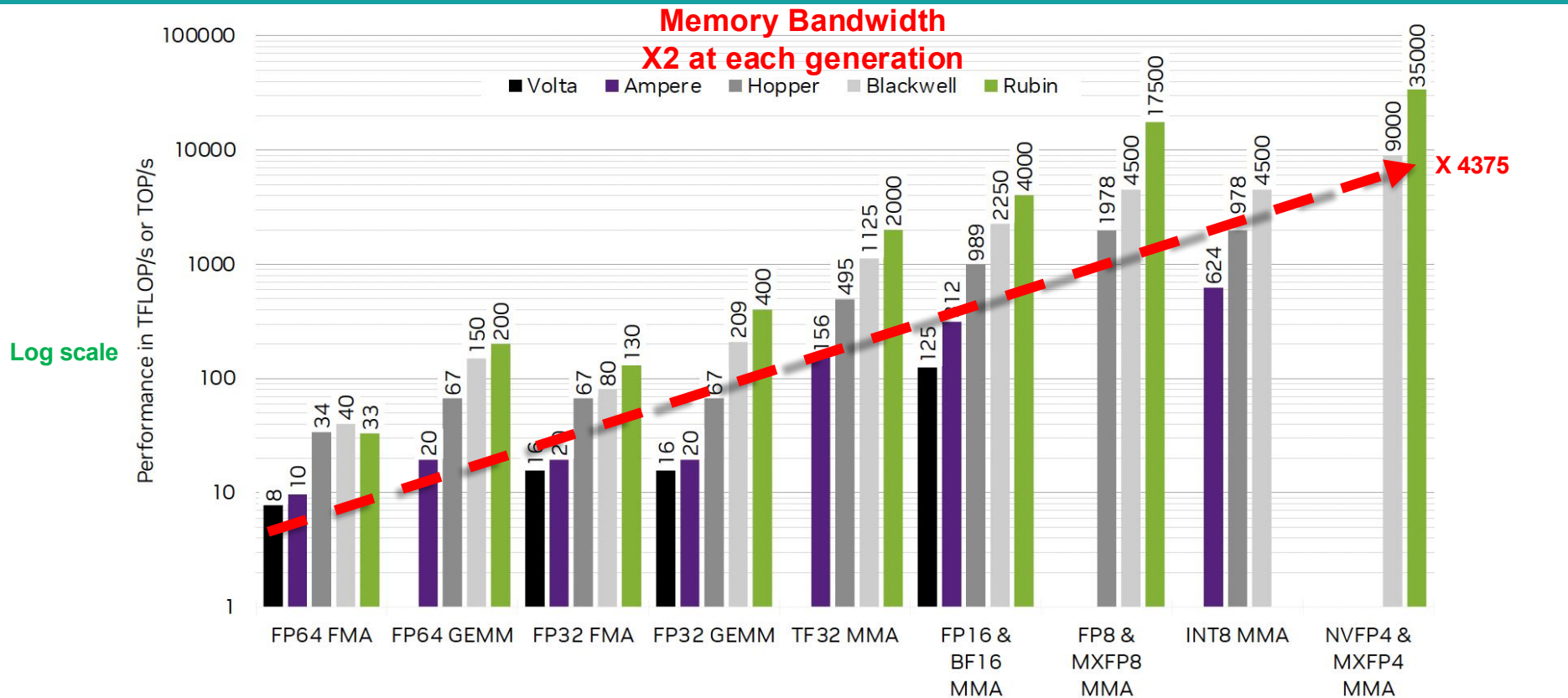
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Vincent Etienne
Amik St-Cyr
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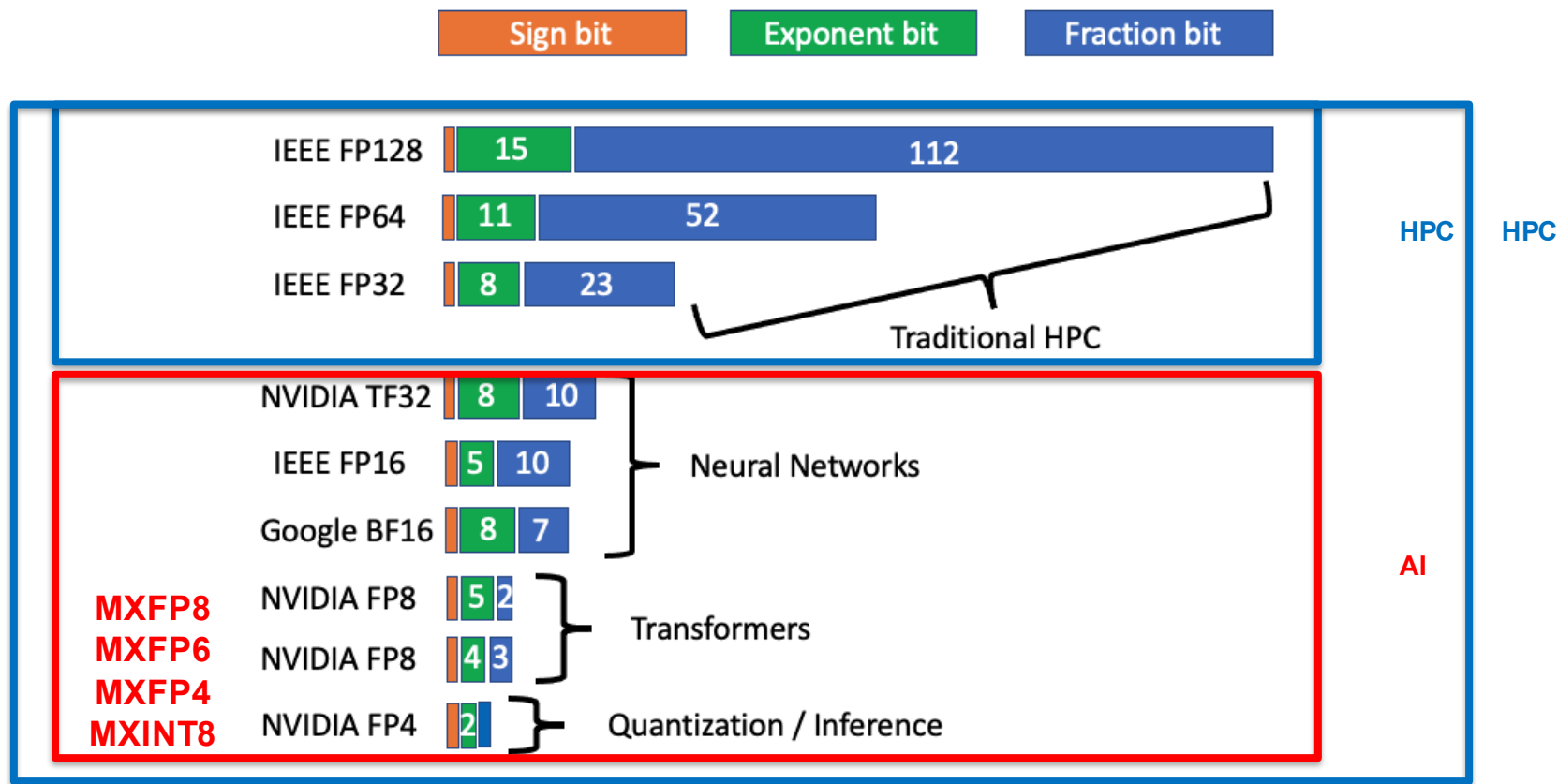
Top10 Fastest Supercomputers for HPL-MxP (Nov'25)

