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Lecture 02: Tile Low-rank Methods and Applications (w/review)

David Keyes
*King Abdullah University of Science and Technology, david.keyes@kaust.edu.sa*

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University of Arkansas Department of Mathematical Sciences
46th Spring Lecture Series

David Keyes
Extreme Computing Research Center
King Abdullah University of Science and Technology
5-9 April 2021

Lecture 2
Tile Low-rank Methods and Applications (w/review)
NLA “renaissance” theme, recapped

- With controllable trade-offs, many numerical linear algebra operations adapt well for high performance on emerging architectures through
  - higher residency on the memory hierarchy
  - greater SIMT/SIMD-style concurrency
  - reduced synchronization and communication
- Rank-structured matrices, based on uniform tiles or hierarchical subdivision play a major role
- Rank-structured matrix software is here for shared-memory, distributed-memory, and GPU environments
- Many applications are benefiting
  - by orders of magnitude in memory footprint & runtime
Algorithmic opportunity

With such new algorithms, we can extend many applications that possess

- memory capacity constraints (e.g., geospatial statistics, PDE-constrained optimization)
- energy constraints (e.g., remote telescopes)
- real-time constraints (e.g., wireless commun)
- running time constraints (e.g., chem, materials, genome-wide associations)
We’ll introduce a hierarchy of ranks …

... and a hierarchy of precisions
Today’s renaissance in numerical linear algebra

A “renaissance” is a rebirth, revival, or renewed interest

Numerical linear algebra has been vital for over 70 years

• has never endured any “dark ages” or “winter”
• it simply became a bottleneck as problem sizes grew
  ▪ dense problems: cubic complexity, quadratic storage
  ▪ sparse problems: memory bandwidth-constrained

Renewal, in the form of reinvention, comes from these:

• many practical accuracy requirements are less stringent than traditional
• many important applications are “data sparse”
• many high-complexity tasks can be performed in lower precision than traditional
• randomness (typically by random selection) beats systematic coverage

A great time to be looking for research topics

• re-examine important existing algorithms in this light
Simple example of data sparsity with the 1D Laplacian

\[ A = \begin{bmatrix} 2 & -1 & \vline & -1 & \vline & 2 & -1 & \vline & -1 \\ -1 & 2 & \vline & -1 & \vline & 2 & -1 & \vline & -1 \\ -1 & 2 & \vline & -1 & \vline & 2 & -1 & \vline & -1 \end{bmatrix} \]

\[ A^{-1} = \frac{1}{8} \times \begin{bmatrix} 7 & 6 & 5 & 4 & 3 & 2 & 1 \\ 6 & 12 & 10 & 8 & 6 & 4 & 2 \\ 5 & 10 & 15 & 12 & 9 & 6 & 3 \\ 4 & 8 & 10 & 12 & 8 & 4 \\ 3 & 6 & 9 & 12 & 8 & 4 \\ 2 & 4 & 6 & 12 & 8 & 4 \\ 1 & 2 & 3 & 4 & 5 & 6 & 7 \end{bmatrix} \]

\[ A \text{ is sparse but } A^{-1} \text{ is dense} \]

Conformal off-diagonal blocks of \( A \) and \( A^{-1} \) admit low-rank representation with the same low rank (Fiedler & Markham, 1986)
Solvers have always evolved beneath “$Ax=b$”

- Advances in algorithmic efficiency rival advances in hardware architecture
- Consider Poisson’s equation on a cube of size $N=n^3$

<table>
<thead>
<tr>
<th>Year</th>
<th>Method</th>
<th>Reference</th>
<th>Storage</th>
<th>Flops</th>
</tr>
</thead>
<tbody>
<tr>
<td>1947</td>
<td>GE (banded)</td>
<td>Von Neumann &amp; Goldstine</td>
<td>$n^5$</td>
<td>$n^7$</td>
</tr>
<tr>
<td>1950</td>
<td>Optimal SOR</td>
<td>Young</td>
<td>$n^3$</td>
<td>$n^4 \log n$</td>
</tr>
<tr>
<td>1971</td>
<td>CG</td>
<td>Reid</td>
<td>$n^3$</td>
<td>$n^{3.5} \log n$</td>
</tr>
<tr>
<td>1984</td>
<td>Full MG</td>
<td>Brandt</td>
<td>$n^3$</td>
<td>$n^3$</td>
</tr>
</tbody>
</table>

