Efficient Computation Through Tuned Approximation

ATPESC 2024

جامعة الملك عبدالله
للعلوم والتقنية
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Science and Technology

David Keyes
and the HiCMA group of KAUST's
Extreme Computing Research Center

Alternative titles

"How to get *four* Gordon Bell Prize Finalist nominations (and counting!) out of *one* simple idea"

"Do linear algebra; see the world!"

Earl Blossom, 1891-1970

ATPESC – What is “extreme” in computing?

Can be “extreme” in:

- scale (as in number of nodes or cores)
- low memory bandwidth per core (as in CPUs)
- low memory capacity per core (as in GPUs)
- low power constraints (as in battery-operated or remote “edge” processors, such as sensors, telescopes, satellites)
- real-time constraints (as in data-streaming apps, like analyzing what comes off particle colliders)
- long running times (as in low-scaling apps, like many density functional theory and molecular dynamics apps)

Some home-grown software targeting extremes

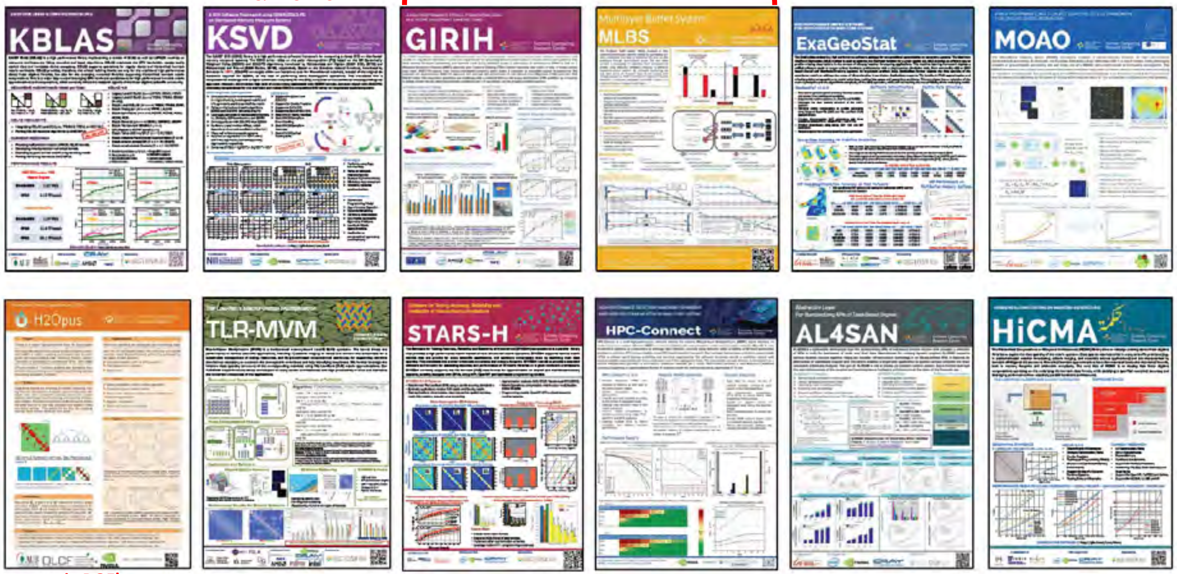
in NVIDIA cuBLAS & NEC NLC

in Cray LibSci & NEC NLC

in Aramco ExaWave

R interface

on sky in Suburu



in DOE's Strumpack

in PyLOPS & MAVIS

Updated annually for SC'xy , at https://github.com/ecrc

Externally hosted software, too

PETSc

Two PETSc developers with extensive line commits are in the ECRC:

Lisandro Dalcin
PETSc, petsc4py, mpi4py, mpi4py-fft, shem4py, …

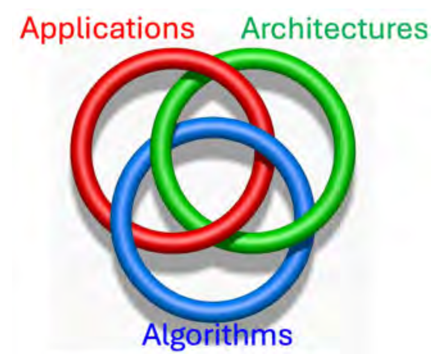
Stefano Zampini
PETSc, OpenFOAM, deal.ii, MFEM, CEED, …

Conclusions, up front

As computational infrastructure demands a growing sector of research budgets and global energy expenditure, we must *all* address the need for greater efficiency

As a community, we have excelled at this historically in three aspects:

- architectures
- applications (redefining *actual outputs of interest*)
- algorithms



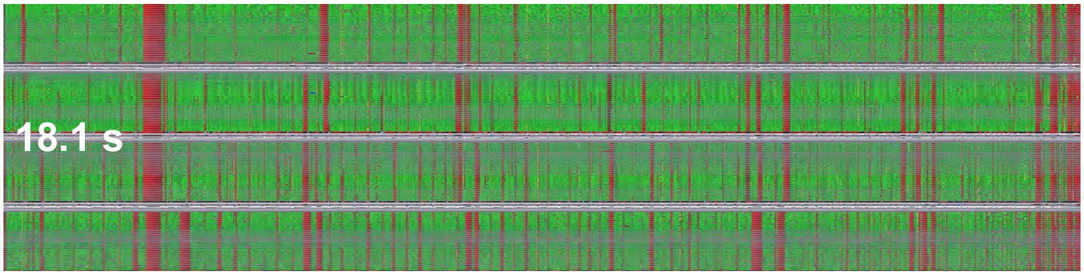
There are *new algorithmic* opportunities in:

- reduced rank representations
- reduced precision representations

Our journey in tuned approximation began in 2018 with these time traces for tile low-rank (TLR) Cholesky

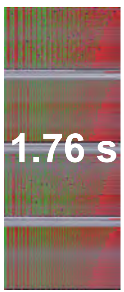
… for factorization of a dense 54K covariance matrix on four 32-core nodes of a Cray XC-40

Dense Tile-based Cholesky factorization (Chameleon)



time →

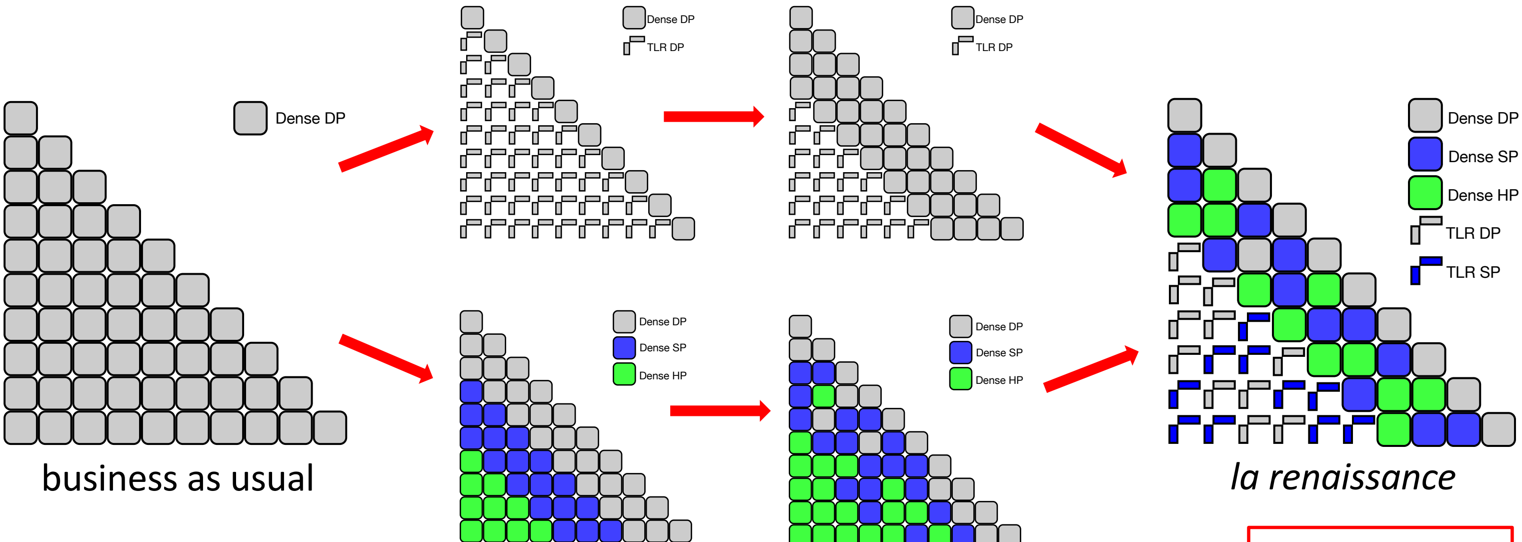
Tile low rank (TLR) Cholesky factorization (HiCMA)



- TLR may score a lower percentage of peak (after squeezing out flops)
- TLR may have poorer load balance (a higher percentage of idle time (red) vs. computation (green))
- TLR may scale less efficiently (less able to cover data motion with computation)
- TLR is, however, **10X superior in time** for required application accuracy, at **about 65% of average power** compared to dense

Akbudak, Ltaief, Mikhalev, Charara & K., *Exploiting Data Sparsity for Large-scale Matrix Computations,* Euro-Par 2018

Computational efficiency through *tuned approximation*: a journey with *tile low rank* and *mixed precision*

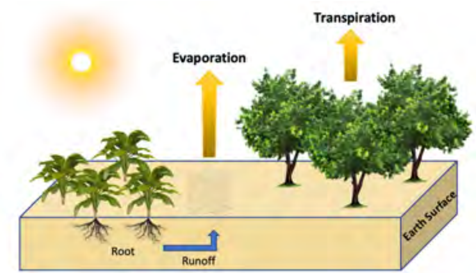


Don’t oversolve: maintain just enough accuracy for the application purpose
Economize on storage: no extra copies of the original matrix

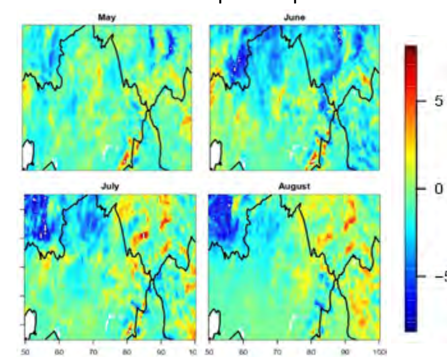
Now using four precisions: FP64, FP32, FP16 & FP8

Efficiency (“science per Joule”) improvement in HPC?

- We consider 3 categories of efficiency improvement
  - from architectures, applications, algorithms
- In 2022, 2023, and a pair of 2024 Gordon Bell finalist papers
- Through efficiency improvements in inner linear algebra operations from exploiting
  - rank structure (related to correlation smoothness)
  - precision structure (related to correlation magnitudes)



time series evapotranspiration



Time-to-solution addresses the energy "elephant"

Frontier (#1 on Top500) delivers about 1 Exaflop/s at about 50 Gigaflop/s per Watt

- **20 MegaWatts consumed continuously**

Representative electricity cost in US is $ 0.20 per KiloWatt-hour

- **$ 200 per MegaWatt-hour**

Powering an exaflop/s system costs about $ 4,000 per hour

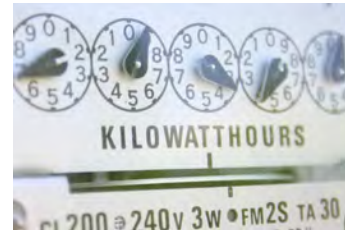
- 10 Kilohour per year (8,760, to be more precise)

→ $40 million annual electricity bill for an exaflop/s system

Carbon footprint of a KiloWatt-hour is about 0.5 kg CO2-equivalent

- 10,000 kg CO2e hourly carbon footprint for an exaflop/s system
- 100,000 metric tons CO2e annually

→ equivalent to 20,000 typical passenger cars in the USA



A 10% improvement:
saves $4M/year
takes 2,000 cars off the road

A 10X improvement:
saves $36M/year
takes 18,000 cars off the road

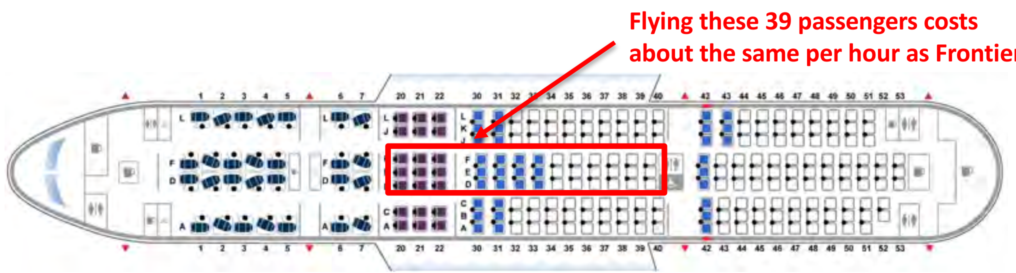
10X is actually achievable in many use cases

CO2 production equivalents

"Science per Joule" is a matter of planetary stewardship

Running on Frontier versus flying commercially

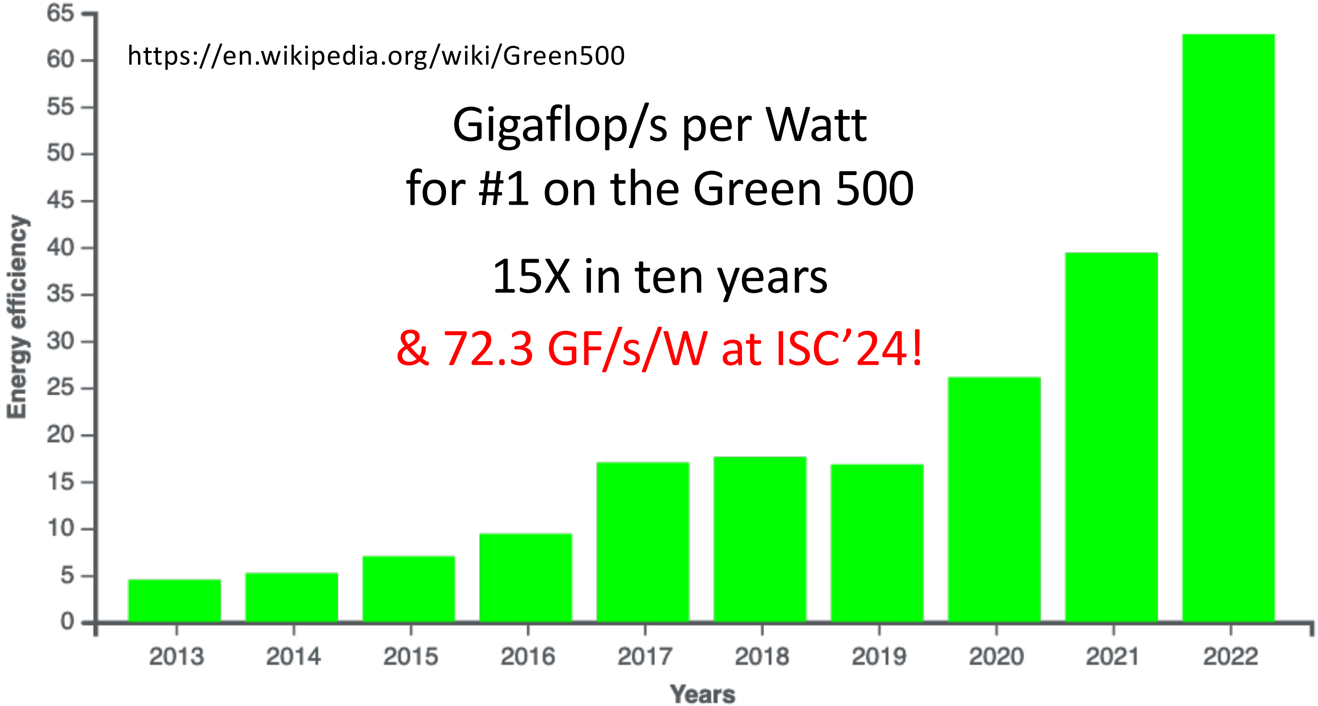
- Carbon footprint of a KiloWatt-hour is 0.5 kg CO2-equivalent
  - 10,000 kg CO2e hourly carbon footprint for an exaflop/s system (10 metric tons)
- Carbon footprint of one passenger-hour of commercial cruise Mach flight is about 0.25 metric tons CO2e
  - 1 hour of exaflop/s is roughly equivalent to 40 passenger-hours of flight



Carbon offset your next flight by efficient programming!