Rank	Site	Computer	Cores	HPL Rmax (Eflop/s)	TOP500 Rank	HPL-MxP (Eflop/s)	Speedup
1	DOE/SC/LLNL USA	El Capitan , HPE Cray 255a, AMD 4th Gen EPYC 24C 1.8 GHz, AMD Instinct MI300A, Slingshot-11	11,340,000	1.809	1	16.7	9.6
2	DOE/SC/ANL USA	Aurora , HPE Cray EX, Intel Max 9470 52C, 2.4 GHz, Intel GPU MAX, Slingshot-11	8,159,232	1.012	3	11.6	11.5
3	DOE/SC/ORNL USA	Frontier , HPE Cray EX235a, AMD Zen-3 (Milan) 64C 2GHz, AMD MI250X, Slingshot-11	8,560,640	1.353	2	11.4	8.4
4	EuroHPC/FZJ Germany	JUPITER Booster , BullSequana XH3000, NVIDIA Grace 72C 3GHz, GH200, NVIDIA Infiniband NDR200	4,801,344	1.0	4	6.25	6.3
5	Softbank Japan	CHIE-4 , NVIDIA DGX B200, Xeon Platinum 8570 56C 2.1 GHz, B200 SXM 180GB, Infiniband NDR400	662,256	0.135	17	3.3	24.4
6	AIST Japan	ABCI 3.0 , HPE Cray XD670, Xeon Platinum 48C 2.1GHz, NVIDIA H200 SXM5 141 GB, Infiniband NDR200	479,232	0.145	16	2.36₈ 1.2₁₆	16.3 ₈ 8.3 ₁₆
7	EuroHPC/CSC Finland	LUMI , HPE Cray EX235a, AMD Zen-3 (Milan) 64C 2GHz, AMD MI250X, Slingshot-11	2,752,704	0.380	9	2.35	6.2
8	RIKEN Center for Computational Science, Japan	Fugaku , Fujitsu A64FX 48C 2.2GHz, Tofu D	7,630,848	0.442	7	2.0	4.5
9	EuroHPC/CINECA Italy	Leonardo , BullSequana XH2000, Xeon Pl. 32C 2.6GHz, NVIDIA A100 SXM4 40 GB, QR NVIDIA HDR100 IB	1,824,768	0.241	10	1.8	7.6
10	KAIST Saudi Arabia	Shaheen III , HOE Cray EX254n, NVIDIA Grace 72C 3.1GHz, NVIDIA GH200, Slingshot-11	574,464	0.123	18	0.7	5.7

FP/TF/INT Performance of 5 Generations of NVIDIA GPUs



Feeling like a kid in a candy store



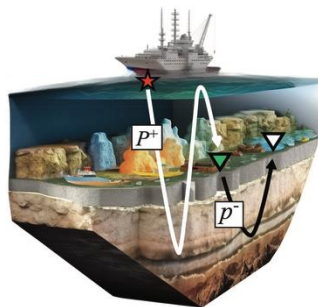
Four Challenging Scientific Applications



Computational Astronomy



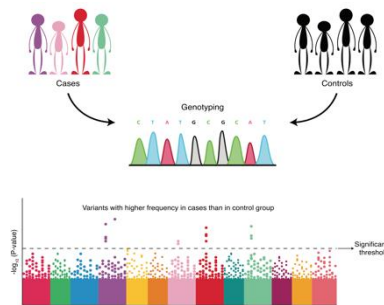
Best Paper
PASC18



Seismic Processing



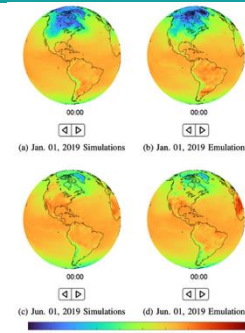
Gordon Bell Finalist
SC23



Computational Biology



Gordon Bell Finalist
SC24



Climate Simulations / Emulations



Gordon Bell Finalist SC22
Gordon Bell Winner SC24

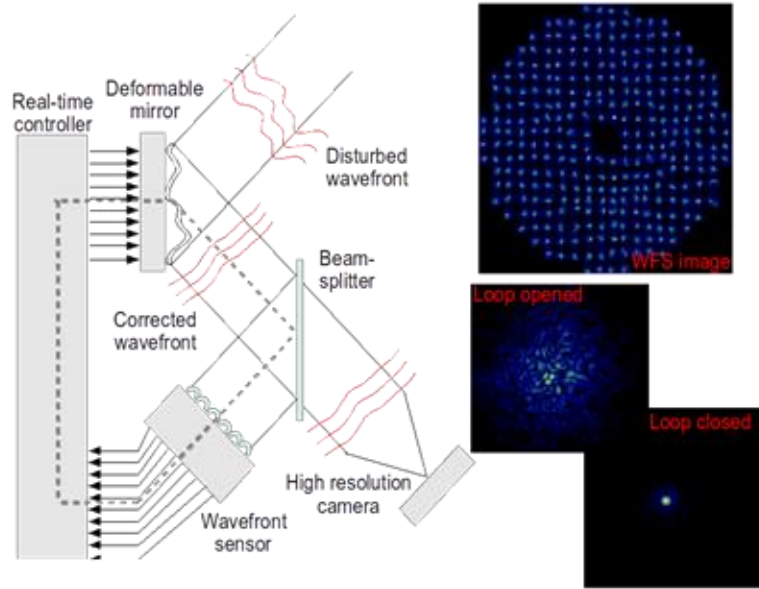
Adaptive optics: outsmarting the atmospheric turbulence