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

*Six months is reduced to 1 second
Solver algorithms and Moore’s Law

- This advance took place over a span of about 36 years, or 24 doubling times for Moore’s Law.
- $2^{24} \approx 16$ million $\Rightarrow$ the same as the factor from algorithms alone!
Large-scale brings focus on complexity

- **Given, for example:**
  - a “physics” phase that scales as $O(N)$
  - a “solver” phase that scales as $O(N^{3/2})$
  - computation is almost all solver after several doublings

- **Increasingly, this is felt in the gut or the utility bills of users**

![Graph showing weak scaling limit, assuming efficiency of 100% in both physics and solver phases.](image)

- Solver takes 50% time on 1 proc
- Solver takes 97% time on 1K procs
A brief review of beneficial background

In a short lecture series that gets to the reinvention, we need to assume the invention, namely knowledge of

• where the problems come from
• how they are traditionally solved

so we undertake next a 15-slide review on

• types of applications that lead to “bottleneck” linear algebra operations
• what results we need to extract
• algebraic building blocks

It could be “homework” tonight to look up what you might be missing

We make convenient assumptions, without the caveats for every possible pathology related to conditioning, etc.
\begin{review}
Primary problem class for my lectures

Symmetric positive definite matrices arising from

• Schur complements within discretizations of elliptic and parabolic PDEs
• integral equations with displacement kernels
• Hessians from PDE-constrained optimization
• fractional differential equations
• covariances in spatial statistics
• radial basis functions from unstructured meshes
• kernel matrices from machine learning applications
Schur complements

Suppose $p$, $q$ are nonnegative integers, and suppose $A$, $B$, $C$, $D$ are respectively $p \times p$, $p \times q$, $q \times p$, and $q \times q$ matrices of complex numbers. Let

$$M = \begin{bmatrix} A & B \\ C & D \end{bmatrix}$$

so that $M$ is a $(p + q) \times (p + q)$ matrix.

If $D$ is invertible, then the **Schur complement** of the block $D$ of the matrix $M$ is the $p \times p$ matrix defined by

$$M/D := A - BD^{-1}C.$$

This eliminates the bottom $q$ unknowns in terms of the remaining $p$ unknowns and is known as “static condensation” in the finite element method.

The Schur complement arising from an SPD matrix is still SPD, but is generally dense even for a sparse original, because $D^{-1}$ is dense.

Schur complements arise when block Gauss elimination is performed to factorize a sparse matrix into its Cholesky (or more generally $LU$) factors, due to such fill in.

⇒ Condensing sparse finite element, finite difference, and finite volume matrices leads to dense blocks that are often data sparse
c/o wikipedia
The most basic type of integral equation is called a *Fredholm equation of the first type*,

\[ f(x) = \int_{a}^{b} K(x, t) \varphi(t) \, dt. \]

One method to solve numerically requires discretizing variables and replacing integral by a quadrature rule

\[ \sum_{j=1}^{n} w_j K(s_i, t_j) u(t_j) = f(s_i), \quad i = 0, 1, \ldots, n. \]

This is \( A \, u = f \), where \( A \) is \( n \times n \). If the kernel \( K(s, t) \) depends only on the distance between \( s \) and \( t \) and not on either separately, it is a “displacement kernel” and invariant upon interchange of argument, so \( A \) is a symmetric matrix and generally dense.