Better yet, please justify my flight here to give this talk ☺

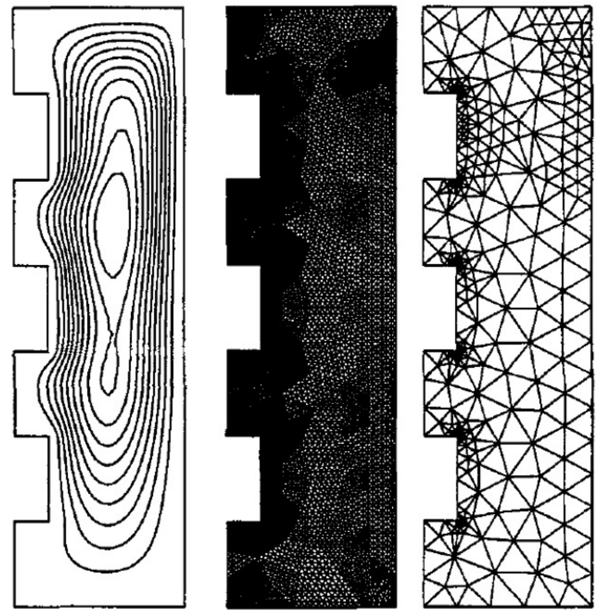
Architecture efficiency tracked by the Green 500



Application “efficiency” from redefining the objective

Sometimes, the output of interest from a computation is not a solution to high accuracy everywhere, but a *functional* of the solution to a *specified accuracy*, e.g.

- compute the convective heat flux across a fluid-solid boundary, obtainable without globally uniform accuracy
- use low fidelity surrogates in early inner iterations of “outer loop problems”



temperature contour — conservative mesh — output bound mesh (flux to 1%)

Machiels, Peraire & Patera, *A posteriori FE Output Bounds for the Incompressible NS Equations*, (2001), J. Comp. Phys. **172**:401

HPC algorithmic efficiency tracked by Poisson solvers

Consider a Poisson solve in a 3D n x n x n box; natural ordering gives bandwidth of n^2

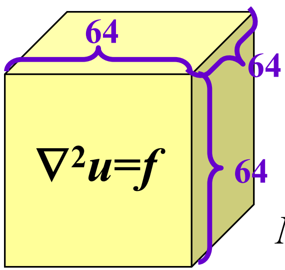
Year	*Method*	*Reference*	*Storage*	*Flops*
1947	**GE (banded)**	**Von Neumann & Goldstine**	n^5	n^7
1950	**Optimal SOR**	**Young**	n^3	$n^4 \log n$
1971/77	**MILU-CG**	**Reid/Van der Vorst**	n^3	$n^{3.5} \log n$
1984	**Full MG**	**Brandt**	n^3	n^3

If $n = 64$, this implies an overall reduction in flops of ~16 million *

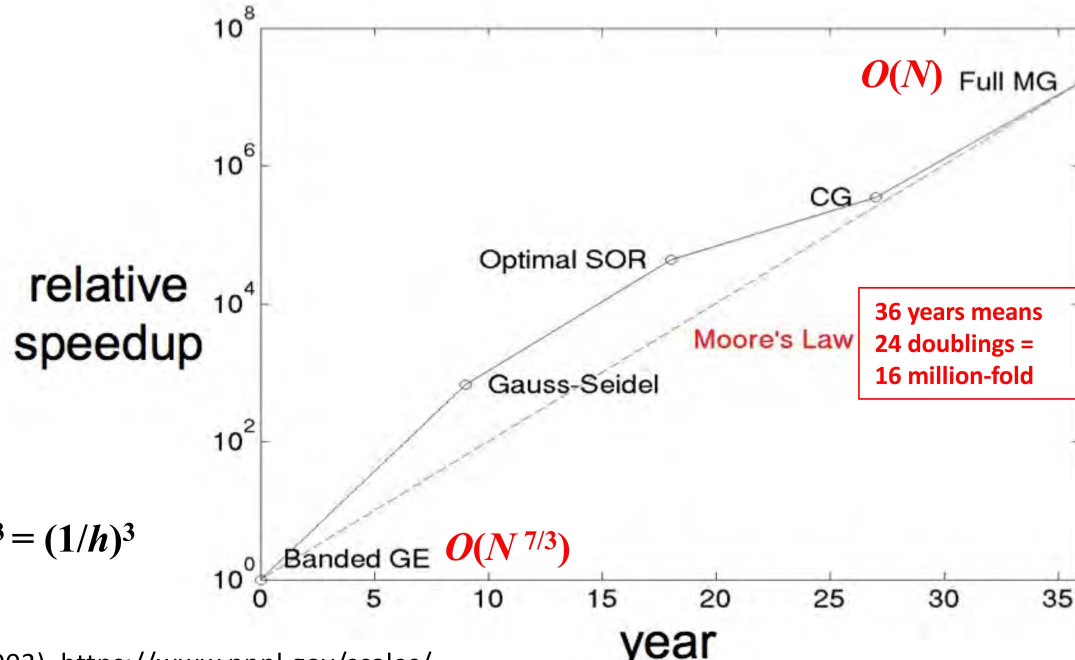
*Six months is reduced to 1 second (recall: 3.154 x 10^7 seconds per year)

“Algorithmic Moore’s Law”

HPC progresses even faster in algorithms than in hardware: *example of Poisson’s equation in a 3D box with 2nd-order FD*



$N = n^3 = (1/h)^3$



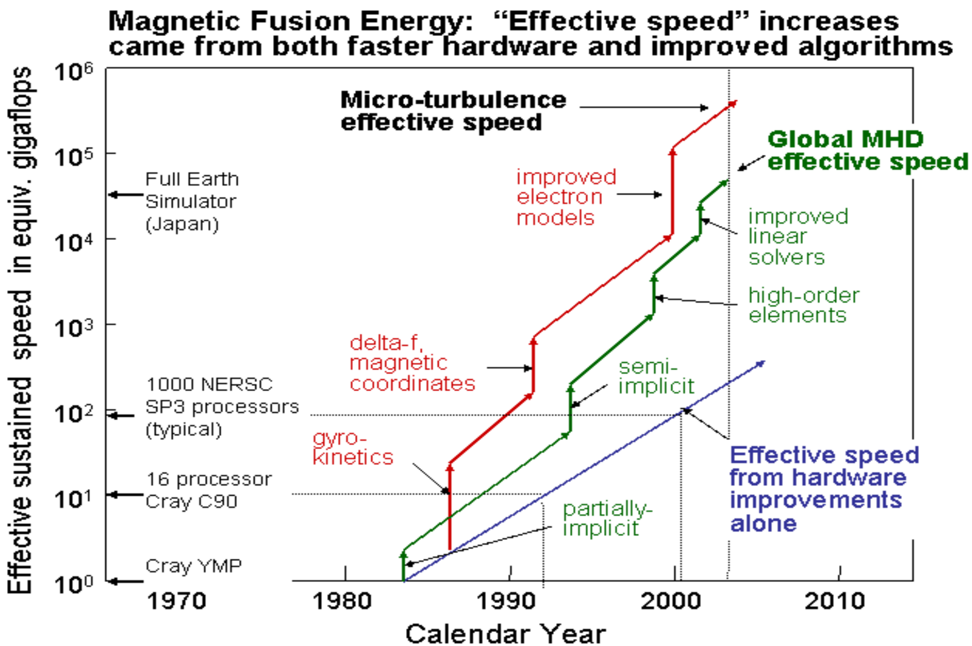
Keyes *et al*., SCaLeS Rpt. Vol. 1 (2003), https://www.pnnl.gov/scales/

“Algorithmic Moore’s Law” for fusion energy simulations

GKT in red

MHD in green

Moore’s Law in blue



“Semi-implicit”:

All waves treated implicitly, but still stability-limited by transport

“Partially implicit”:

Fastest waves filtered, but still stability-limited by slower waves

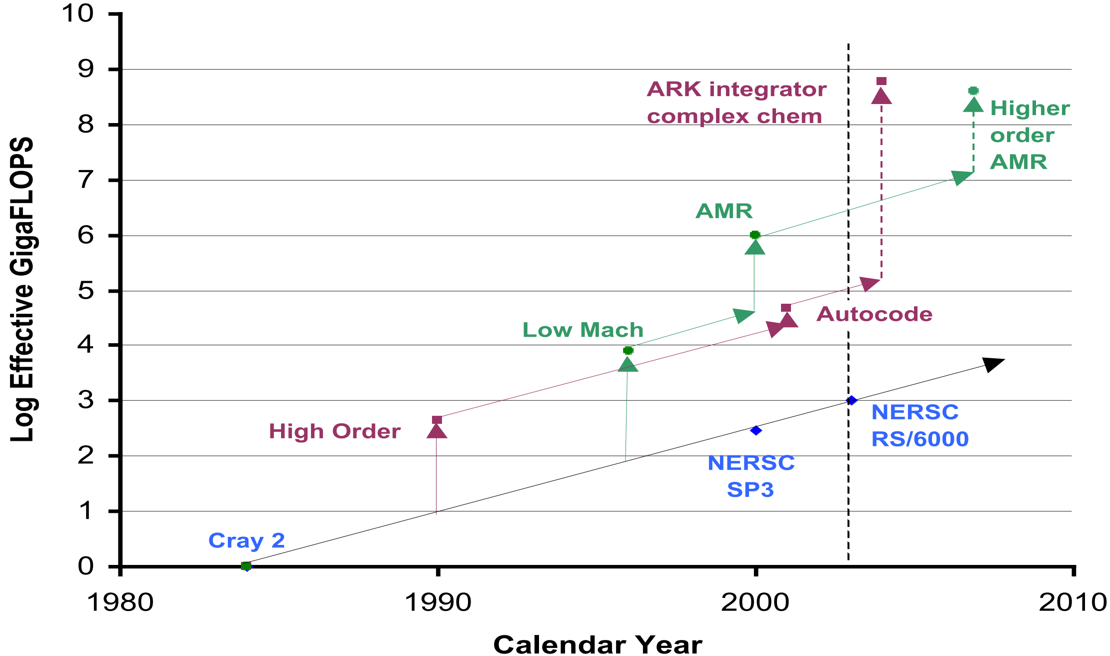
Keyes *et al.*, SCaLeS Rpt. Vol 2 (2004), https://www.pnnl.gov/scales/

“Algorithmic Moore’s Law” for combustion simulations

Complex kinetics in maroon

CFD in green

Moore’s Law in blue



Keyes *et al.*, SCaLeS Rpt. Vol. 2 (2004), https://www.pnnl.gov/scales/

Algorithms improve exponents; Moore only adjusts the base

- To scale to extremes, one must start with algorithms with optimal asymptotic complexity, $O(N \log^p N)$, $p = 0, 1, 2$
- These are typically (not exclusively) recursively hierarchical
- Some such algorithms through the decades:
  - Fast Fourier Transform (1960's): $N^2 \rightarrow N \log N$
  - Multigrid (1970's): $N^{4/3} \log N \rightarrow N$
  - Fast Multipole (1980's): $N^2 \rightarrow N$
  - Sparse Grids (1990's): $N^d \rightarrow N (\log N)^{d-1}$
  - $\mathcal{H}$ matrices (2000's): $N^3 \rightarrow k^2 N (\log N)^2$
  - Multilevel Monte Carlo (2000's): $N^{3/2} \rightarrow N (\log N)^2$
  - Randomized matrix algorithms (2010's): $N^3 \rightarrow N^2 \log k$
  - ??? (2020's): ??? → ??? (*your* challenge!)

Hints for contributions for the 2020's

You are going to replace inefficient first-order convergent neural network training methods by, e.g.,

- communication-reducing hierarchically preconditioned second-order methods
- matrix-free nonlinear acceleration methods

You are going replace inefficient ML inference by, e.g.,

- by pruned, compressed forms of "attention"

"With great computational power comes great algorithmic responsibility."
– Longfei Gao, ALCF (PhD 2013, KAUST)

Hints for contributions for the 2020's

You are going to attach QPUs to classical supercomputers to farm out tasks that offer exponential speedup over their classical counterparts

- when offered sufficiently many sufficiently reliable qubits to confer quantum advantage

You are going master hybridized mod-sim/ML/QC workflows

- using few instances of high fidelity, high resolution simulations supplemented by many instances of machine-learned surrogates
- each modality being employed where it is the most energy efficient

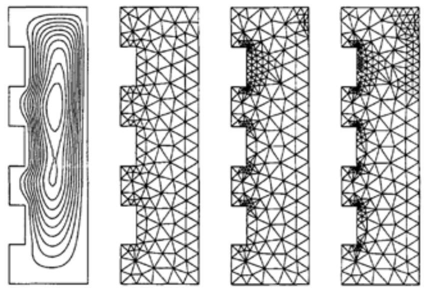
"With great computational power comes great algorithmic responsibility."
– Longfei Gao, ALCF (PhD 2013, KAUST)

Science per Joule – summary so far

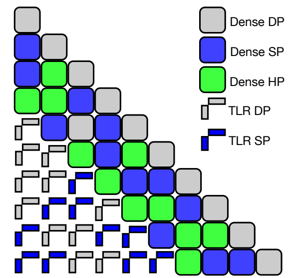
Improving the "science per Joule" (or per unit time) involves:

architecture

application



algorithm/software



In a fortunate world, these are orthogonal: the *desired app* can employ the *best algorithm* on the most *efficient hardware.*

Algorithmic "secret sauce"

Where possible, without losing accuracy:

- Replace default double precision (64-bit IEEE standard) with lower precisions
  - Save storage
  - Save data motion
  - Exploit special-purpose hardware optimized for low precision
- Replace default full rank blocks of discrete linear operators or discrete field data with lower rank blocks
  - Save storage
  - Save data motion
  - Exploit special-purpose hardware optimized for BLAS3

Two natural questions

- How did double precision become the default for scientific computing in the first place?
  - When should we be cautious of low precision?

- What is the intuition behind low-rank approximation?
  - When should we expect it to be practical?

Lessons from the 1D Laplacian

Two concepts we need to understand in our pursuit of computational efficiency in linear algebra:

- conditioning (implications on precision)
- rank structure (implications on sparsification)

can be motivated with reference to the 1D Laplacian (to be precise, its negative $-\Delta$), discretized here to second-order in FD, FE, or FV:

$$\begin{bmatrix} 2 & -1 & & & & & \\ -1 & 2 & -1 & & & & \\ & -1 & 2 & -1 & & & \\ & & -1 & 2 & -1 & & \\ & & & -1 & 2 & -1 & \\ & & & & -1 & 2 & -1 \\ & & & & & -1 & 2 \end{bmatrix}$$

Laplacian ill-conditioned stresses precision

Let $n = 1/h$ and consider Dirichlet end conditions with n**-1** interior points. Then:

$$\lambda_1 \;= 2\,[1 - \cos \pi/n] \qquad \sim (\pi/n)^2$$
$$\lambda_{n-1} = 2\,[1 - \cos (n-1)\pi/n] \;\sim\; 4$$

As n gets large and the mesh resolves more Fourier components, the condition number grows like the square of the matrix dimension (inverse mesh parameter):

$$\kappa \;=\; \lambda_{n-1} / \lambda_1 \;\sim\; (4/\pi^2)\, n^2$$

In single precision real arithmetic, κ approaches the reciprocal of macheps (10^{-7}) for an n as small as 2^{10} ($\sim 10^3$). Laplacian-like operators arise throughout modeling and simulation (diffusion, electrostatics, gravitation, stress, graphs, etc.), implying $O(1)$ error in the result, so HPC has traditionally demanded double precision by default. GPUs were accepted only when they offered hardware DP (2008, NVIDIA GTX 280).