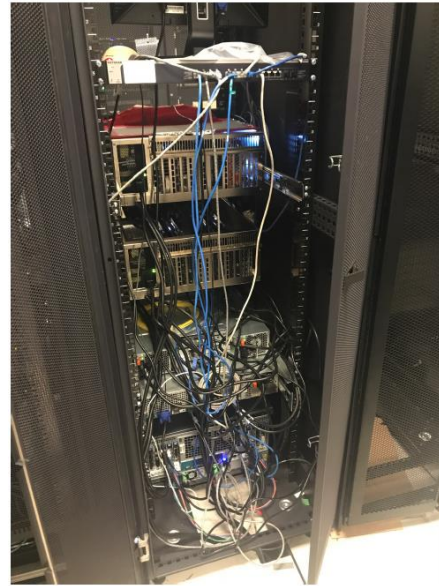
The sun observed with a compact camera

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

Adaptive Optics: tomographic reconstructor, real-time controller



The Advanced Machinery



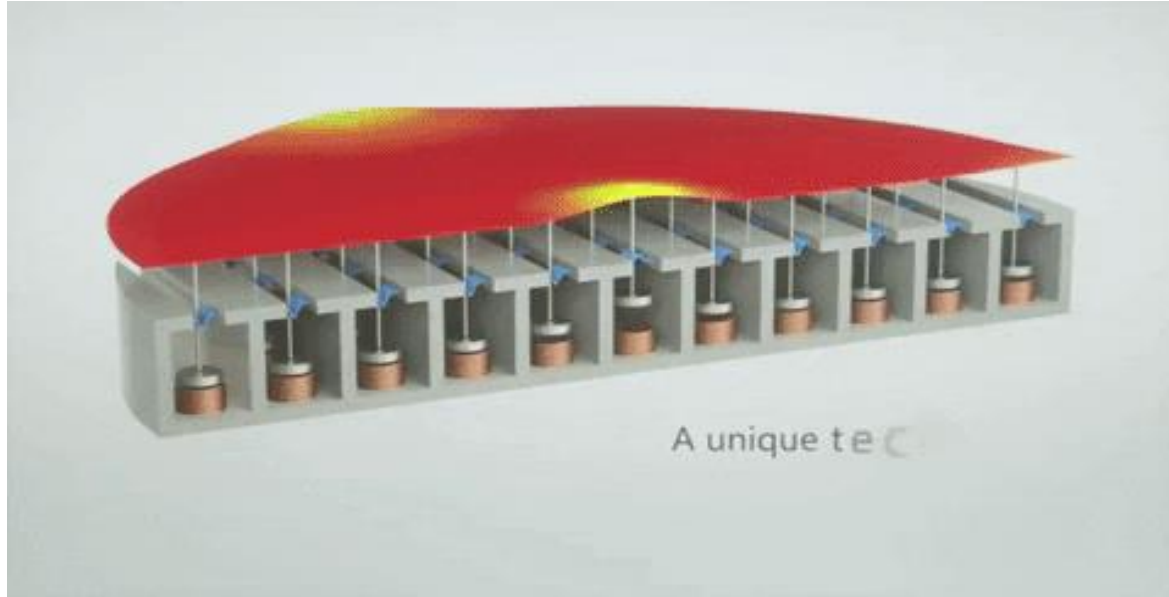
Operating at 14,000 feet



Surviving at 14,000 feet

N. Doucet, HL, D. Gratadour and D. Keyes, *Mixed-Precision Tomographic Reconstructor Computations on Hardware Accelerators*, IEEE/ACM SC19 IA3 Workshop.
HL, D. Sukkari, O. Guyon, and D. Keyes, *Extreme Computing for Extreme Adaptive Optics: The Key to Finding Life Outside our Solar System*, ACM PASC18.
HL, J. Cranney, D. Gratadour, Y. Hong, L. Gatineau, and D. Keyes, *Meeting the real-time challenges of ground-based telescopes using low-rank matrix computations*, IEEE/ACM SC21.

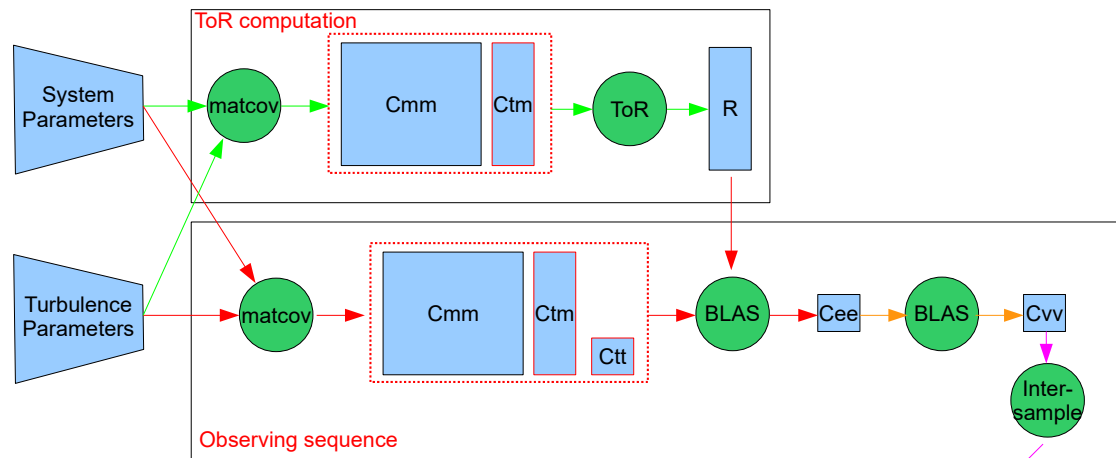
Adaptive Optics: deformable mirrors



A unique telescope

N. Doucet, HL, D. Gratadour and D. Keyes, *Mixed-Precision Tomographic Reconstructor Computations on Hardware Accelerators*, IEEE/ACM SC19 IA3 Workshop.
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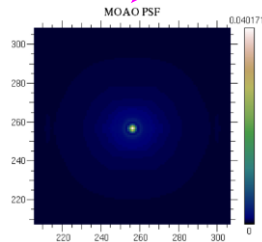
Adaptive Optics: deformable mirrors