For a *second type Fredholm* integral equation, the unknown \( u \) also appears outside, giving diagonal weight to \( A = I + K \).

\[ \Rightarrow \text{Integral equations of interest are often strongly diagonally dominant and data-sparse (leading, e.g., to fast multipole methods)} \]

c/o wikipedia
Hessian matrices

Suppose \( f : \mathbb{R}^n \to \mathbb{R} \) is a function taking as input a vector \( \mathbf{x} \in \mathbb{R}^n \) and outputting a scalar \( f(\mathbf{x}) \in \mathbb{R} \). If all second partial derivatives of \( f \) exist and are continuous over the domain of the function, then the Hessian matrix \( \mathbf{H} \) of \( f \) is a square \( n \times n \) matrix, usually defined and arranged as follows:

\[
\mathbf{H}_f = \begin{bmatrix}
\frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\
\frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\
\vdots & \vdots & \ddots & \vdots \\
\frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n^2}
\end{bmatrix}, \text{ symmetric by interchange of partial derivatives.}
\]

Hessian matrices are used in large-scale optimization problems within Newton-type methods because they are the coefficient of the quadratic term of a local Taylor expansion of a function. That is,

\[
y = f(\mathbf{x} + \Delta \mathbf{x}) \approx f(\mathbf{x}) + \nabla f(\mathbf{x}) \Delta \mathbf{x} + \frac{1}{2} \Delta \mathbf{x}^T \mathbf{H}(\mathbf{x}) \Delta \mathbf{x}
\]

where \( \nabla f \) is the gradient \( \left( \frac{\partial f}{\partial x_1}, ..., \frac{\partial f}{\partial x_n} \right) \). Computing and storing the full Hessian matrix takes \( \Theta(n^2) \) memory, which is infeasible for high-dimensional functions such as the loss functions of neural nets, conditional random fields, and other statistical models with large numbers of parameters. For such situations, truncated-Newton and quasi-Newton algorithms have been developed.

\( \Rightarrow \) Hessian matrices require approximation for optimization

Often sum of compact and low-rank and often hierarchically low rank

c/o wikipedia
Fractional derivatives

A fairly natural question to ask is whether there exists a linear operator $H$, or half-derivative, such that

$$ H^2 f(x) = D f(x) = \frac{d}{dx} f(x) = f'(x). $$

It turns out that there is such an operator, and indeed for any $a > 0$, there exists an operator $P$ such that

$$ (P^a f)(x) = f'(x), $$

or to put it another way, the definition of $\frac{d^a f}{dx^a}$ can be extended to all real values of $a$.

There is the Caputo fractional derivative defined as:

$$ D^\nu f(t) = \frac{1}{\Gamma(n-\nu)} \int_0^t (t-u)^{(n-\nu-1)} f^{(n)}(u) du \quad (n-1) < \nu < n $$

where $n$ is the smallest integer larger than the fractional power $\nu$. When discretized, the operator $D^\nu$ is symmetric and dense except when $\nu$ is an integer. For instance, if $n = 2$, we get the discrete 1D Laplacian matrix, which is sparse, with trivially low-rank off-diagonal blocks. For fractional values of $\nu$ we lose sparsity, but we still have data sparsity. The off-diagonal blocks have low rank.

⇒ Discretized fractional derivative operators – which are currently extremely hot – are natural candidates for hierarchically low-rank approximation, which is crucial in dimensions higher than one.
Covariance matrices

Remember that for a scalar-valued random variable \( X \)

\[
\sigma^2_X = \text{var}(X) = \mathbb{E}[(X - \mathbb{E}[X])^2] = \mathbb{E}[(X - \mathbb{E}[X]) \cdot (X - \mathbb{E}[X])].
\]

If the entries in the column vector

\[
\mathbf{X} = (X_1, X_2, \ldots, X_n)^T
\]

are random variables, each with finite variance and expected value, then the covariance matrix \( K_{XX} \) is the matrix whose \((i, j)\) entry is the covariance\(^1\) p. 177

\[
K_{X_i X_j} = \text{cov}[X_i, X_j] = \mathbb{E}[(X_i - \mathbb{E}[X_i])(X_j - \mathbb{E}[X_j])]
\]

where the operator \( \mathbb{E} \) denotes the expected value (mean) of its argument.