For the biharmonic, even double precision gives out at $n = 2^{10}$. Some multiscale codes require quadruple precision, often available only in software.

Laplacian off-diagonal smoothness relaxes ranks

A is full-rank, but its off-diagonal blocks have low rank

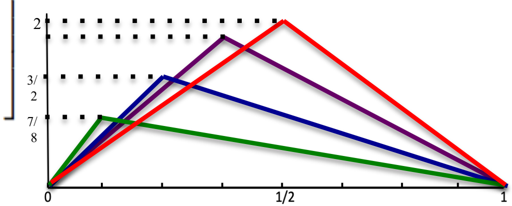
$$A = \left[\begin{array}{ccc|cccc} 2 & -1 & & & & & \\ -1 & 2 & -1 & & & & \\ & -1 & 2 & -1 & & & \\ \hline & & -1 & 2 & -1 & & \\ & & & -1 & 2 & -1 & \\ & & & & -1 & 2 & -1 \\ & & & & & -1 & 2 \end{array}\right]$$

$$\Leftrightarrow \; = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \begin{bmatrix} -1 & 0 & 0 & 0 \end{bmatrix}$$

Its inverse is dense, but it inherits the same rank structure

$$A^{-1} = \frac{1}{8} \times \left[\begin{array}{ccc|cccc} 7 & 6 & 5 & 4 & 3 & 2 & 1 \\ 6 & 12 & 10 & 8 & 6 & 4 & 2 \\ 5 & 10 & 15 & 12 & 9 & 6 & 3 \\ \hline 4 & 8 & 12 & 16 & 12 & 8 & 4 \\ 3 & 6 & 9 & 12 & 15 & 10 & 5 \\ 2 & 4 & 6 & 8 & 10 & 12 & 6 \\ 1 & 2 & 3 & 4 & 5 & 6 & 7 \end{array}\right]$$

$$\Leftrightarrow \; = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} \begin{bmatrix} 4 & 3 & 2 & 1 \end{bmatrix}$$

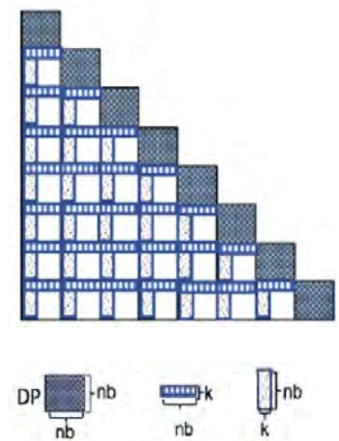


A renaissance in numerical linear algebra (1)

It turns out that many formally dense matrices arising from

- **integral equations** with smooth Green's functions
- **covariances** in statistics
- **Schur complements** within discretizations of PDEs
- **Hessians** from PDE-constrained optimization
- **nonlocal operators** from fractional differential equations
- **radial basis functions** from unstructured meshing
- **kernel matrices** from GWAS & machine learning applications

have exploitable low-rank structure in "most" their off-diagonal blocks (if well ordered)

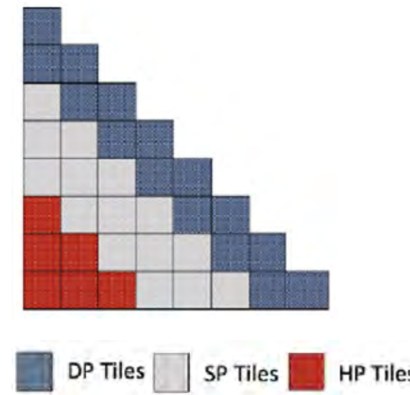


A renaissance in numerical linear algebra (2)

It turns out that many matrices arising in applications have blocks of **relatively small norm** and can be replaced with **reduced precision.**

Mixed precision algorithms have a long history, e.g., iterative refinement (1963, Wilkinson), where multiple copies of the matrix are kept in different precisions for different purposes.

There are many such new algorithms; see Higham & Mary, *Mixed precision algorithms in numerical linear algebra*, Acta Numerica (2022).



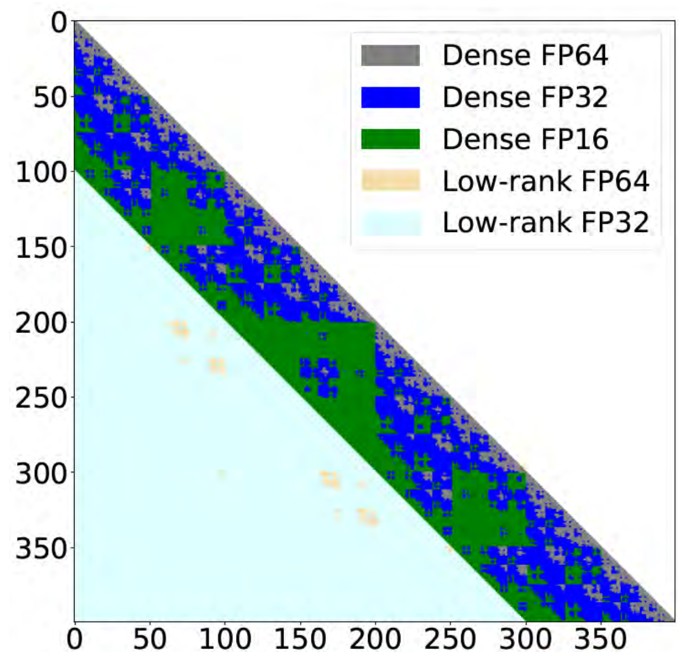
A renaissance in numerical linear algebra (3)

Moreover, these ideas can be combined, as in this 1M x 1M dense symmetric covariance matrix:

- Original in DP: 4 TB
- Replacement: 0.915 TB

Smaller workingsets mean larger problems fit in GPUs and last-level caches on CPUs, for data movement savings

- Also, net computational savings
- Data structures and programs are more complex



Rank: a tuning knob

- Replace dense blocks with reduced rank representations, whether "born dense" or as arising during matrix operations
  - use high accuracy (high rank) to build "exact" solvers
  - use low accuracy (low rank) to build preconditioners
- Consider hardware parameters in tuning block sizes and maximum rank parameters, to complement mathematical considerations
  - e.g., cache sizes, warp sizes
- Select from already broad and ever broadening algorithmic menu to form low-rank blocks (next slide)
  - traditionally a flop-intensive vendor-optimized GEMM-based flat algorithm
- Implement in "batches" of leaf blocks
  - flattening trees in the case of hierarchical methods

Low-rank approximations for compressible tiles

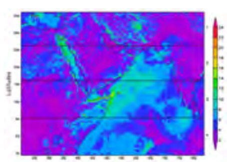
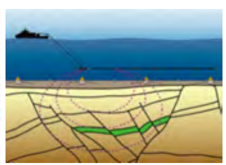
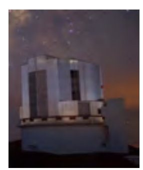
Options for forming data sparse representations of the amenable off-diagonal blocks

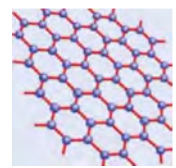
- standard SVD: $O(n^3)$, too expensive, especially for repeated compressions after additive tile manipulations
- randomized SVD (Halko *et al*., 2011): $O(n^2 \log k)$ for rank k, requires only a small number of passes over the data, saving over the SVD in memory accesses as well as operations
- adaptive cross approximation (ACA) (Bebendorf, 2000): $O(k^2 n \log n)$, motivated by integral equation kernels
- matrix skeletonization (representing a matrix by a representative collection of row and columns), such as CUR, sketching, or interpolatory decompositions based on proxies

Application opportunities

With such new algorithms, today's HPC can extend many applications that possess

- memory capacity constraints (e.g., geospatial statistics, PDE-constrained optimization)
- power constraints (e.g., remote telescopes)
- real-time constraints (e.g., wireless communication)
- running time constraints (e.g., chemistry, materials, genome-wide associations)




Example: covariance matrices from spatial statistics

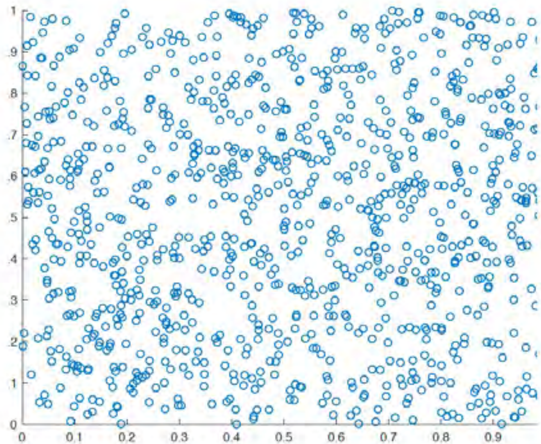
- Climate and weather applications have many measurements located regularly or irregularly in a region; prediction is needed at other locations
- Modeled as realization of Gaussian or Matérn spatial random field, with parameters to be fit
- Leads to evaluating, inside an optimization loop, the log-likelihood function involving a large dense (but data sparse) covariance matrix $\boldsymbol{\Sigma}$

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

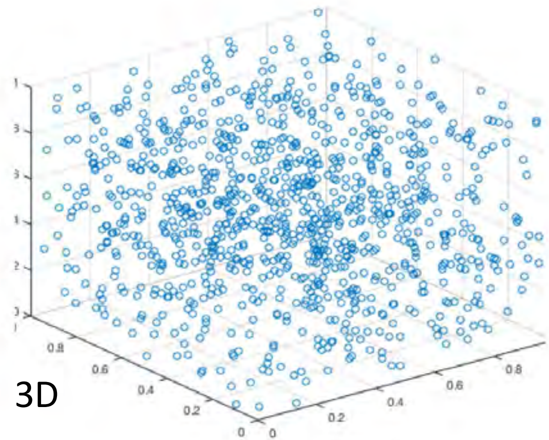
- Apply inverse $\boldsymbol{\Sigma}^{-1}$ and determinant $|\ \boldsymbol{\Sigma}\ |$ with Cholesky

Synthetic scaling test

Random coordinate generation within the unit square or unit cube with Matérn kernel decay, each pair of points connected by square exponential decay, $a_{ij} \sim \exp(-c|x_i - x_j|^2)$



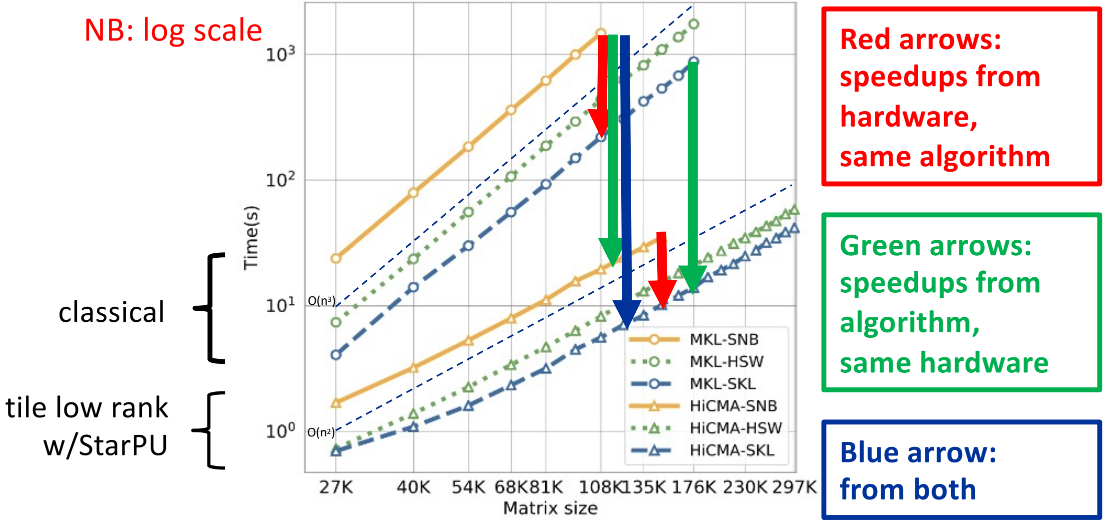
2D



3D

HiCMA TLR vs. Intel MKL on shared memory

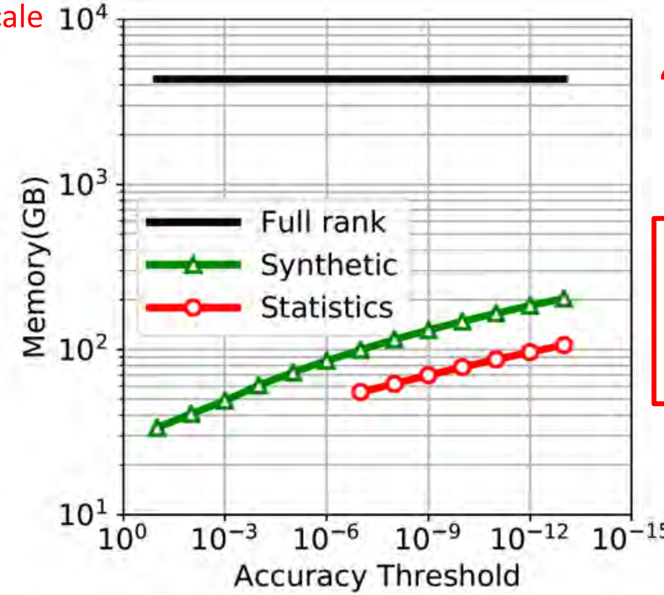
- Gaussian kernel to accuracy 1.0e-8 in each tile
- Three generations of Intel manycore (Sandy Bridge, Haswell, Skylake)
- Two generations of linear algebra (classical dense and tile low rank)



Akbudak, Ltaief, Mikhalev, Charara & K., *Exploiting Data Sparsity for Large-scale Matrix Computations,* Euro-Par 2018

Memory footprint for TLR fully DP matrix of size 1M

NB: log scale



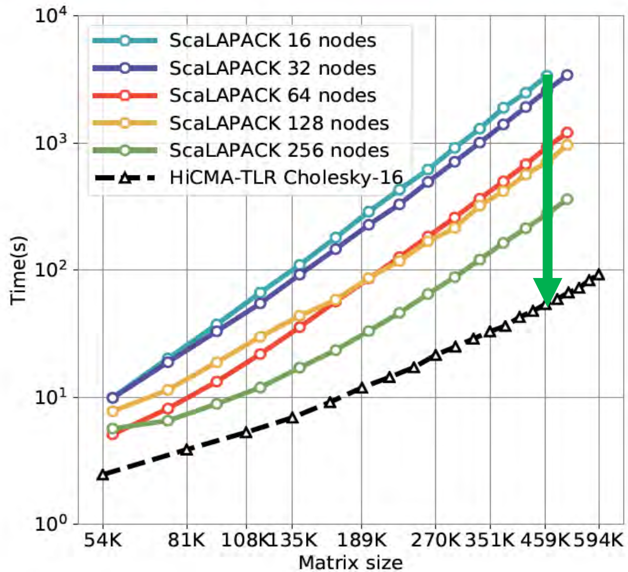
4 TB

1 to 2 orders of magnitude less, depending upon accuracy (x-axis)