$$R = C_{tm} \cdot C_{mm}^{-1}$$

$$C_{ee} = C_{tt} - C_{tm} R^t - R C_{tm}^t + R C_{mm} R^t$$

$$C_{vv} = D^\dagger C_{ee} D^{\dagger t}$$

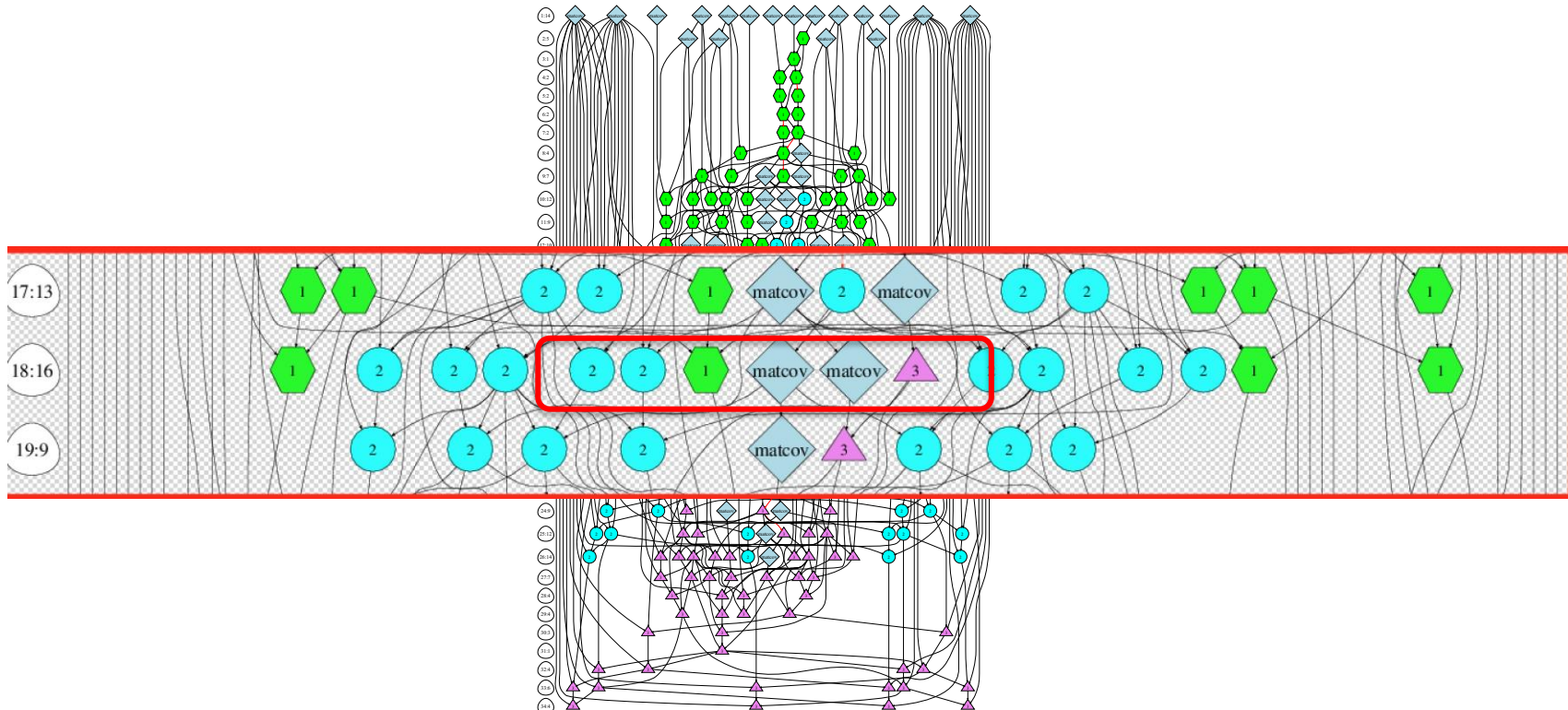


N. Doucet, HL, D. Gratadour and D. Keyes, *Mixed-Precision Tomographic Reconstructor Computations on Hardware Accelerators*, IEEE/ACM SC19 IA3 Workshop.

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HL, J. Cranney, D. Gratadour, Y. Hong, L. Gatineau, and D. Keyes, *Meeting the real-time challenges of ground-based telescopes using low-rank matrix computations*, IEEE/ACM SC21.

Asynchronous Many Tasks Execution



N. Doucet, HL, D. Gratadour and D. Keyes, *Mixed-Precision Tomographic Reconstructor Computations on Hardware Accelerators*, IEEE/ACM SC19 IA3 Workshop.
HL, D. Sukkari, O. Guyon, and D. Keyes, *Extreme Computing for Extreme Adaptive Optics: The Key to Finding Life Outside our Solar System*, ACM PASC18.
HL, J. Cranney, D. Gratadour, Y. Hong, L. Gatineau, and D. Keyes, *Meeting the real-time challenges of ground-based telescopes using low-rank matrix computations*, IEEE/ACM SC21.

The *First* MxP Cholesky Factorization

Algorithm 1 Mixed-Precision Cholesky factorization.

```

1: for k=0..NT-1 do
2:    $A[k][k] \leftarrow \text{spotrf}(A[k][k])$ 
3:   for m=k+1..NT-1 do
4:      $A[m][k] \leftarrow \text{strsm}(A[k][k], A[m][k])$ 
5:      $H[m][k] \leftarrow \text{SP2HP}(A[m][k])$ 
6:   end for
7:   for n=k+1..NT-1 do
8:      $A[n][n] \leftarrow \text{ssyrk}(A[n][k], A[n][n])$ 
9:     for m=n+1..NT-1 do
10:       $\text{precision} \leftarrow \text{heuristic}(m, n)$ 
11:      if precision == float then
12:         $A[m][n] \leftarrow \text{sgemm}(A[m][k], A[n][k], A[m][n])$ 
13:      else if precision == half then
14:        if variant == 1 or 2 then
15:           $H[m][n] \leftarrow \text{SP2HP}(A[m][n])$ 
16:           $H[m][n] \leftarrow \text{hgemm}(H[m][k], H[n][k], H[m][n])$ 
17:           $A[m][n] \leftarrow \text{SP2HP}(H[m][n])$ 
18:        else
19:           $A[m][n] \leftarrow \text{hgemm}(H[m][k], H[n][k], A[m][n])$ 
20:        end if
21:      end if
22:    end for
23:  end for
24: end for

```

TABLE I

32/16-BIT MIXED PRECISION `CUBLASGEMMEX` SUPPORTED FUNCTION.

GEMM variants	A/B type	C type	Compute type	Alpha / Beta
HP3	16-bit	16-bit	16-bit	16-bit
HP2	16-bit	16-bit	32-bit	32-bit
HP1	16-bit	32-bit	32-bit	32-bit
SP	32-bit	32-bit	32-bit	32-bit

The first column will be used to specify the function's precision in the following.