In other words,

\[
K_{XX} = \begin{bmatrix}
\mathbb{E}[(X_1 - \mathbb{E}[X_1])(X_1 - \mathbb{E}[X_1])] & \mathbb{E}[(X_1 - \mathbb{E}[X_1])(X_2 - \mathbb{E}[X_2])] & \cdots & \mathbb{E}[(X_1 - \mathbb{E}[X_1])(X_n - \mathbb{E}[X_n])]
\mathbb{E}[(X_2 - \mathbb{E}[X_2])(X_1 - \mathbb{E}[X_1])] & \mathbb{E}[(X_2 - \mathbb{E}[X_2])(X_2 - \mathbb{E}[X_2])] & \cdots & \mathbb{E}[(X_2 - \mathbb{E}[X_2])(X_n - \mathbb{E}[X_n])]
\vdots & \vdots & \ddots & \vdots \\
\mathbb{E}[(X_n - \mathbb{E}[X_n])(X_1 - \mathbb{E}[X_1])] & \mathbb{E}[(X_n - \mathbb{E}[X_n])(X_2 - \mathbb{E}[X_2])] & \cdots & \mathbb{E}[(X_n - \mathbb{E}[X_n])(X_n - \mathbb{E}[X_n])]
\end{bmatrix}
\]

This matrix is the generalization of the scalar variance to \( n \) dimensions.

The entries on the diagonal are the variances of each individual element of \( \mathbf{X} \).

⇒ Covariance matrices are symmetric and positive semi-definite with elements that generally decay with distance by causality, and data sparse when properly ordered (e.g., space-filling curves)

c/o wikipedia
Solvers and their nestedness

To “go big” and achieve the potential of emerging architectures for scientific applications, we need implementations of fast

- linear and least squares solvers
- eigensolvers & singular value solvers
- nonlinear and optimization solvers
- time integrators & sensitivity solvers
- stencil solvers

that

- offer tunable accuracy-time-space tradeoffs
- exploit data sparsity
- exploit hierarchy of precisions
- may require more flops but complete earlier, thanks to more concurrency or less communication or synchronization
- are energy efficient
# A week of solvers 😊

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<tr>
<th>Mon, April 5th</th>
<th>Tue, April 6th</th>
<th>Wed, April 7th</th>
<th>Thu, April 8th</th>
<th>Fri, April 9th</th>
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<tr>
<td><strong>9:00am</strong></td>
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<td>David Keyes</td>
<td>David Keyes</td>
<td>David Keyes</td>
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<tr>
<td></td>
<td>Universals of Extreme Scale</td>
<td>Tile Low Rank Methods &amp;</td>
<td>Hierarchically Low Rank Methods</td>
<td>Convergence of Big</td>
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<td></td>
<td>Computing</td>
<td>Applications</td>
<td>&amp; Applications</td>
<td>Data and Extreme</td>
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<td><strong>10:15am</strong></td>
<td>Ulrike Yang</td>
<td>Laura Grigori</td>
<td>Xiao-Chuan Cai</td>
<td>Rio Yokota</td>
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<td>Algebraic Multigrid Methods</td>
<td>Multilevel and Randomized</td>
<td>Nonlinear Preconditioning</td>
<td>Low-rank &amp; Kroenecker Methods</td>
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<td><strong>11:30am</strong></td>
<td>Edmond Chow</td>
<td>Jack Dongarra</td>
<td>Carol Woodward</td>
<td>Sherry Li</td>
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<td>Preconditioned Iterative</td>
<td>Dense Linear</td>
<td>Time Integration Methods</td>
<td>Low-rank Factorization Methods</td>
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<td>Methods</td>
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<td><strong>6:00pm</strong></td>
<td>Ann Almgren</td>
<td>AWM Panel</td>
<td>Women in STEM</td>
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<td></td>
<td>Mathematics for High Performance</td>
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<td></td>
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</table>
Since Householder (1954), direct matrix computations have been built on a foundation of decompositions or factorizations:

- $A = LL^T = LDL^T$ (Cholesky, $L$, $L$ lower tri)
- $A = LU$ (LU (pivots not shown), $L$ lower tri, $U$ upper tri)
- $A = QR$ (QR, $Q$ orthogonal, $R$ right tri)
- $A = UH$ (Polar, $U$ unitary, $H$ HPD if $A$ has full rank)
- $A = UTU^H$ (Schur, $U$ unitary, $T$ upper tri)
- $A = V\Lambda V^T$ (Eigen, $V$ orthogonal if $A$ symmetric, $\Lambda$ diagonal,)
- $A = U\Sigma V^T$ (Singular, $U$, $V$ unitary, $\Sigma$ diagonal)

Mathematically, these decompositions were all known by 1910.

If $A$ is $n \times n$, dense, and full rank, their complexities are all $O(n^3)$.

In factored form, determinants, inverses for repeat solves, and low-rank updates are comparatively inexpensive.
Linear solvers of iterative type

Linear iterative methods are primarily useful for sparse problems, because their inner loops typically contain matrix-vector multiplications and (approximate) preconditioning solves.

These typically exploit special spectral, mathematical, or geometric structure, e.g., coming from a PDE:

- stationary iterative methods
- Chebyshev iterative methods
- Krylov subspace iterative methods
- multilevel iterative methods

and may thus achieve a complexity as low as $O(n)$.

(Sparse problems are also solved by direct methods, especially those coming from PDE discretizations, in less than $O(n^3)$ by exploiting geometric structure, e.g., nested dissection.)
Nonlinear solvers

Nonlinear solvers for $f(x) = 0$ are invariably iterative. For high-dimensional problems, they are of fixed-point type

$$x_{k+1} = g(x_k)$$

or accelerated (e.g., Anderson), or are variants of Newton’s method

$$x_{k+1} = x_k - J(x_k)^{-1}f(x_k)$$

where the inverse of the Jacobian is effected by incomplete application of an iterative linear method, often on an approximate Jacobian. Jacobian-free Newton-Krylov methods that access $J(x_k)$ only by Fréchet derivatives

$$J(u)v \approx \frac{1}{\varepsilon} [F(u + \varepsilon v) - F(u)]$$

are popular. Newton’s method may be nonlinearly preconditioned and is usually “globalized” by line-search, trust-region, or physics-informed “continuation” methods.

Continuation can be in the form of problem resolution (mesh), problem parameters (Reynolds), or artificial means.
Time integration solvers

Integrators for $f(x_t, x) = 0$ with important special case $x_t + F(x) = 0$ are usually semi-discretized in space, and sometimes fed to an explicit ODE integrator.

When arising in parabolic, differential algebraic, or mixed contexts, they are typically implicitly discretized in time because the temporal stability bound is typically more severe than the accuracy bound.

Hyperbolic systems admitting wave behavior tend to have accuracy and stability limits of the same order and may be solved explicitly.

However, in multi-wavespeed systems, fast wave phenomena may be unimportant to the dynamics of interest, so implicit methods are used. As such, time integrators tend to reduce on each timestep to a nonlinear solve, which, in turn through Newton reduces to a linear solve.

Time-integration methods may carry extra sensitivity variables along, which provide a form of uncertainty quantification.
Optimization solvers

Large-scale optimization problems typically come with PDE constraints and piggyback on implicit nonlinear solvers.

Consider the rootfinding problem derived from the necessary gradient conditions for minimization, with design variables $u$.

- **Objective** $\min_u \Phi(x,u) \ ; \ \Phi \in \mathbb{R}$
- **Constraints** $f(x,u) = 0 \ ; \ x \in \mathbb{R}^N \ ; \ u \in \mathbb{R}^M \ ; \ f \in \mathbb{R}^N$
- **Lagrangian** $\Phi(x,u) + \lambda^T f(x,u) \ ; \ \lambda \in \mathbb{R}^N$
- **Form the gradient of the Lagrangian with respect to each of $x, u$, and $\lambda$ to get a large coupled root-finding problem:**

\[
\begin{align*}
\Phi_x (x,u) + \lambda^T f_x (x,u) &= 0 \\
\Phi_u (x,u) + \lambda^T f_u (x,u) &= 0 \\
f(x,u) &= 0
\end{align*}
\]
Newton Reduced Sequential Quadratic Programming (RSQP)