Akbudak, Ltaief, Mikhalev, Charara & K., *Exploiting Data Sparsity for Large-scale Matrix Computations*, EuroPar 2018

HiCMA TLR vs. ScaLAPACK on distributed memory

NB: log scale



Green arrow: speedup from algorithm, same 16 nodes

Shaheen II at KAUST: a Cray XC40 system with 6,174 compute nodes, each of which has two 16-core Intel Haswell CPUs running at 2.30 GHz and 128 GB of DDR4 main memory

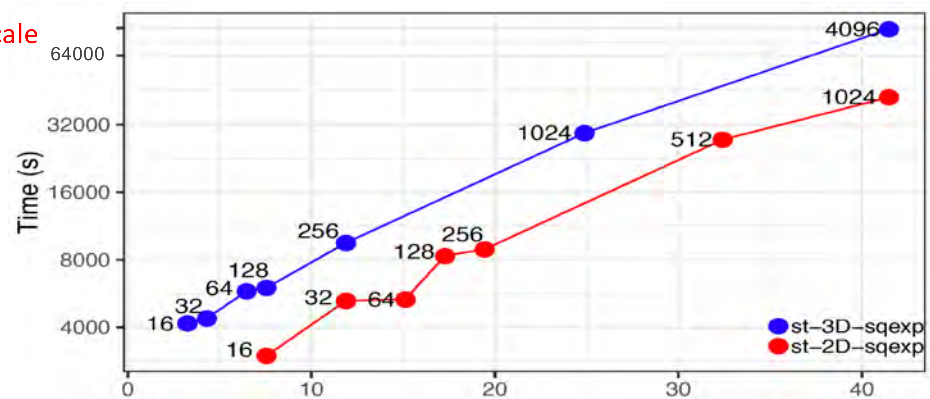
Akbudak, Ltaief, Mikhalev, Charara & K., *Exploiting Data Sparsity for Large-scale Matrix Computations,* Euro-Par 2018

Extreme Tile Low Rank

Cholesky factorization of a TLR matrix derived from Gaussian covariance of random distributions, up to 42M DOFs, on up to 4096 nodes (131,072 cores) of a Cray XC40

- would require 7.05 PetaBytes in dense DP (using symmetry)
- would require 77 days by ScaLAPACK (at the TLR rate of 3.7 Pflop/s)

NB: log scale



Fully dense computation would have cost about $1.03M in electricity and generated about 2500 metric tons of CO_2e

Cao, Pei, Akbudak, Mikhalev, Bosilca, Ltaief, K. & Dongarra, *Extreme-Scale Task-Based Cholesky Factorization Toward Climate and Weather Prediction Applications*. PASC'20 (ACM)

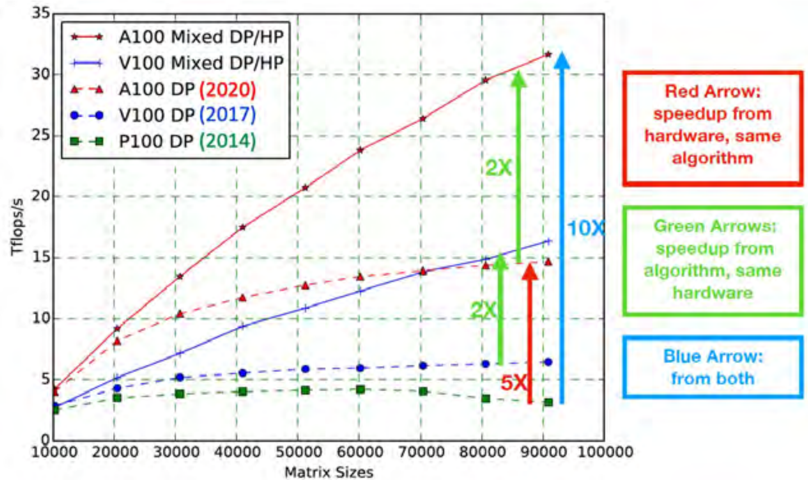
Two motivations for mixed precision

- Mathematical: (much) better than “no precision”
  - Statisticians often approximate remote diagonals as *zero* after performing a diagonally clustered space-filling curve ordering, so their coefficients must be orders of magnitude down from the diagonals
  - not just *smoothly decaying* in the low-rank sense, but actually *small*
- Computational: faster time to solution
  - hence lower energy consumption and higher performance, especially by exploiting heterogeneity

Peak Performance in TF/s	V100 NVLink	A100 NVLink	H100 SXM
FP64	7.5	9.7	34
FP32		19.5	67
FP64 Tensor Core	15	19.5	67
FP32 Tensor Core	8x	156 16x	495 16x
FP16 Tensor Core	120	312	989
	rel. 2017	rel. 2020	rel. 2023

Mixed precision geospatial statistics on GPUs

- Gaussian kernel to accuracy 1.0e-9 in each tile
- Three generations of NVIDIA GPU (Pascal, Volta, Ampere)
- Two generations of linear algebra (double precision and mixed DP/HP)



Ltaief, Genton, Gratadour, K. & Ravasi, 2022, *Responsibly Reckless Matrix Algorithms for HPC Scientific Applications*, Computing in Science and Engineering

2022 Gordon Bell Finalist justification

Reshaping Geostatistical Modeling and Prediction for Extreme-Scale Environmental Applications

I. JUSTIFICATION FOR THE GORDON BELL PRIZE

Synergistic combination of mixed-precision computations and low-rank matrix approximations. Dynamic task-based runtime system and data movement. Scalability on 16K Fugaku nodes (786,432 cores) for maximum log-likelihood estimation (MLE). Performance speedup up to 12X over FP64 execution while attaining application-worthy accuracy. Incorporation into path-finding software framework for geostatistical applications.

2022 Gordon Bell Finalist attributes

II. PERFORMANCE ATTRIBUTES

Performance Attributes	Our submission
Problem Size	Nine million geospatial locations[1]
Category of achievement	Time-to-solution and scalability
Type of method used	Maximum Likelihood Estimation (MLE)
Results reported on basis of	Whole application
Precision reported	Double, single, and half precision
System scale	16K Fujitsu A64FX nodes of Fugaku[1]
Measurement mechanism	Timers; FLOPS; Performance modeling

GB’22 collaborators

KAUST Supercomputing Core Lab, HLRS-Stuttgart, Oak Ridge LCF, RIKEN, and:

Qinglei Cao

Yu Pei

George Boslica

Jack Dongarra

Rabab Alomairy

Pratik Nag

Sameh Abdulah

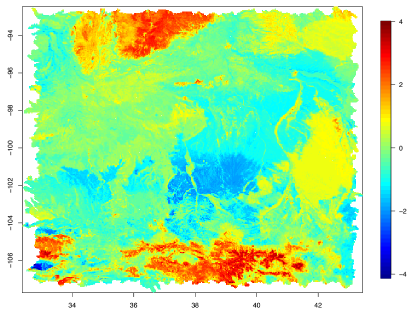
Hatem Ltaief

Ying Sun

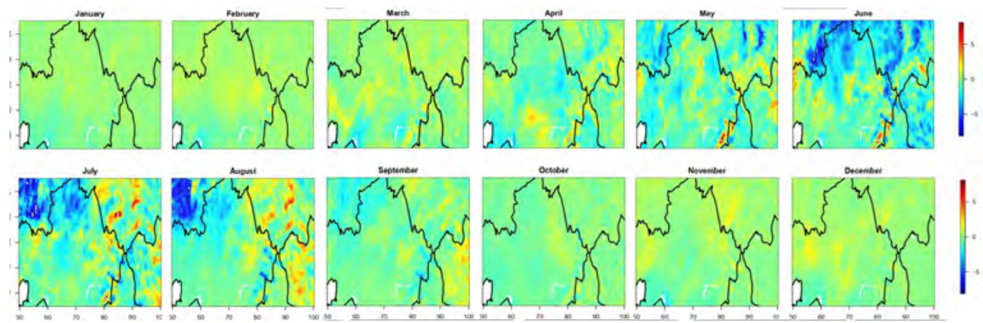
Marc Genton

App: spatial & spatio-temporal environmental statistics

Space and space-time modeling using Maximum Likelihood Estimation (MLE) on two environmental datasets



2D soil moisture data at the top layer of the Mississippi River basin



2021 monthly evapotranspiration (ET) over Central Asia

[means are subtracted out in these plots]

Statistical “emulation” (complementary to simulation)

- Predicts quantities directly from data (*e.g.*, weather, climate)
  - assumes a correlation model
  - data may be from observations or from first-principles simulations
  - statistical alternative to large-ensemble simulation averages
- Relied upon for economic and policy decisions
  - predicting demands, engineering safety margins, mitigating hazards, siting renewable resources, etc.
  - such applications are among principal supercomputing workloads
- Whereas simulations based on PDEs are usually memory bandwidth-bound, emulations based on covariance matrices are usually compute-bound (achieve a high % of bandwidth peak)

The computational challenge

- Contemporary observational datasets can be huge
  - Collect p observations at each of n locations $Z_p(x_n, y_n, z_n, t_n)$
  - Find optimal fit of the observations Z to a plausible function
  - Infer values at missing locations of interest
- Maximum Likelihood Estimate (MLE)
  - model for estimating parameters required to perform inference
- Complexity:
  - Arithmetic cost: solve systems with and calculate determinant of n-by-n covariance matrix
  - $O((pn)^3)$ floating-point operations and $O((pn)^2)$ memory
  - Memory footprint: 10^6 locations require 4 TB memory (double precision, invoking symmetry, for $p = 1$)

The computational ~~challenge~~ opportunity

- Contemporary observational datasets can be huge
  - Collect p observations at each of n locations $Z_p(x_n, y_n, z_n, t_n)$
  - Find optimal fit of the observations Z to a plausible function
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  - Memory footprint: 10^6 locations require 4 TB memory (double precision, invoking symmetry, for $p = 1$)

Motivation: High Performance Computational Statistics (HPCS)

"Increasing amounts of data are being produced (e.g., by remote sensing instruments and numerical models), while techniques to handle millions of observations have historically lagged behind… Computational implementations that work with irregularly-spaced observations are still rare." - Dorit Hammerling, NCAR, July 2019

1M × 1M dense sym DP matrix requires 4 TB, $N^3 \sim 10^{18}$ Flops

Traditional approaches:

Global low rank

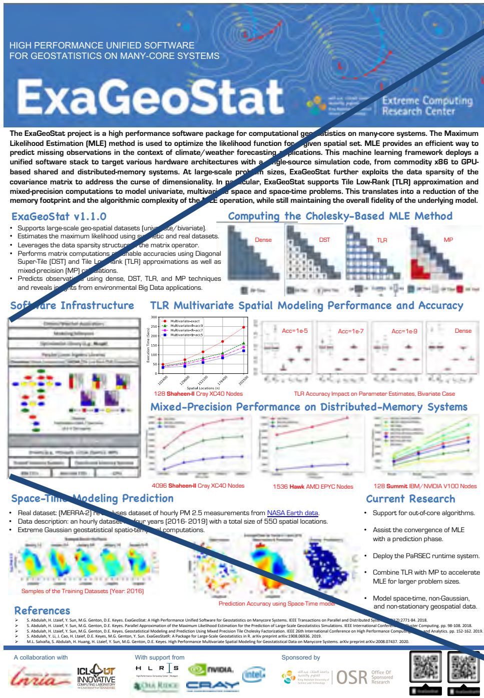
Zero outer diagonals

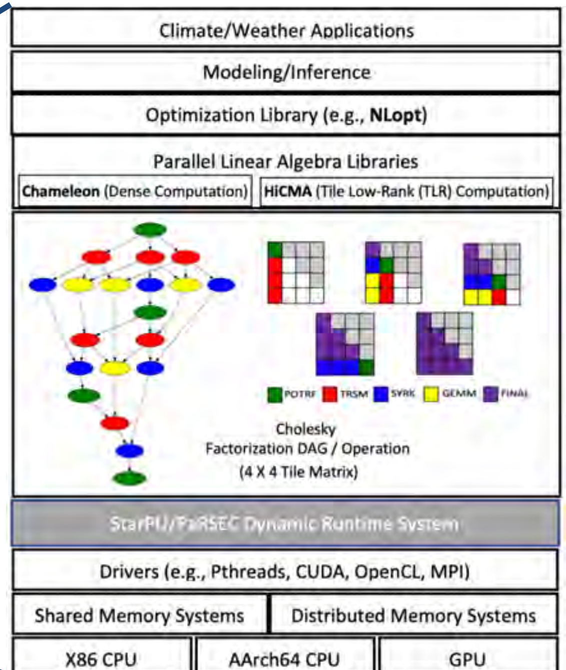
Better approaches:

Hierarchical low rank

Reduced precision outer diagonals

https://github.com/ecrc/exageostat

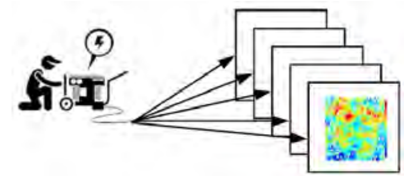




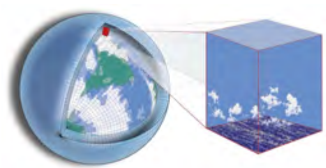
Sameh Abdulah,
Research Scientist
ECRC, KAUST

ExaGeoStat's 3-fold framework

- Synthetic Dataset Generator
  - Generates large-scale geospatial datasets which can be used separately as benchmark datasets for other software packages



- Maximum Likelihood Estimator (MLE)
  - Evaluates the maximum likelihood function on large-scale geospatial datasets
  - Supports dense full machine precision, Tile Low-Rank (TLR) approximation, low-precision approximation accuracy, and now TLR-MP



- ExaGeoStat Predictor
  - Infers unknown measurements at new geospatial locations from the MLE model

The portable ExaGeoStat software stack

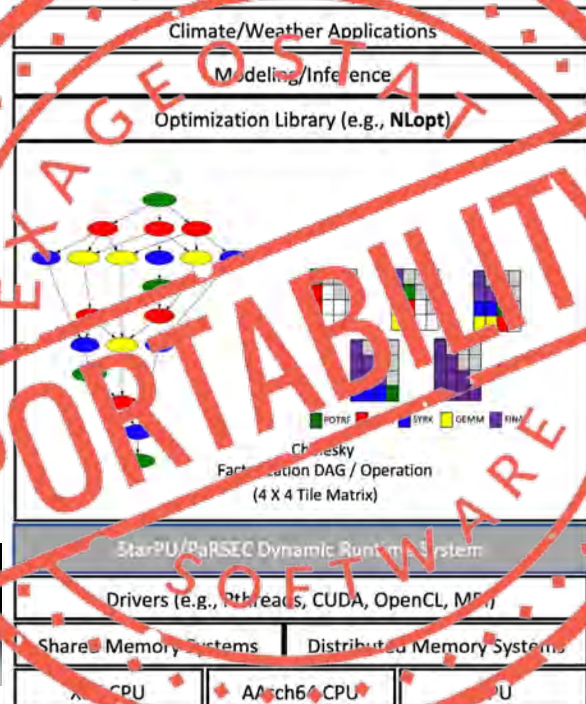
Nov 2023
Top500 data

AMD EPYC

Fujitsu A64FX

NVIDIA V100

Intel X86



#1 Frontier

#4 Fugaku

#7 Summit

#141 Shaheen-2

Maximum Likelihood Estimator (MLE)