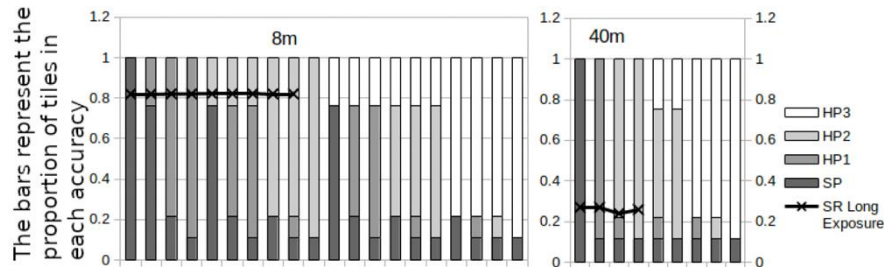
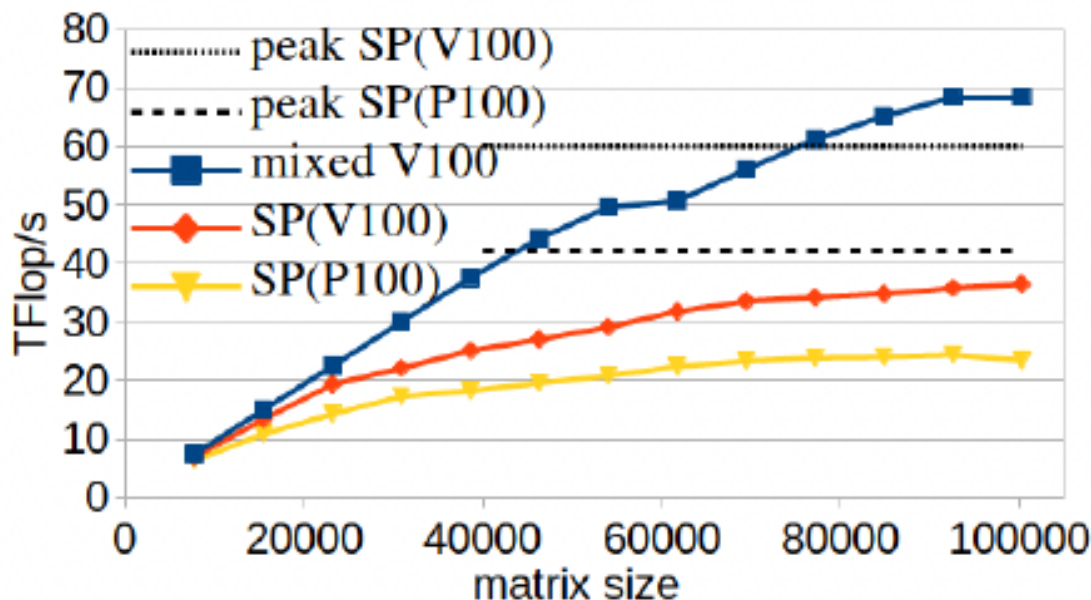
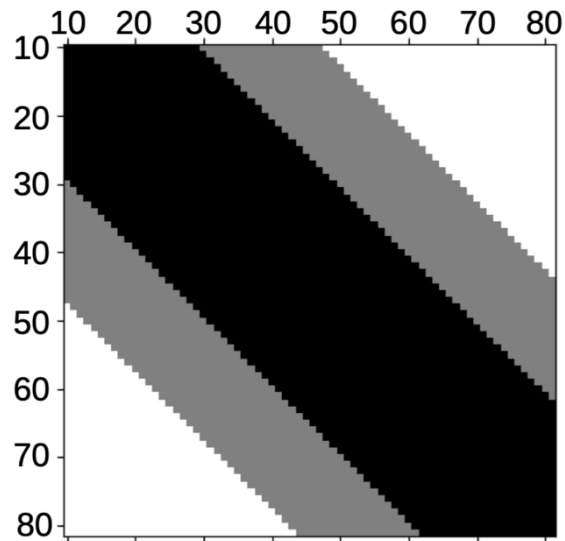


Fig. 5. Proportion of the different GEMM precision and associated ToR accuracy on a eight meter telescope with 17k measurements (left) and an forty meter telescope with 50k measurements (right).

Adaptive Optics: tomographic reconstructor, real-time controller and deformable mirrors

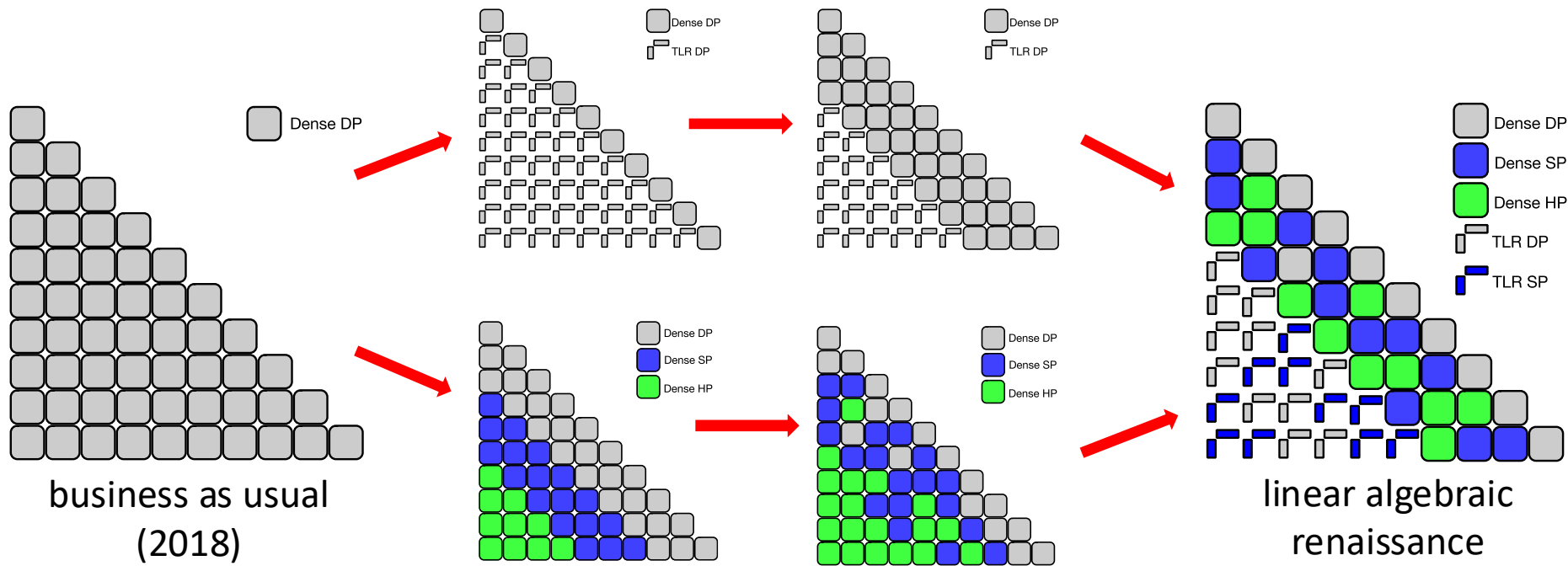


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The journey toward linear algebra *Renaissance*



Don't over-solve: maintain just enough accuracy for the application purpose (2022)

Don't over-store: no extra copies of the original matrix

HiCMA Powered by PaRSEC: Released at SC25

Hierarchical Computations on Manycore Architectures
Powered by the PaRSEC Runtime System

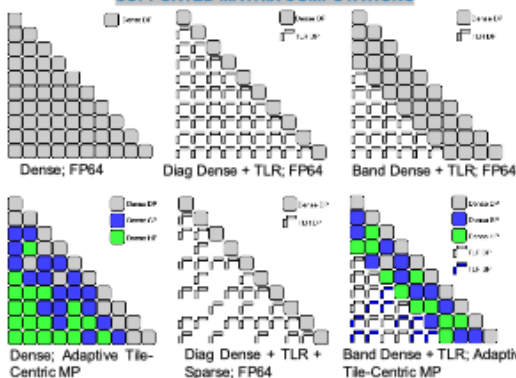
HiCMA

Powered by PaRSEC

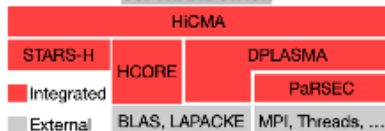
Qinglei Cao, Rabab Alomairy, George Bosilca, Sameh Abdulah, Hatem Ltaief, and David E. Keyes

The Hierarchical Computations on Manycore Architectures (HiCMA) library, which is powered by the PaRSEC runtime system, extends dense linear algebra libraries toward hierarchical computations on distributed many-core, heterogeneous architectures. The core idea of HiCMA is to develop fast linear algebra computations on dense, low-rank, mixed-precision, and sparse data formats for scientific and AI applications, while satisfying specified numerical accuracy and leveraging massively parallel heterogeneous hardware.