- Applying Newton’s method leads to the KKT system for states $x$, designs $u$, and multipliers $\lambda$

$$
\begin{bmatrix}
W_{xx} & W_{ux} & (J_x^T \\
W_{ux} & W_{uu} & J_u^T \\
J_x & J_u & 0
\end{bmatrix}
\begin{bmatrix}
\delta x \\
\delta u \\
\delta \lambda
\end{bmatrix}
= 
- \begin{bmatrix}
g_x \\
g_u \\
f
\end{bmatrix}
$$

- Newton Reduced SQP solves the Schur complement system $H \delta u = g$, where $H$ is the reduced Hessian

$$
H = W_{uu} - J_u^T J_x^T W_{ux} - (J_u^T J_x^T W_{xx} - W_{ux}) J_x^T J_x
$$

$$
g = -g_u + J_u^T J_x^T g_x - (J_u^T J_x^T W_{xx} - W_{ux}) J_x^T f
$$

- Then

$$
J_x \delta x = -f - J_u \delta u
$$

$$
J_x^T \delta \lambda = -g_x - W_{xx} \delta x - W_{ux}^T \delta u
$$
Stencil ops: 4 very different types of $y = Ax$

**Explicit positions**
- Explicit values

$$y_i = d_i x_i - \sum_{j \in S_i} c_{ij} x_j$$
- General sparse matvec

**Implicit positions**
- Explicit values

$$y_i = d_i x_i - \sum_{j=i+K} c_{ij} x_j$$
- Diffusion on Cartesian mesh, $\nabla \cdot A \nabla$

**Explicit positions**
- Implicit values

$$y_i = d_i x_i - \sum_{j \in S_i} x_j$$
- Graph Laplacian

$$d_i = |S_i|$$

**Implicit positions**
- Implicit values

$$y_i = dx_i - \sum_{j=i+K} x_j$$
- Laplacian on Cartesian mesh, $\nabla^2$

$$d = |K|$$

e.g., for 1D Laplacian, $K = \{-1, +1\}$ and $d = 2$
Rank-structured operators

- **Advantages**
  - shrink memory footprints to live higher on the memory hierarchy
    - higher means quick access (↑ arithmetic intensity)
  - reduce operation counts
  - tune work to accuracy requirements
    - e.g., preconditioner versus solver

- **Disadvantages**
  - pay cost of (re-)compression
  - not all operators compress well
Data sparsity from rank-structured matrices*

- **Tile low rank (TLR)**
  - all blocks at a single level of subdivision (could in principle vary in size)

- **Hierarchically low rank (HLR)**
  - blocks are left at various levels upon recursive subdivision
  - weak and strong “admissibility” variants

- **HLR more than two decades old**
  - Fiedler (1993) defined “structure ranks”

- **Prevalent topic in SIAM Applied Linear Algebra conferences**

* A rank-structured matrix is a matrix with enough low-rank blocks that it pays to take advantage of them (paraphrasing Wilkinson on sparse matrices)
Reduce memory footprint and operation complexity with low rank

• 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
  ▪ e.g., cache sizes, warp sizes

• Use randomized SVD (Halko, Martinsson & Tropp, 2009) to form low-rank blocks
  ▪ a flop-intensive GEMM-based flat algorithm

• Implement in “batches” of leaf blocks
  ▪ flattening trees in the case of HLR
Complexities of rank-structured factorization

For a square dense matrix of $O(N)$:

- **“Straight” $LU$ or $LDL^T$**
  - **Operations** $O(N^3)$
  - **Storage** $O(N^2)$

- **Tile low-rank** (Amestoy, Buttari, L’Excellent & Mary, *SISC*, 2016)*
  - **Operations** $O(k^{0.5}N^2)$
  - **Storage** $O(k^{0.5}N^{1.5})$
  - for uniform blocks with size chosen optimally for max rank $k$ of any compressed block, bounded number of uncompressed blocks per row