- The log-likelihood function: $\ell(\boldsymbol{\theta}) = -\frac{n}{2}\log(2\pi) - \frac{1}{2}\log|\boldsymbol{\Sigma}(\boldsymbol{\theta})| - \frac{1}{2}\mathbf{Z}^\top\boldsymbol{\Sigma}(\boldsymbol{\theta})^{-1}\mathbf{Z}.$
- Optimization over $\boldsymbol{\theta}$ to maximize the likelihood function estimation until convergence
  - generate the covariance matrix $\boldsymbol{\Sigma}(\boldsymbol{\theta})$ using a specified kernel
  - evaluate the log determinant and the inverse operations, which require a Cholesky factorization of the given covariance matrix
  - update $\boldsymbol{\theta}$
- NLOPT* is typically used to maximize the likelihood
- Parallel PSwarm optimization algorithm runs several likelihood estimation steps at the same time (an embarrassingly parallel outer loop)

*open-source library by Prof. Steve Johnson of MIT

Covariance functions supported in ExaGeoStat

Univariate Matern Kernel

$$C(r;\boldsymbol{\theta}) = \frac{\theta_1}{2^{\theta_3-1}\Gamma(\theta_3)}\left(\frac{r}{\theta_2}\right)^{\theta_3}\mathcal{K}_{\theta_3}\left(\frac{r}{\theta_2}\right)$$

(3 parameters to fit: variance, range, smoothness)

Space/Time Nonseparable Kernel

$$C(\mathbf{h},u) = \frac{\sigma^2}{a_t|u|^{2\alpha}+1}\mathcal{M}_\nu\left\{\frac{\|\mathbf{h}\|/a_s}{(a_t|u|^{2\alpha}+1)^{\beta/2}}\right\},$$

(6 parameters to fit, add: time-range, time-smoothness, and separability)

Multivariate Parsimonious Kernel

$$C_{ij}(\|\mathbf{h}\|;\boldsymbol{\theta}) = \frac{\rho_{ij}\sigma_{ii}\sigma_{jj}}{2^{\nu_{ij}-1}\Gamma(\nu_{ij})}\left(\frac{\|\mathbf{h}\|}{a}\right)^{\nu_{ij}}\mathcal{K}_{\nu_{ij}}\left(\frac{\|\mathbf{h}\|}{a}\right)$$

Tukey g-and-h Non-Gaussian Field with Kernel

$$\rho_Z(h) = \frac{1}{\Gamma(\nu)2^{\nu-1}}\left(4\sqrt{2\nu}\frac{h}{\phi}\right)^{\nu}\mathcal{K}_\nu\left(4\sqrt{2\nu}\frac{h}{\phi}\right)$$

Multivariate Flexible Kernel

$$C(\mathbf{h};u) = \frac{\sigma^2}{2^{\nu-1}\Gamma(\nu)(a|u|^{2\alpha}+1)^{\delta+\beta d/2}}\left(\frac{c\|\mathbf{h}\|}{(a|u|^{2\alpha}+1)^{\beta/2}}\right)^{\nu} \times K_\nu\left(\frac{c\|\mathbf{h}\|}{(a|u|^{2\alpha}+1)^{\beta/2}}\right), \quad (\mathbf{h};u)\in\mathbb{R}^d\times\mathbb{R},$$

Powered Exponential Kernel

$$C(r;\boldsymbol{\theta}) = \theta_0\exp\left(\frac{-r^{\theta_2}}{\theta_1}\right)$$

How to choose the rank?

- Tiles are compressed to low rank based on user-supplied tolerance parameter, based on the first neglected singular value-vector pair.
- A tile-centric, structure-aware heuristic decides at runtime whether the tile should remain in low rank form or converted back to dense, based on estimates of the overheads of maintaining and operating with the compressed form.
- The structure-aware runtime decision is based only the estimated number of flops and time to solution, while the precision-aware runtime decision (next slide) is based only on the accuracy requirements of representing the matrix in the Frobenius norm.

How to choose the precision?

- Consider 2-precision case, with machine epsilons (unit roundoffs) u_{high} and u_{low} , resp.
- Let $\| A \|_F$ be the Frobenius norm of the global matrix square matrix A, which is computable by streaming A through just once
- Let n_T be the number of tiles in each dimension of A
- Then any tile A_{ij} such that

$$\| A_{ij} \|_F / (\| A \|_F / n_T) < u_{high} / u_{low}$$

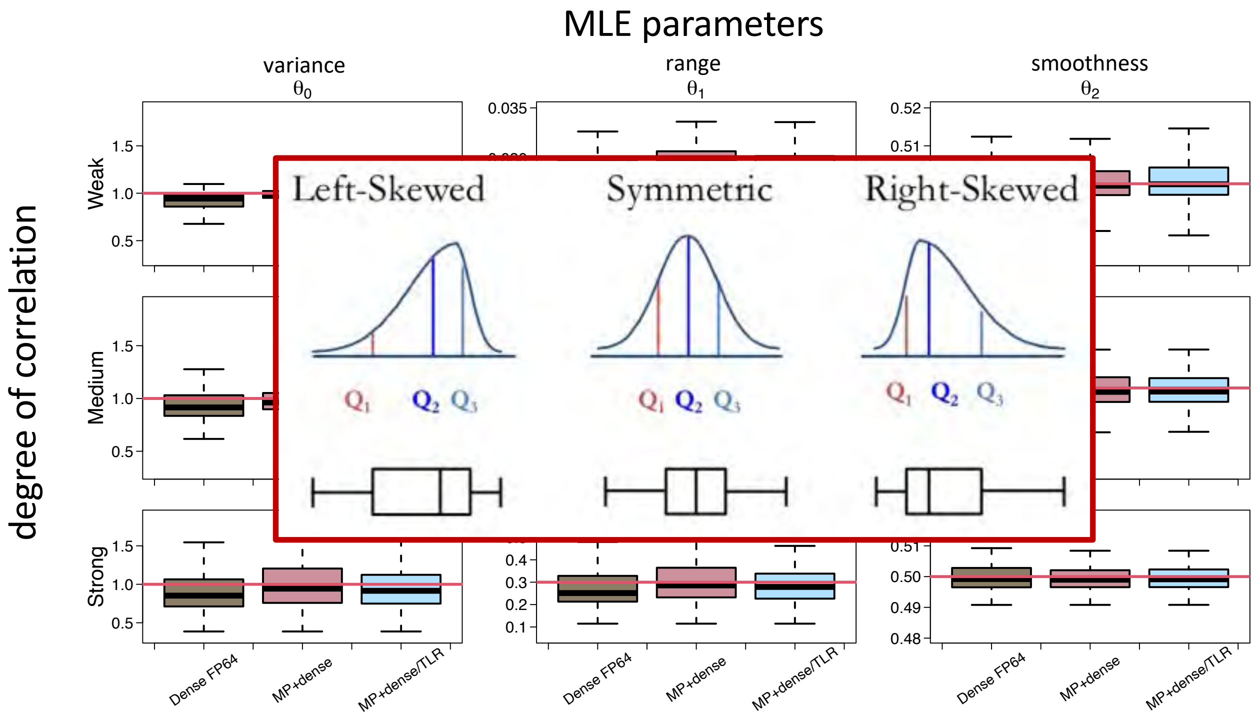
  is stored in low precision; otherwise kept in high
- The mixed precision tiled matrix $\mathcal{A}$ thus formed satisfies

$$\| \mathcal{A} - A \|_F < u_{high} \| A \|_F$$

- Generalizes to multiple precisions
- Tiles can be converted dynamically at runtime

Higham & Mary, *Mixed Precision Algorithms in Numerical Linear Algebra* (2022), Acta Numerica, pp. 347-414

Accuracy on synthetic 2D space dataset



Accuracy on real 3D (2D space + time) dataset

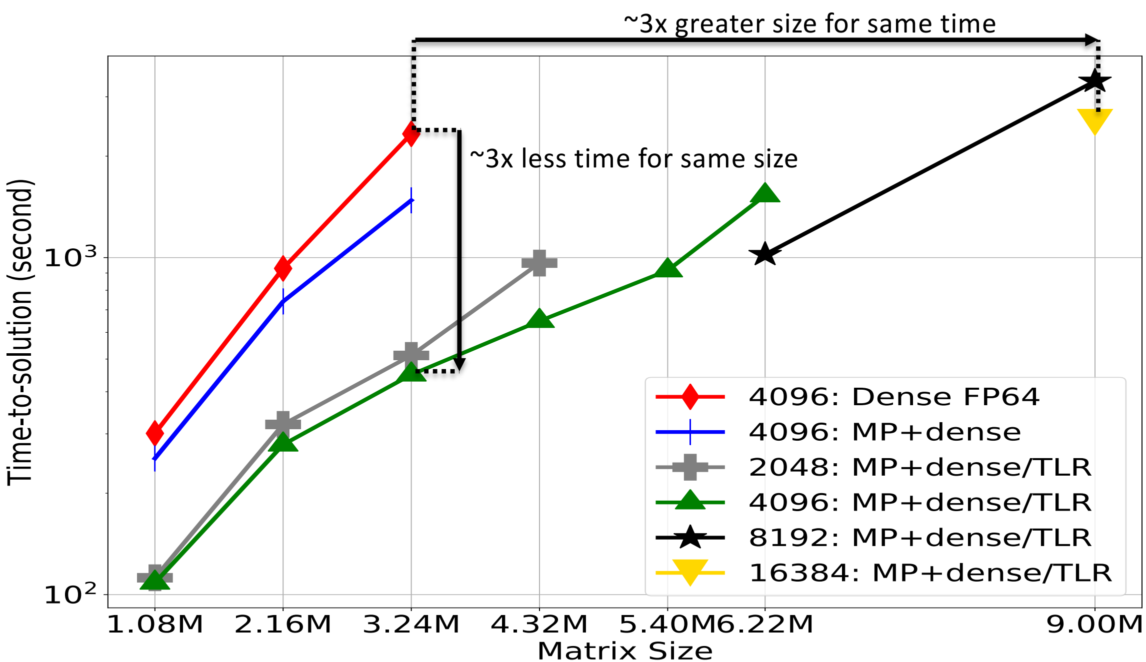
Variants	Variance (θ_0)	Range (θ_1)	Smoothness (θ_2)
Dense FP64	1.0087	3.7904	0.3164
MP+dense	0.9428	3.8795	0.3072
MP+dense/TLR	0.9247	3.7756	0.3068

Variants	Range-time (θ_3)	Smoothness-time (θ_4)	Nonsep-param (θ_5)
Dense FP64	0.0101	3.4890	0.1844
MP+dense	0.0102	3.4941	0.1860
MP+dense/TLR	0.0102	3.5858	0.1857

Variants	Log-Likelihood (llh)	MSPE
Dense FP64	-136675.1	0.9345
MP+dense	-136529.0	0.9348
MP+dense/TLR	-136541.8	0.9428

mean-square prediction error

Performance on up to 16K nodes of Fugaku



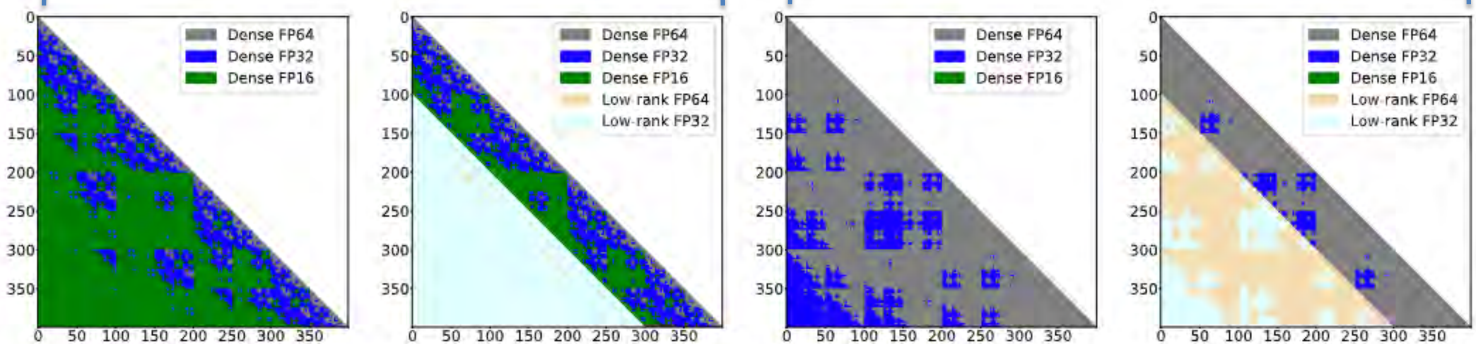
To be improved:

Still tuning runtime system PaRSEC on Fugaku's 32GB/node

Tile map for 2D space kernel with ~1M points

370 tiles of size 2700 in each dimension

weak correlation | strong correlation



memory footprint 1.6 TB

memory footprint 0.9 TB

memory footprint 3.8 TB

memory footprint 1.8 TB

default dense double is ~4 TB

Impact for spatial statistics

*The potential for this combination in spatial statistics generally is high... The authors have demonstrated **controllable and high accuracy typical of universal double precision, while exploiting mostly half precision, and keeping relatively few tiles clustered around the diagonal in their original fully dense format.** The result is reduction in time to solution of an order of magnitude or more, with the ratio of improvement growing with problem size, but already transformative.*

-- Professor Sudipto Banerjee, UCLA

Impact for spatial statistics

The innovations described in numerical linear algebra and in dynamic runtime task scheduling deliver an order of magnitude or more of reduction in execution time for a sufficiently large spatial or spatial-temporal data set using the Maximum Likelihood Estimation (MLE) and kriging paradigm. Perhaps more importantly, ***by reducing the memory footprint of such models, they allow much larger datasets to be accommodated within given computational resources. The advance this creates for spatial statisticians – geophysical and otherwise – is potentially immense****, given that this result is now available through ExaGeoStat.*

-- Professor Doug Nychka, Colorado School of Mines

Impact for spatial statistics

An especially attractive aspect of the submission is the innovation that it required in the a64fx ARM architecture of Fugaku, namely the accumulation in 32 bits of the 16-bit floating point multiply. I regard this aspect of the KAUST-UT-RIKEN collaboration of abiding benefit beyond the particular application of this submission.

As you know, my mottos for data science are that "Statistics is the 'Physics' of Data" and "Statistics is to Machine Learning as Physics is to Engineering." ***Your Gordon Bell campaign is accelerating the use of spatial statistics to allow it to keep up with exascale hardware.***

-- Dr. George Ostrouchov, ORNL

2023 Gordon Bell Finalist justification

Scaling the "Memory Wall" for Multi-Dimensional Seismic Processing with Algebraic Compression on Cerebras CS-2 Systems

I. JUSTIFICATION FOR THE GORDON BELL PRIZE

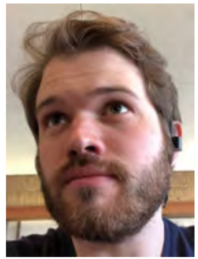
High-performance matrix-vector multiplication using low-rank approximation. Memory layout optimizations and batched executions on massively parallel Cerebras CS-2 systems. Leveraging AI-customized hardware capabilities for seismic applications for a low-carbon future. Application-worthy accuracy (FP32) with a sustained bandwidth of 92.58PB/s (for 48 CS-2s) would constitute the third-highest throughput from June'23 Top500.