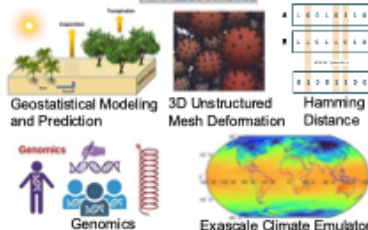
SUPPORTED MATRIX COMPUTATIONS



SOFTWARE STACK



APPLICATIONS



CURRENT FEATURES

- Matrix Computations:** Cholesky factorization, Matrix-matrix multiplication, Symmetric rank k update
- Tile-Centric Mixed-Precision** (FP64, FP32, FP16, FP8, INT8, 1Bit), **Tile Low-Rank** (TLR) Approximation, and **Sparse** Computations
- Memory Layout:** LAPACK and DPLASMA/tile
- Hardware Supports:** CPUs and GPUs (Nvidia and AMD), Shared and distributed-memory environments

FUTURE DIRECTIONS

- Julia Integration
- LU and QR Factorizations
- Tile Low-Rank on GPUs
- Sparse Direct Solvers
- NVIDIA CUTLASS
- Precision Emulation

GITHUB REPO



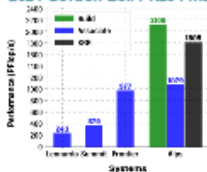
2024 Gordon Bell Prize for Climate Modelling



Paper: Boosting Earth System Model Outputs and Saving Petabytes in Their Storage Using Exascale Climate Emulators

Stochastically capture spatio-temporal variability, accelerate computation, improve emulator accuracy, and yield insights on climate change and extremes.

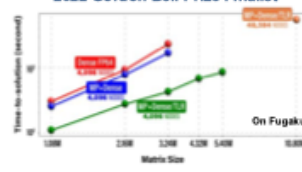
2024 Gordon Bell Prize Finalist



Paper: Toward Capturing Genetic Epistasis from Multivariate Genome-Wide Association Studies Using Mixed-Precision Kernel Ridge Regression

Enhance Kernel Ridge Regression (KRR) and achieve a performance improvement of five orders of magnitude over the state-of-the-art CPU-only REGEM

2022 Gordon Bell Prize Finalist



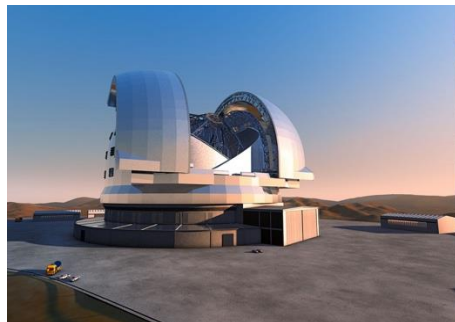
Paper: Reshaping Geostatistical Modeling and Prediction for Extreme-Scale Environmental Applications

Extend the capability of space-time geostatistical modeling using algebraic approximations and illustrate application-expected accuracy worthy of double precision from majority low-precision computations and low-rank matrix approximations.

A collaboration of



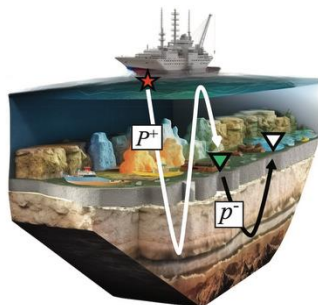
Four Challenging Scientific Applications



Computational Astronomy



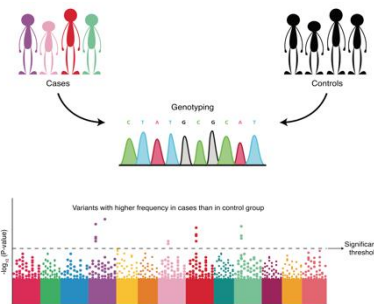
Best Paper
PASC18



Seismic Processing



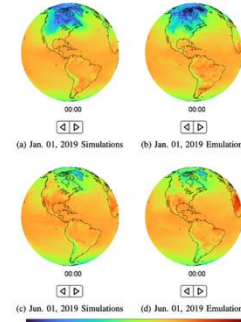
Gordon Bell Finalist
SC23



Computational Biology



Gordon Bell Finalist
SC24

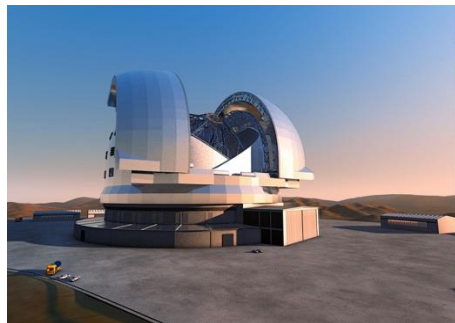


Climate Simulations / Emulations



Gordon Bell Finalist SC22
Gordon Bell Winner SC24

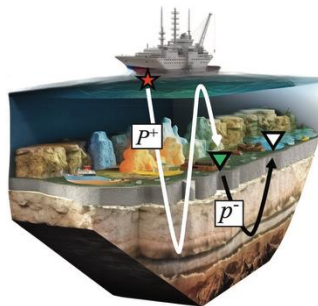
Four Challenging Scientific Applications



**Computational
Astronomy**



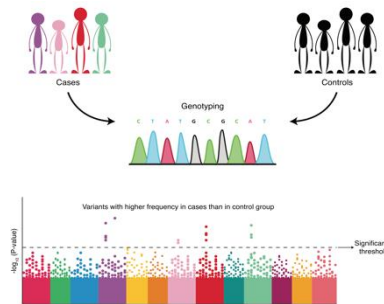
Best Paper
PASC18



**Seismic
Processing**



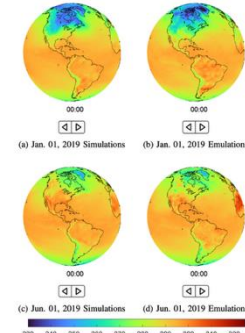
Gordon Bell Finalist
SC23



**Computational
Biology**



Gordon Bell Finalist
SC24



**Climate
Simulations / Emulations**



Gordon Bell Finalist SC22
Gordon Bell Winner SC24

Challenges with ML-based Climate/Weather Forecasting Simulations

- Today, weather and climate data are usually **huge**!
 - A set of univariate/multivariate **Z observations** $\in \mathbb{R}^n$ at given **n** locations on one or more time slots.
 - **Z observations** could be temperature, precipitation, humidity, air pollution ... etc
- **Maximum Likelihood Function**: a statistical approach used to estimate the parameters of a model. This method is particularly useful in spatial analysis due to its ability to handle complex spatial dependencies and heterogeneity