2023 Gordon Bell Finalist attributes

Performance Attributes	Our submission
Problem Size	Broadband 3D seismic dataset ($\sim 20k$ sources and receivers and frequencies up to $50Hz$)
Category of achievement	Sustained bandwidth Scalability
Type of method used	Algebraic compression
Results reported on basis of	Whole application (for GPU cluster) Main kernel (for Cerebras cluster)
Precision reported	Single precision complex
System scale	Up to 48 Cerebras CS-2 systems, i.e., $35,784,000$ processing elements[1]
Measurement mechanism	Timers; Memory accesses; Performance modeling

GB’23 collaborators

Group42 (Abu Dhabi), KAUST Supercomputing Core Lab and:



Leighton Wilson

Mathias Jacquelin

Yuxi Hong

Hatem Ltaief

Matteo Ravasi

Cerebras CS-2 Wafer-Scale Engine (WSE)

2023 Gordon Bell submission

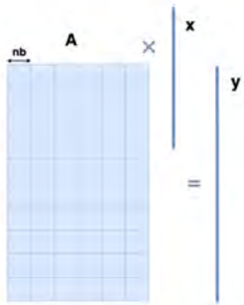


Fig. 2: Original dense MVM.

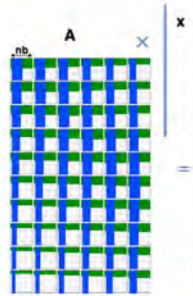


Fig. 3: Rank-compressed operator.

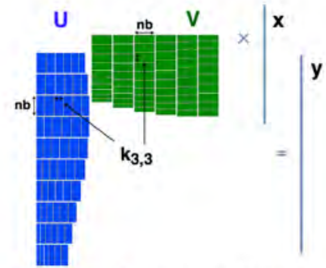


Fig. 4: Stacked bases U and V.

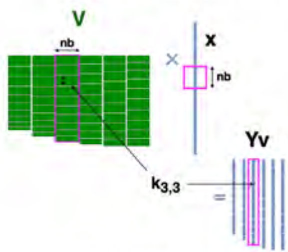


Fig. 5: V-batch stage of MVM.

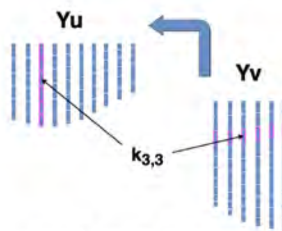


Fig. 6: Shuffle from V to U bases.

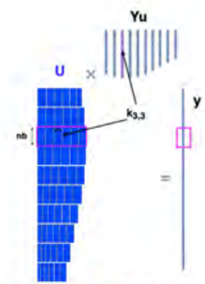
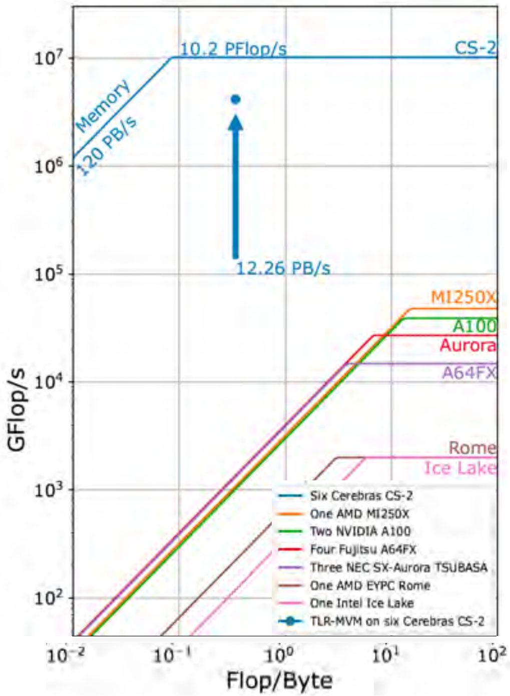


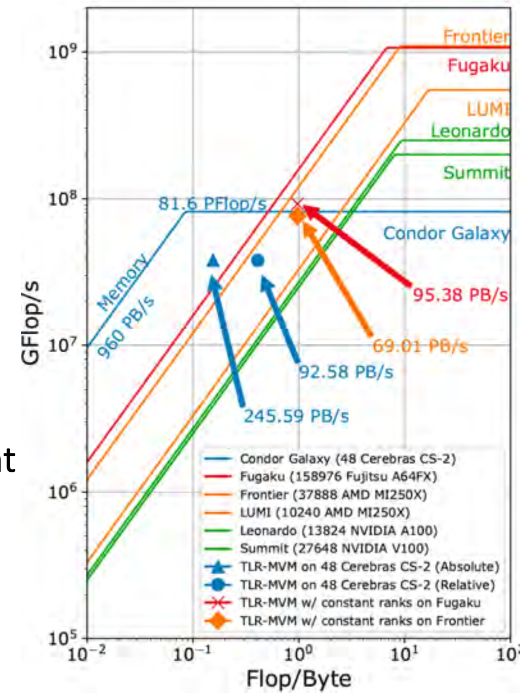
Fig. 7: U-batch of MVM.

2023 Gordon Bell submission

Roofline models of 6 CS-2's compared with other solutions



Roofline models of 48 CS-2's compared with current top 5



Impact for geophysical imaging

For the past 3 decades, we have needed large-scale convolutions for multiple applications to tackle subsurface challenges – which are now greater than ever for the energy transition, such as rapid, wide-scale monitoring of subsurface hydrogen storage – but have never achieved it due to the unsurmountable bottleneck imposed by the size of datasets (starting at TBs).

This project, with its balanced focus on accuracy and practical performance, is likely to finally break through a decades-old barrier in geophysical imaging.

– Dr. Ivan Vasconcelos, Shearwater Geoservices

Impact for geophysical imaging

The impact that the efficient implementation of multi-dimensional convolution with low-rank tiles that Ltaief and co-authors have developed is better understood if we bear in mind that multidimensional convolution and deconvolution are ubiquitous operations in seismic processing.

This new implementation may lead to a drastic reduction of the turnaround time of seismic data processing projects. *The consequence is that the decision-makers, regardless of whether they use seismic images for conventional hydrocarbon exploration or for other applications, will receive valuable information in a timely manner.*

– Dr. Claudio Bagaini, SLB (Schlumberger)

Impact for geophysical imaging

Conventional algorithms for MDD would not have mapped onto the Cerebras CS-2 engines because their N^3 arithmetic complexity is prohibitive. Only the algebraically compressed form of the problem fits. All parts of this interdisciplinary project are thus necessary for its success.

As the title indicates, this team is 'scaling the memory wall' that has loomed over computational science & engineering at the high end for, by now, three decades. Their algorithms and CS-2 implementation have enormous implications for our community, since their application is representative of many important CS&E problems.

– Professor Omar Ghattas, U Texas

2024 Gordon Bell Climate Finalist justification

Boosting Earth System Model Outputs And Saving PetaBytes in their Storage Using Exascale Climate Emulators

I. JUSTIFICATION FOR THE GORDON BELL PRIZE

Exascale climate emulator developed using 318 billion hourly and 31 billion daily observations for generating climate emulations at ultra-high spatial resolution ($0.034^\circ \sim 3.5$ km). Modeling climate data using spherical harmonics. Mixed-precision computations. `PaRSEC` dynamic runtime system. Running on 9,025 nodes on Frontier, 1,936 nodes on Alps, 1,024 nodes on Leonardo, and 3,072 nodes on Summit, with the hybrid Flop/s rates 0.976 EFlop/s, 0.739 EFlop/s, 0.243 EFlop/s, and 0.375 EFlop/s, respectively.

2024 Gordon Bell Climate Finalist attributes

Problem size	54,486,360 spatial locations across the globe at a spatial resolution of 0.034° (∼3.5 km)
Category of achievement Type of method used	Scalability and peak performance Spherical Harmonic Transform (SHT) and Cholesky factorization
Results reported on basis of Precision reported System scale	Cholesky factorization Double and mixed-precision - 0.976 EFlop/s on 9,025 nodes of Frontier (36,100 AMD MI250X multi-chip module (MCM) GPUs) equivalent to 72,200 AMD Graphics Compute Dies (GCDs) - 0.739 EFlop/s on 1,936 nodes of Alps (7,744 NVIDIA Grace-Hopper Superchips (GH200)) - 0.243 EFlop/s on 1,024 nodes of Leonardo (4,096 NVIDIA A100 GPUs) - 0.375 EFlop/s on 3,072 nodes of Summit (18,432 NVIDIA V100 GPUs)
Measurement mechanism	Timers, Flops

GB'24 climate prize collaborators

KAUST Supercomputing Core Lab, Oak Ridge LCF, CSCS Alps, CINECA Leonardo, and:


Allison Baker


George Boslica


Qinglei Cao


Stefano Castruccio


Gera Stenchikov


Sameh Abdulah


Marc Genton


Zubair Khalid

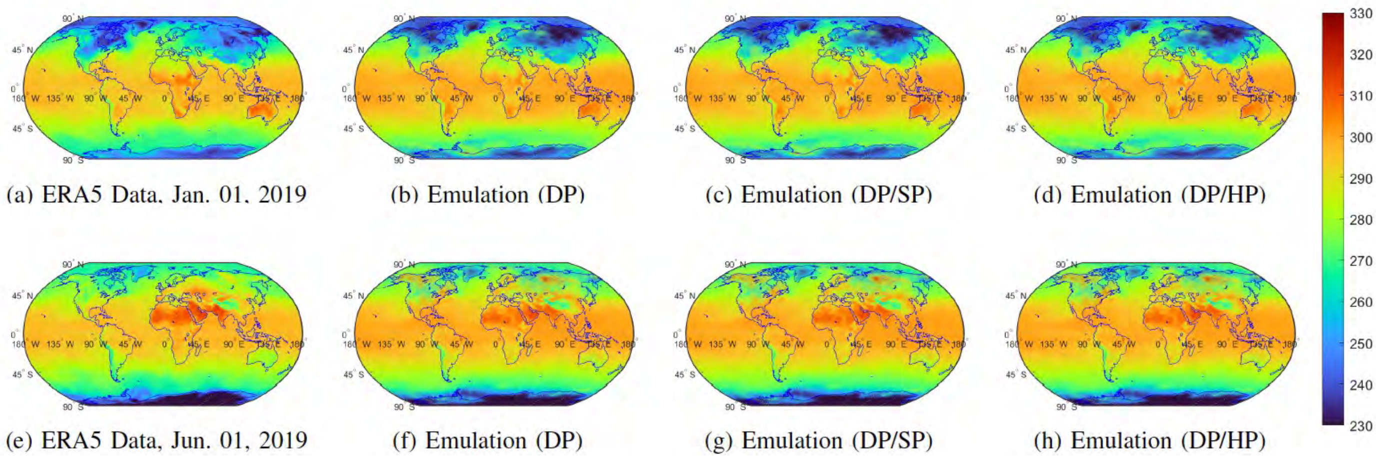

Hatem Ltaief


Yan Song


Ying Sun

Motivation for climate emulation

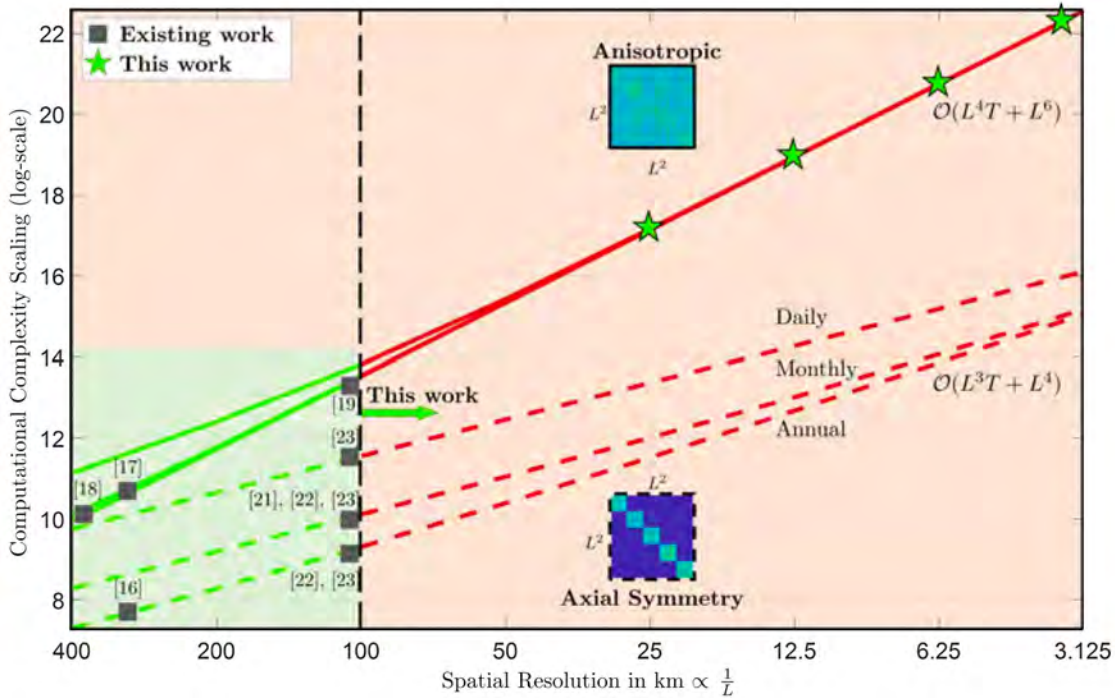
- 45-institution Coupled Model Intercomparison Project (CMIP)
- CMIP6 campaign recently generated 28 PB of data, at a cost of $45/TB/year
- emulation trained on simulation generates realizations with same statistics
- efficient basis for compact storage, e.g., spherical harmonics



(a) ERA5 Data, Jan. 01, 2019 (b) Emulation (DP) (c) Emulation (DP/SP) (d) Emulation (DP/HP)

(e) ERA5 Data, Jun. 01, 2019 (f) Emulation (DP) (g) Emulation (DP/SP) (h) Emulation (DP/HP)

Expanding emulation capabilities



Performance on four Top10 systems (eff. Pflops/s)

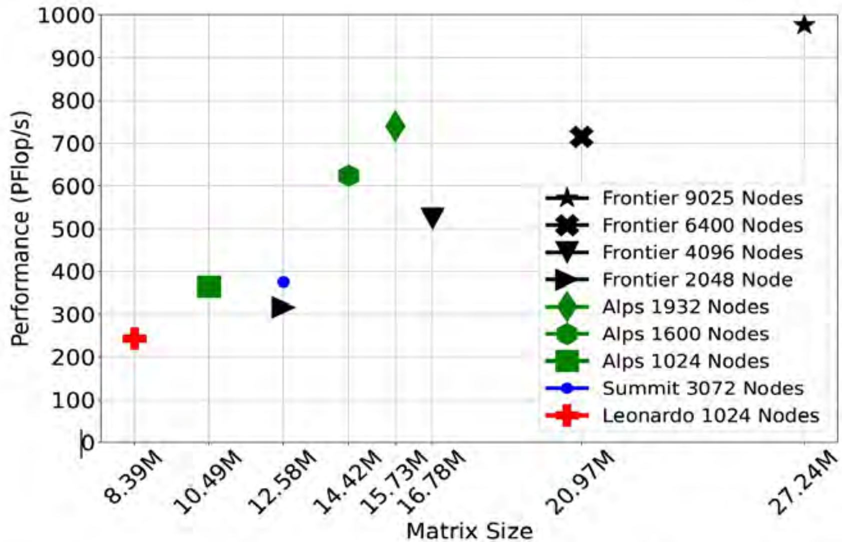


Fig. 8: Performance of largest runs on Summit, Leonardo, Alps, and Frontier; with additional run-up points on Alps and Frontier, all using the DP/HP precision variant.

Per node performance on a 1024-node subsystem

TABLE I: DP/HP Performance on 1,024 nodes of the four systems, i.e., Frontier, Alps, Leonardo, and Summit.

System	**Frontier**	**Alps**	**Leonardo**	**Summit**
Vendor	AMD	NVIDIA		
Chip	MI250X	GH200	A100	V100
# GPUs	4,096	4,096	4,096	6,144
Matrix Size	8.39M	10.49M	8.39M	6.29M
Performance (PFflop/s)	223.7	384.2	243.1	153.6
TFlop/s/GPU	54.6	93.8	57.2	25

2024 Gordon Bell Prize Finalist justification

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

I. JUSTIFICATION FOR THE GORDON BELL PRIZE

High-performance tile-centric matrix computations for kernel ridge regression. End-to-end GWAS software supporting the largest-ever multivariate study of 305K patients from UK BioBank. Application-worthy FP64 accuracy using four precisions. Sustained throughput exceeding 11X over FP 64 on A100s. Near-perfect weak-scaling on one-third of Leonardo, projecting to 2 MP Eflops/s on full system.

2024 Gordon Bell Prize Finalist attribution

Performance Attributes	Value
Problem Size	305K UK BioBank patients [real data] 8M patients [synthetic data]
Category of achievement	Scalability, performance, time to solution
Type of method used	Kernel Ridge Regression
Results reported on basis of	Whole-application GWAS Cholesky factorization
Precision reported	FP64, FP32, FP16, FP8, INT8
System scale	2/3 of Summit [1] 1/3 of Leonardo [1] - projected to $\sim$ 2 MP Eflop/s with weak scaling on full Leonardo system
Measurement mechanism	Timers, Flops

GB'24 prize collaborators

KAUST Supercomputing Core Lab, Oak Ridge LCF, CSCS Alps, CINECA Leonardo, and:


Rached Abdelkhalek


Rabab Alomairy


Qinglei Cao


Benedikt Dorschner


Thorsten Kurth


David Ruau


Lotfi Slim

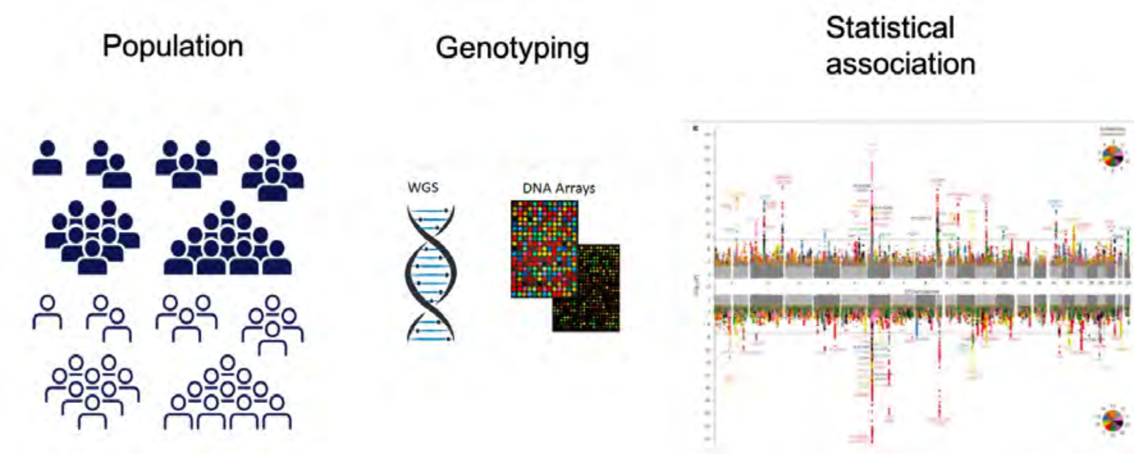

Salim Bougaffa


Hatem Ltaief


Jie Ren

Motivation for epistatic genome association studies

- Train statistical model on genotype/environmental-to-phenotype data
- Use to predict disease and other genetic/environmental characteristics
- Ridge regression is a linear association that considers individual SNPs
- Kernel ridge regression is correlates instances of multiple SNPs



Motivation for epistatic genome association studies

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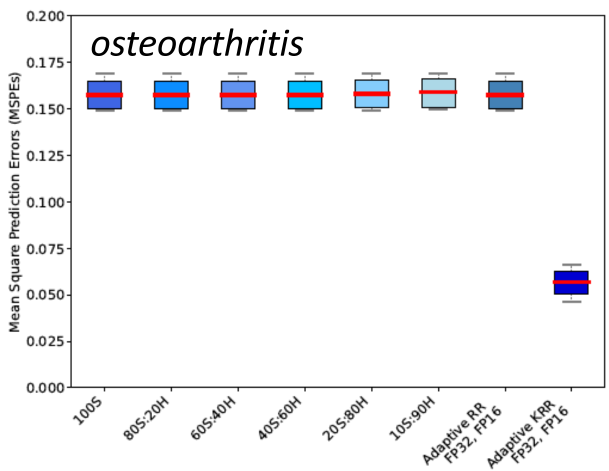
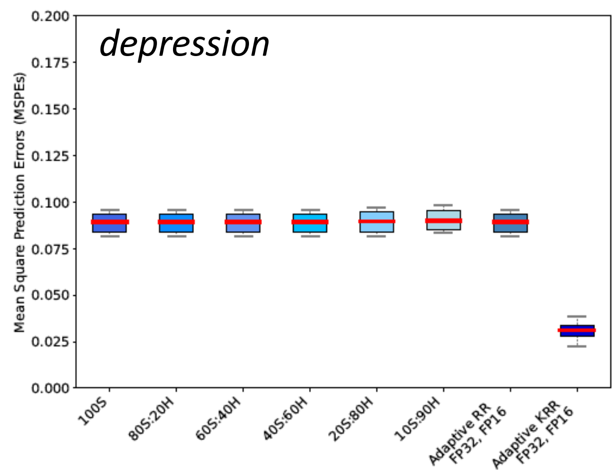




Submitted to the 2024 Gordon Bell Prize

TABLE I: Comparing RR vs. KRR Pearson correlations.

Phenotypes	**RR**	**KRR**
`Hypertension`	0.2983	0.8071
`Asthma`	0.2517	0.8205
`Allergic Rhinitis`	0.2008	0.8652
`Osteoarthritis`	0.3189	0.8386
`Depression`	0.2041	0.8454

Kernel Ridge Regression is just linear algebra

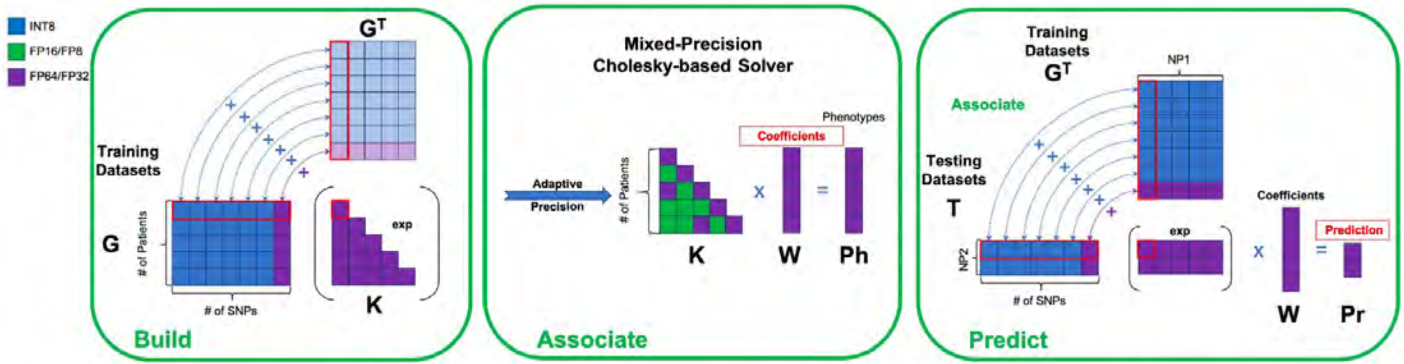
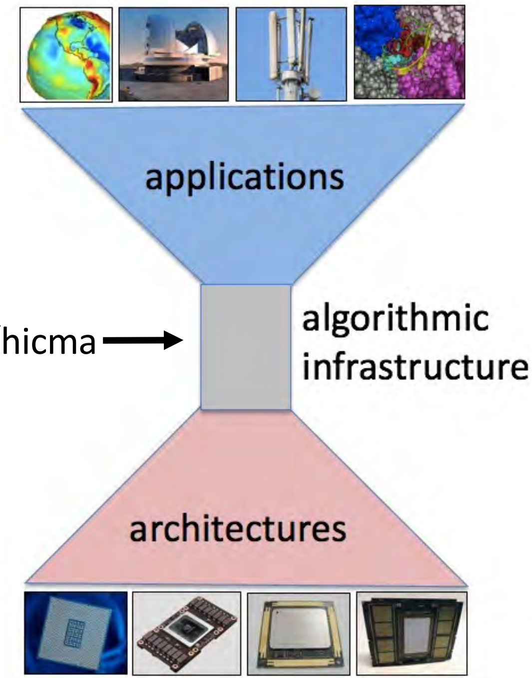


Fig. 3: Leveraging the INT8 / FP8 / FP16 / FP32 / FP64 multivariate KRR-based GWAS for genetic epistasis.

Hourglass model of software

https://github.com/ecrc/hicma



Conclusions, recapped

As computational infrastructure demands a growing sector of research budgets and global energy expenditure, we must *all* address the need for greater efficiency

As a community, we have excelled at this historically in three aspects:

- architectures
- applications (redefining *actual outputs of interest*)
- algorithms

There are *new algorithmic* opportunities in:

- reduced rank representations
- reduced precision representations

Sustainable computing – two meanings

Computing sustainably

- or at least efficiently – not computing more than necessary for a given scientific target

Computing to *support* sustainability

- renewable energy
- affordable energy

For follow-up

1) *Parallel Approximation of the Maximum Likelihood Estimation for the Prediction of Large-Scale Geostatistics Simulations,* S. Abdulah, H. Ltaief, Y. Sun, M. G. Genton & D. Keyes, 2018, IEEE International Conference on Cluster Computing (CLUSTER), 2018, pp. 98-108, doi: 10.1109/CLUSTER.2018.00089.
2) *Hierarchical Algorithms on Hierarchical Architectures*, D. Keyes, H. Ltaief & G. Turkiyyah, 2020, Philosophical Transactions of the Royal Society, Series A 378:20190055, doi 10.1098/rsta.2019.0055
3) *Responsibly Reckless Matrix Algorithms for HPC Scientific Applications*, H. Ltaief, M. G. Genton, D. Gratadour, D. Keyes & M. Ravasi, 2022, Computing in Science and Engineering, doi 10.1109/MCSE.2022.3215477.
4) *Reshaping Geostatistical Modeling and Prediction for Extreme-Scale Environmental Applications*, Q. Cao, S. Abdulah, R. Alomairy, Y. Pei, P. Nag, G. Bosilca, J. Dongarra, M. G. Genton, D. E. Keyes, H. Ltaief & Y. Sun, 2022, in proceedings of the International Conference for High Performance Computing, Networking, Storage, and Analysis (SC'22), IEEE Computer Society (ACM Gordon Bell Finalist), doi 10.1109/SC41404.2022.00007.
5) *Mixed Precision Algorithms in Numerical Linear Algebra*, 2022, N. J. Higham & T. Mary, Acta Numerica, pp. 347—414, doi:10.1017/S0962492922000022.
6) *Scaling the “Memory Wall” for Multi-Dimensional Seismic Processing with Algebraic Compression on Cerebras CS-2 Systems, H. Ltaief, Y. Hong, L. Wilson, M. Jacquelin, M. Ravasi, & David Keyes, 2023,* , in proceedings of the International Conference for High Performance Computing, Networking, Storage, and Analysis (SC'22), IEEE Computer Society (ACM Gordon Bell Finalist), doi 10.1145/3581784.362704.


Thank you
شكرا
جامعة الملك عبدالله
للعلوم والتقنية
King Abdullah University of
Science and Technology

Extra slides

Review: mean and covariance of random process Z

The mean function of $Z(\boldsymbol{s})$ is

$$\mu(\boldsymbol{s}) = \mathbb{E}\{Z(\boldsymbol{s})\}$$

The covariance function of $Z(\boldsymbol{s})$ is

$$C(\boldsymbol{s}_1, \boldsymbol{s}_2) = \text{cov}\{Z(\boldsymbol{s}_1), Z(\boldsymbol{s}_2)\} = \mathbb{E}[\{Z(\boldsymbol{s}_1) - \mu(\boldsymbol{s}_1)\}\{Z(\boldsymbol{s}_2) - \mu(\boldsymbol{s}_2)\}],$$

where $\boldsymbol{s}_1$ and $\boldsymbol{s}_2$ are two spatial locations

Review: covariance matrix of random process Z

The covariance matrix Σ is

$$\Sigma = \begin{bmatrix} \mathrm{E}[(X_1 - \mathrm{E}[X_1])(X_1 - \mathrm{E}[X_1])] & \mathrm{E}[(X_1 - \mathrm{E}[X_1])(X_2 - \mathrm{E}[X_2])] & \cdots & \mathrm{E}[(X_1 - \mathrm{E}[X_1])(X_n - \mathrm{E}[X_n])] \\ \mathrm{E}[(X_2 - \mathrm{E}[X_2])(X_1 - \mathrm{E}[X_1])] & \mathrm{E}[(X_2 - \mathrm{E}[X_2])(X_2 - \mathrm{E}[X_2])] & \cdots & \mathrm{E}[(X_2 - \mathrm{E}[X_2])(X_n - \mathrm{E}[X_n])] \\ \vdots & \vdots & \ddots & \vdots \\ \mathrm{E}[(X_n - \mathrm{E}[X_n])(X_1 - \mathrm{E}[X_1])] & \mathrm{E}[(X_n - \mathrm{E}[X_n])(X_2 - \mathrm{E}[X_2])] & \cdots & \mathrm{E}[(X_n - \mathrm{E}[X_n])(X_n - \mathrm{E}[X_n])] \end{bmatrix}$$

Σ is symmetric and positive semi-definite

Diagonal elements are the variances

Inference (kriging)

The estimated $\boldsymbol{\theta}$ can be used to predict missing measurements at some other location in the same region. Prediction can be performed from a multivariate normal joint distribution model with m missing measurements $\mathbf{Z}_m$ and n known measurements $\mathbf{Z}_n$ [13], [14]:

$$\begin{bmatrix} \mathbf{Z}_m \\ \mathbf{Z}_n \end{bmatrix} \sim \mathcal{N}_{m+n}\left(\begin{bmatrix} \boldsymbol{\mu}_m \\ \boldsymbol{\mu}_n \end{bmatrix}, \begin{bmatrix} \boldsymbol{\Sigma}_{mm} & \boldsymbol{\Sigma}_{mn} \\ \boldsymbol{\Sigma}_{nm} & \boldsymbol{\Sigma}_{nn} \end{bmatrix} \right), \tag{2}$$

with $\boldsymbol{\Sigma}_{mm} \in \mathbb{R}^{m\times m}$, $\boldsymbol{\Sigma}_{mn} \in \mathbb{R}^{m\times n}$, $\boldsymbol{\Sigma}_{nm} \in \mathbb{R}^{n\times m}$, and $\boldsymbol{\Sigma}_{nn} \in \mathbb{R}^{n\times n}$. The associated conditional distribution is:

$$\begin{aligned} \mathbf{Z}_m | \mathbf{Z}_n \sim \mathcal{N}_m(\boldsymbol{\mu}_m + \boldsymbol{\Sigma}_{mn}\boldsymbol{\Sigma}_{nn}^{-1}(\mathbf{Z}_n - \boldsymbol{\mu}_n), \\ \boldsymbol{\Sigma}_{mm} - \boldsymbol{\Sigma}_{mn}\boldsymbol{\Sigma}_{nn}^{-1}\boldsymbol{\Sigma}_{nm}). \end{aligned} \tag{3}$$