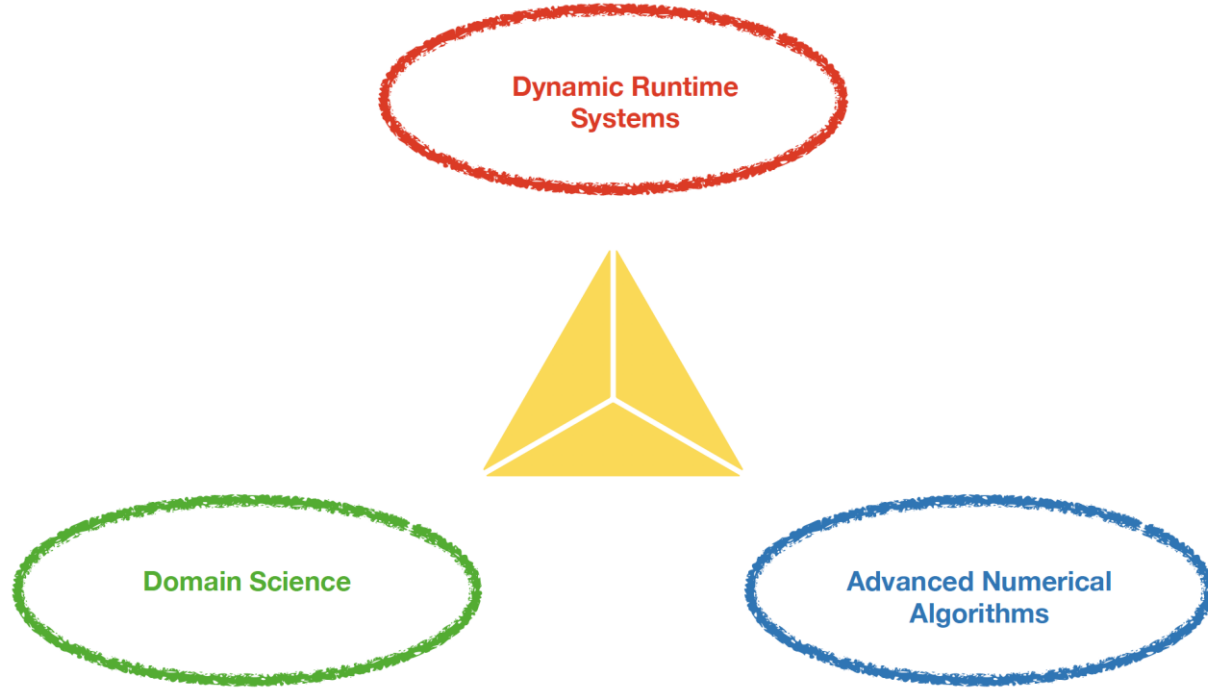
- Prohibitive computational Cost and memory requirements:

$$l(\theta) = -\frac{1}{2}Z^T\Sigma(\theta)^{-1}Z - \frac{1}{2}\log|\Sigma(\theta)|$$

$\Sigma(\theta)$

- The linear solver and log-determinant involving floating point operations on **n -by- n** covariance matrix **$\Sigma(\theta)$** with **$O(n^3)$** complexity and **$O(n^2)$** memory footprint
 - For instance: **10^6** locations require **8TB** Memory!

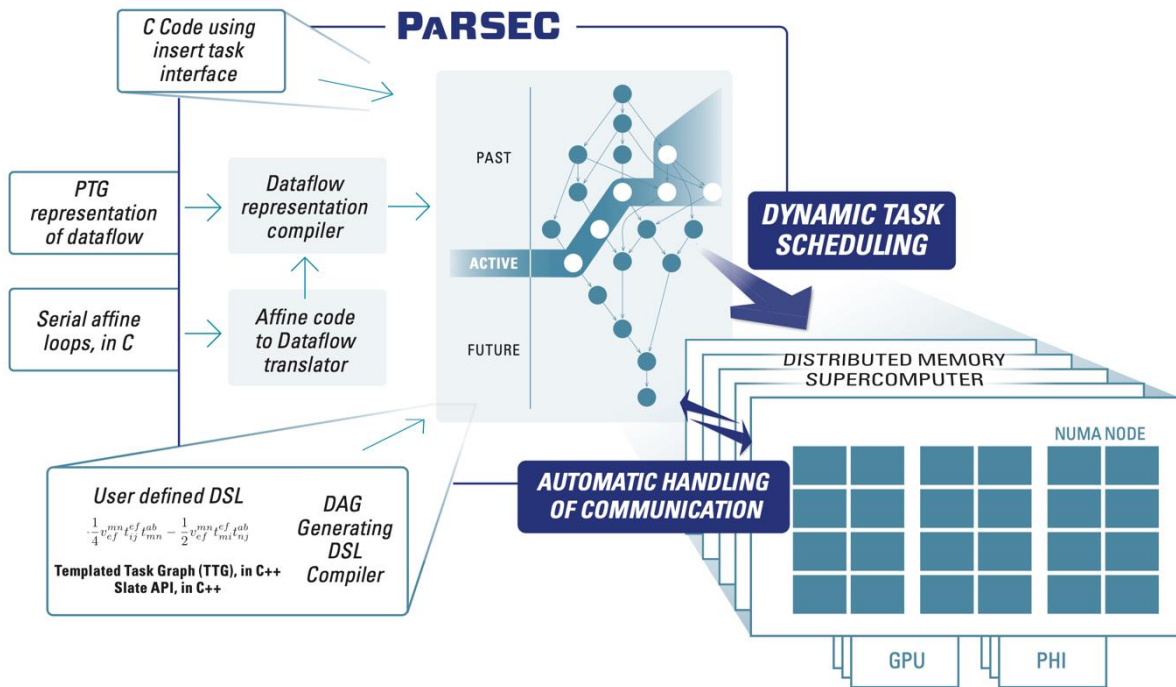
Key Approach Based on a Separation of Concerns



PaRSEC: a dynamic runtime system of the DOE ECP

DAG: directed acyclic graph
PTG: parameterized task graph
DSL: domain specific language

Master
Of
Ceremonies

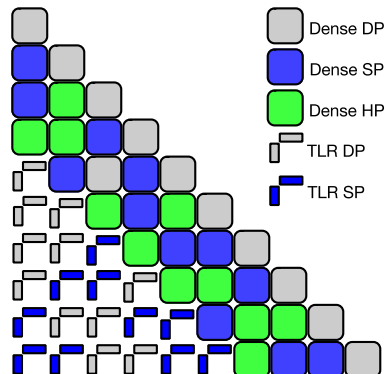


Elapsed Time and Energy Consumption on Shaheen-III

# Nodes	Problem Matrix Size	Time (s) Dense FP64	Time (s) SC		Time (s) MC		Time (s) WC	
			Dense+MP	TLR+MP	Dense+MP	TLR+MP	Dense+MP	TLR+MP
256	2.16M	2859	2847	1036	2180	921	1600	891
512	3.24M	4745	4742	1791	3009	1579	2649	1470
1024	4.32M	4910	4907	2213	4361	1906	3191	1767
2048	6.22M	6202	6207	3890	5575	3206	4962	2456

2020 MJ

linear algebraic
renaissance
(2022)



1065 MJ

575 MJ



Can we do more? Microscaling coming to rescue

Open Compute Project • OCP Microscaling Formats (MX) Specification



OPEN
Compute Project

OCP Microscaling Formats (MX) Specification

Version 1.0

Format Name	Element Data Type	Element Bits (d)	Scaling Block Size (k)	Scale Data Type	Scale Bits (w)
MXFP8	FP8 (E5M2)	8	32	E8M0	8
	FP8 (E4M3)				
MXFP6	FP6 (E3M2)	6	32	E8M0	8
	FP6 (E2M3)				
MXFP4	FP4 (E2M1)	4	32	E8M0	8
MXINT8	INT8	8	32	E8M0	8

Table 1. Format names and parameters of concrete MX-compliant formats.