Inference (kriging)

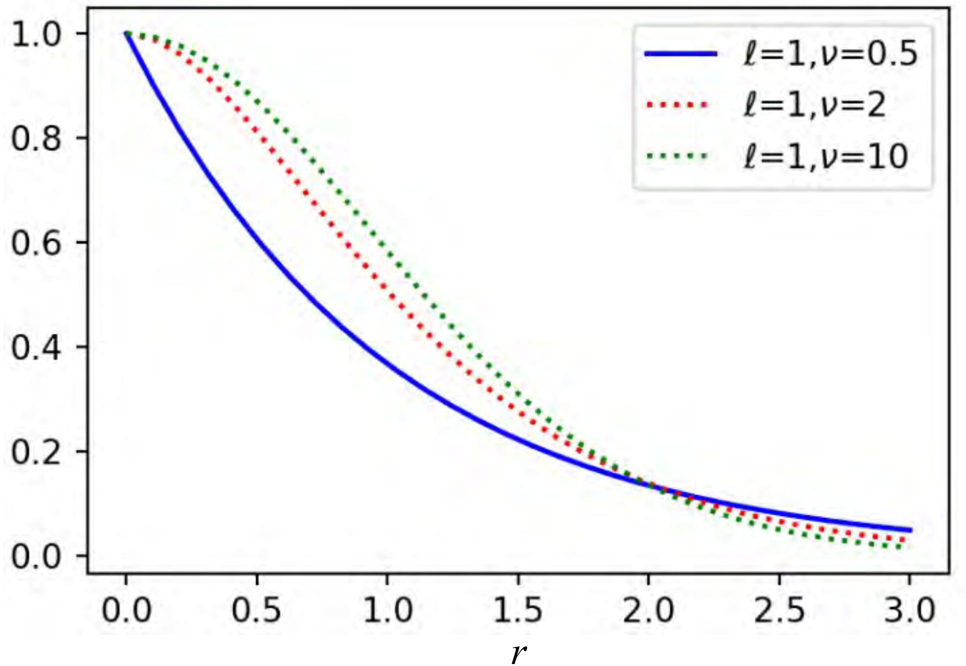
Assuming that the observed vector $\mathbf{Z}_n$ has a zero-mean function (i.e., $\boldsymbol{\mu}_n = \mathbf{0}$, hence $\boldsymbol{\mu}_m = \mathbf{0}$), the unknown vector $\mathbf{Z}_m$ can be predicted [13] by solving:

$$\mathbf{Z}_m = \boldsymbol{\Sigma}_{mn} \boldsymbol{\Sigma}_{nn}^{-1} \mathbf{Z}_n. \tag{4}$$

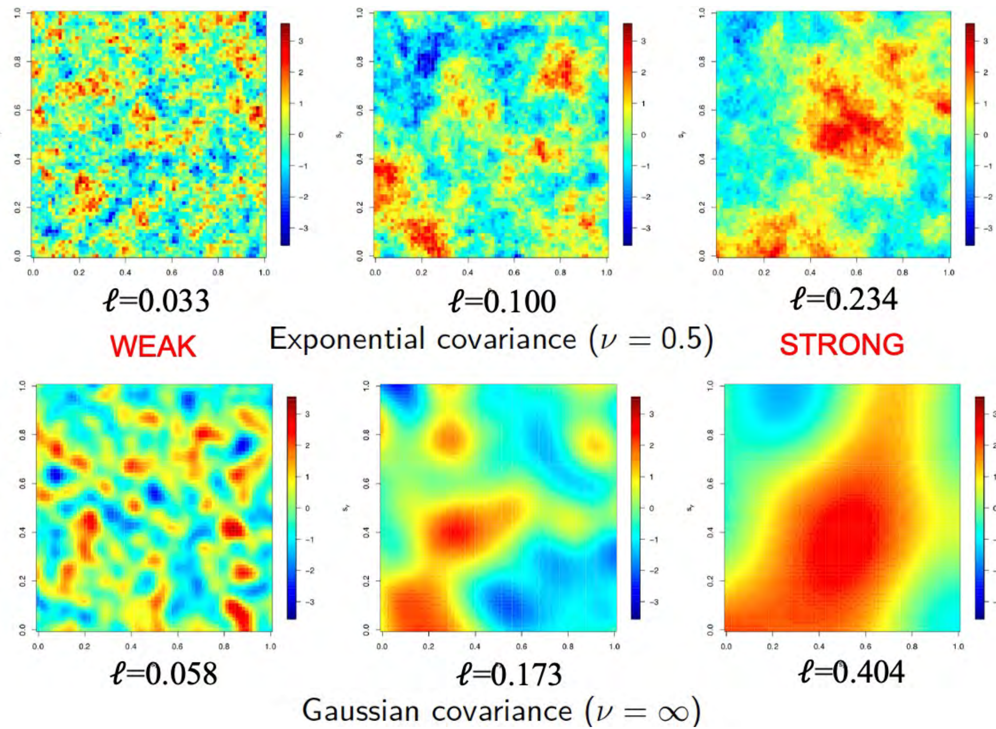
The associated prediction uncertainty is given by:

$$\mathbf{U}_m = \mathrm{diag}[\boldsymbol{\Sigma}_{mm} - \boldsymbol{\Sigma}_{mn} \boldsymbol{\Sigma}_{nn}^{-1} \boldsymbol{\Sigma}_{nm}] \tag{5}$$

Matern distribution for various Hankel indices, θ_3 (= ν)



Range parameter θ_3 (= ℓ) sets correlation length



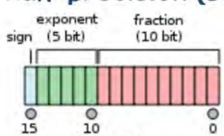
Adapt precision to accuracy requirements

Precision	Type	Bits: Signif (t)	Bits: Exp	Range	$u = 2^{-t}$
half	bfloat16	8	8	$10^{\pm 38}$	3.9×10^{-3}
half	fp16	11	5	$10^{\pm 5}$	4.9×10^{-4}
single	fp32	24	8	$10^{\pm 38}$	6.0×10^{-8}
double	fp64	53	11	$10^{\pm 308}$	1.1×10^{-16}

fp64, fp32, fp16 defined by IEEE standard

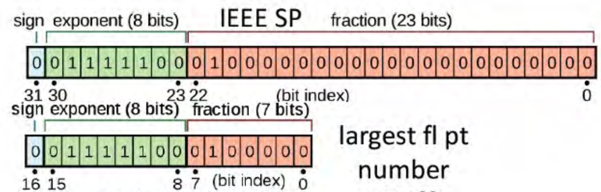
Bfloat16: Google, Intel, ARM, NVIDIA

Note the number range with half precision (16 bit fl.pt.)



float16

largest fl pt number 65,504



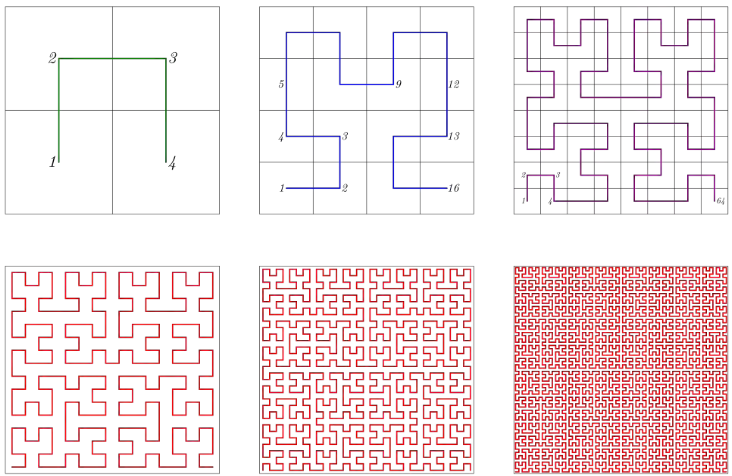
Google TPU: bfloat16

largest fl pt number $O(10^{38})$

c/o Nick Higham (2021), Jack Dongarra (2021)

Diagonal-based reasoning depends on good orderings

Points near each other in 1D memory must be near each other, on average, in N-dimensional space, using space-filling curves

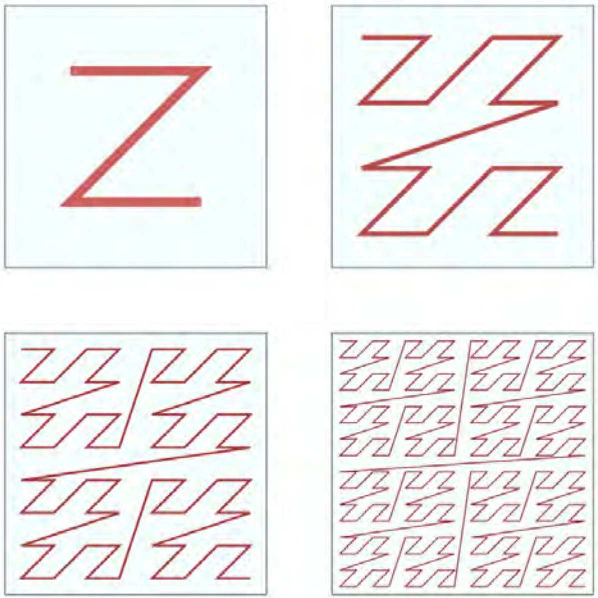


2D Hilbert curves

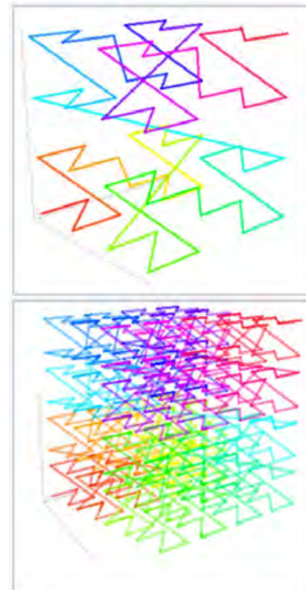
3D Hilbert curves
equipartitioned by color

mons.wikimedia.org/w/index.php?curid=47570255

Diagonal-based reasoning depends on good orderings



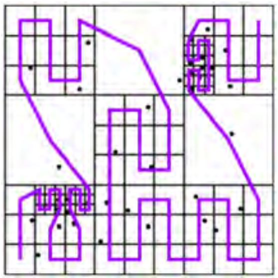
2D Morton curves

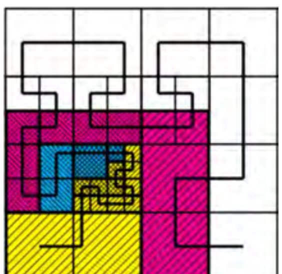


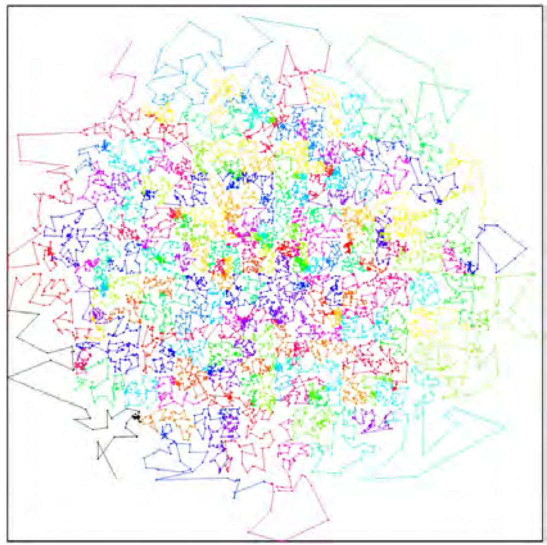
3D Morton curves
equipartitioned by color

mons.wikimedia.org/w/index.php?curid=3879675

Good compression requires good ordering: Hilbert







10,000 points in 200 groups of 50 each

1891 invention by David Hilbert

1997 presented in partitioning context at SC'97 by John Salmon and Mike Warren

2018 won "Test of Time" award at SC'18

Statistical model generalizations

- Multivariate
  - exploits correlations between different fields at same point in addition to same field at different points
- Nonstationary
  - parameters may vary in space and/or time
- Anisotropic
  - correlations may depend on orientation, not just distance in space or time

Extensions in computing environment

- Exploiting better low precision support
  - requirements for statistics (and likely other science and engineering applications) may require more hardware support than training in machine learning
- Achieving greater scalability
  - becoming a finalist will open doors to current and incoming systems
- Delivering greater portability
  - must continue to hide implementation details beneath a convenient API

TLR (complex) LU factorization

Algorithm 1. Dense Tile *LU* factorization of a N-by-N matrix A composed of $nb \times nb$ tiles and solve.

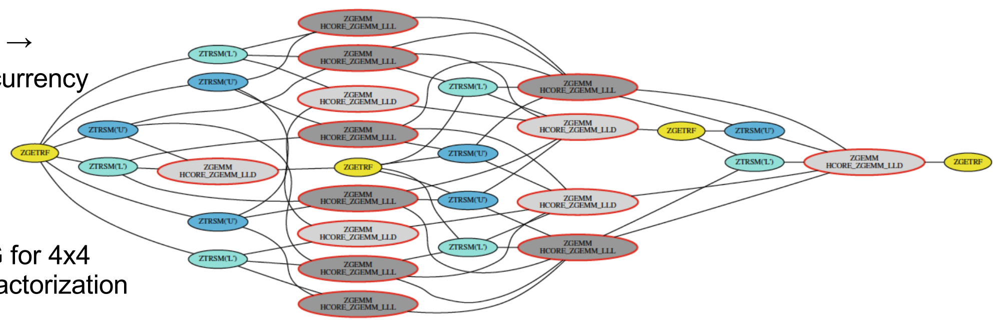
```
p = N / nb                                  ▷ number of tiles
for k = 1 to p do
    ZGETRF(A[k][k])
    for m = k+1 to p do
        ZTRSM('U', A[k][k], A[m][k])
    for n = k+1 to p do
        ZTRSM('L', A[k][k],A[k][n])
        for m = k+1 to p do
            ZGEMM(A[m][k],A[k][n],A[m][n])  ▷
```

Conventional tile LU factorization (shown with complex data types, left) is converted to a TLR LU factorization with replacement of off diagonal blocks with low rank compressed

```
for m = k+1 to p do
    if m == n then
        HCORE_ZGEMM_LLD(U[n][k],    V[n][k],
            U[k][n], V[k][n], D[n][n])
    else
        HCORE_ZGEMM_LLL(U[m][k],    V[m][k],
            U[k][n],    V[k][n],    U[m][n],
            V[m][n], rank, acc)
```

time →

concurrency ↓



DAG for 4x4 LU factorization

Compress (once) on the fly, solve many with TLU

Exterior Helmholt

SUPERCOMPUTING AT THE LEADING EDGE

GCS
Gauss Centre for Supercomputing
ISC 2020

The Board of Directors of the Gauss Centre for Supercomputing (GCS) is pleased to award the

GCS AWARD 2020

to

- Ms. Noha Al-Harthi
- Ms. Rabab Alomairy
- Dr. Kadir Akbudak
- Mr. Rui Chen
- Dr. Hatem Ltaief
- Dr. Hakan Bagci
- Dr. David Keyes

of King Abdullah University of Science and Technology (KAUST), Thuwal, KSA

for their outstanding scientific work, submitted for the ISC 2020 research paper session:

SOLVING ACOUSTIC BOUNDARY INTEGRAL EQUATIONS USING HIGH PERFORMANCE TILE LOW-RANK LU FACTORIZATION

Berlin, June 22, 2020

Prof. Dr.-Ing. Michael M. Resch
Chairman of the International GCS Award Committee
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Al-Harthi, Alomairy, Akbudak, Chen, Ltaief, Ba ... ng High Performance Tile Low Rank LU *Factorization*, Proceedings of ISC High Perforr