1. License

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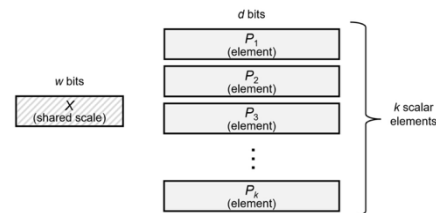
AMD, Arm, Intel, Meta, Microsoft, NVIDIA, Qualcomm

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5.1 Microscaling (MX)

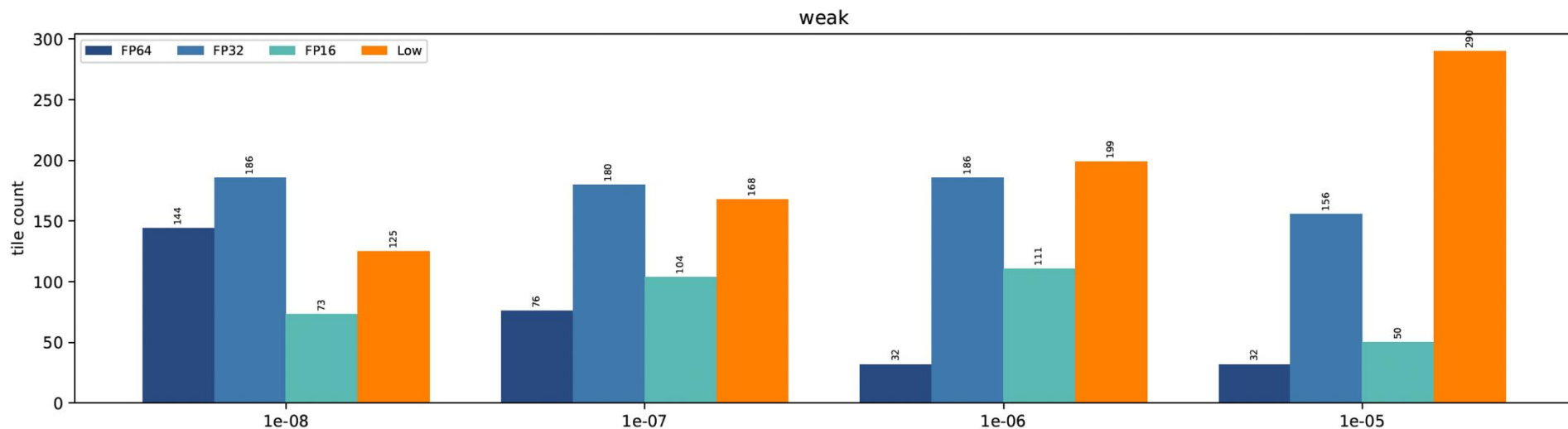
An MX-compliant format is characterized by three components:

- Scale (X) data type / encoding
- Private elements (P_i) data type / encoding
- Scaling block size (k)



Can we do more? Microscaling coming to rescue

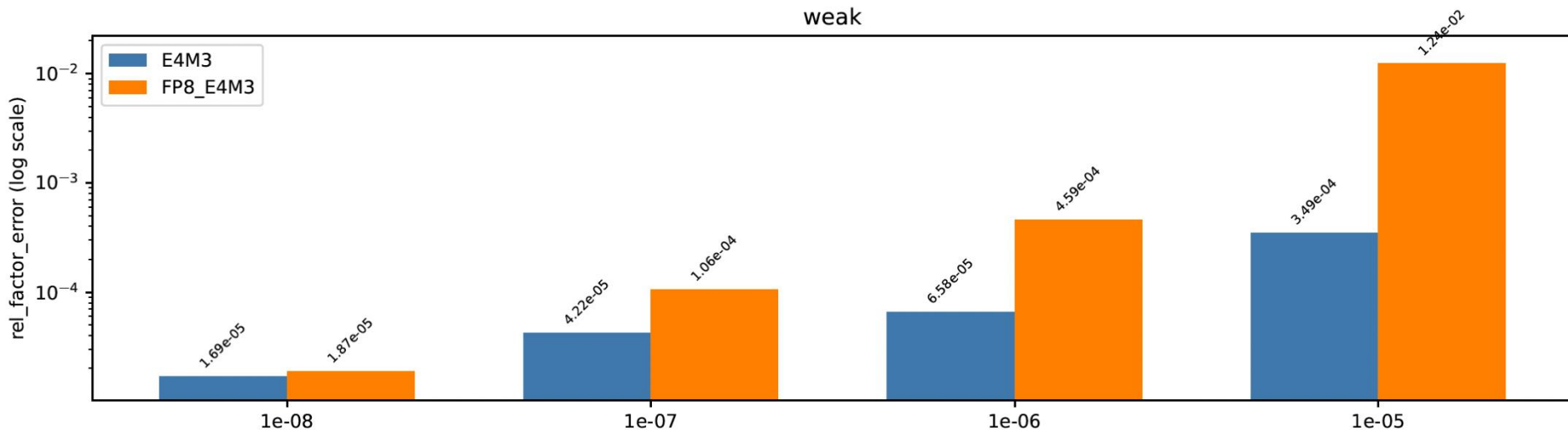
Figure 2 (n=8192, mode=block, nb=256): tile counts for FP32+FP16 bucket (FP64, FP32, FP16, Low)



w/ A. Abdurakhmanov / S.
Fahmy / D. Keyes @KAUST
and T. Mary @Sorbonne

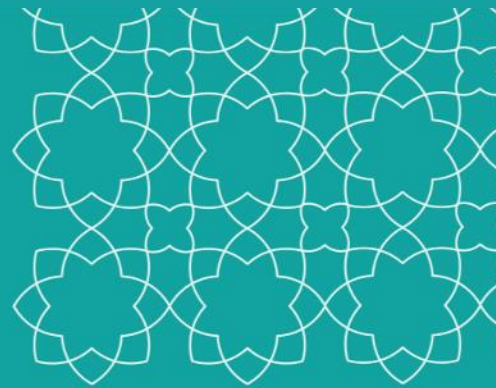
Can we do more? Microscaling coming to rescue

Figure 1 (n=8192, mode=block, nb=256): FP32+FP16 bucket, E4M3 vs FP8_E4M3



w/ A. Abdurakhmanov / S.
Fahmy / D. Keyes @KAUST
and T. Mary @Sorbonne

Do Linear Algebra, See the World!



Thanks,

QUESTIONS?