- **Hierarchically low-rank** (Grasedyck & Hackbusch, *Computing*, 2003)
  - **Operations** $O(k^2N \log^2N)$
  - **Storage** $O(kN)$
  - for strong admissibility, where $k$ is max rank of any compressed block

* First reported $O(k^{0.5}N^{2.5})$, then later $O(k^{0.5}N^2)$ for variant that reorders updates and recompression
Rank-structure also relevant to sparse problems

Classical factorizations fill in with elimination

For 3D Poisson solver on a cube with $O(N)$ degrees of freedom:

- Classical nested dissection generally requires $O(N^2)$ operations
- Tile low-rank can yield $O(N^{4/3})$ operations
  (Amestoy, Buttari, L’Excellent & Mary, *SISC*, 2016)
- Hierarchically low-rank methods can yield $O(N)$ operations
- Gains come from low-rank treatment of the resulting Schur complements
Tile Low Rank begins with tile algorithms

- **PLASMA**, **Chameleon**, and **FLAME** implementations
- Dense matrix is divided into tiles
- Remove artifactual synchronization by bringing task parallelism to the fore

Tile Cholesky of a 4x4 matrix

for \( k = 1 \) to \( T \) do
  \textbf{POTRF}(D(k,k))
  for \( i = k+1 \) to \( T \) do
    \textbf{TRSM}(V(i,k), D(k,k))
  for \( j = k+1 \) to \( T \) do
    \textbf{SYRK}(D(j,j), U(j,k), V(j,k))
  for \( i = j+1 \) to \( T \) do
    \textbf{GEMM}(U(i,k), V(i,k), U(j,k), V(j,k), U(i,j), V(i,j), acc)
Tile Cholesky factorization (dense)

\[
T = \frac{N}{B} \quad \# \text{B is block size; } T \text{ is tiles per dimension}
\]

for \( k = 1 \) to \( T \) do

\textbf{POTRF}(D(k,k))

for \( i = k+1 \) to \( T \) do

\textbf{TRSM}(V(i,k), D(k,k))

for \( j = k+1 \) to \( T \) do

\textbf{SYRK}(D(j,j), U(j,k), V(j,k))

for \( i = j+1 \) to \( T \) do

\textbf{GEMM}(U(i,k), V(i,k), U(j,k), V(j,k), U(i,j), V(i,j), acc)

\[
\text{Kernel} \quad \text{Dense Cholesky}
\]

<table>
<thead>
<tr>
<th>Kernel</th>
<th>Dense Cholesky</th>
</tr>
</thead>
<tbody>
<tr>
<td>POTRF</td>
<td>( \frac{1}{3} \times B^3 )</td>
</tr>
<tr>
<td>TRSM</td>
<td>( B^3 )</td>
</tr>
<tr>
<td>SYRK/LR_SYRK</td>
<td>( B^3 )</td>
</tr>
<tr>
<td>GEMM/LR_GEMM</td>
<td>( 2 \times B^3 )</td>
</tr>
<tr>
<td>Total</td>
<td>( O(N^3) )</td>
</tr>
</tbody>
</table>

A serial and incompressible critical path of TLR Cholesky:

\[
(T-1) \times \left( \text{POTRF} + \text{TRSM} + \text{SYRK} \right) + \text{POTRF}
\]

The block algorithm has \( T \) steps down the diagonal, each of which is \( O(T^2) \) for updates, and the block update operations are each \( O(B^3) \), so there is no reduction in complexity,

\[
T^3 \times B^3 = N^3 ,
\]

just better scheduling.
Dynamic runtime systems

- Operate directly from the sequential code
- Ensure that data dependencies are not violated
- Schedule the tasks across appropriate available hardware resources
- Optimize memory placement for nonuniform access
- Enhance software productivity by abstracting the hardware
- Examples (all avail for shared memory, distributed memory, and GPUs):
  - OpmSs
    - BSC, Barcelona
    - Pragma-based, extending OpenMP to asynchronous execution
  - ParSEC
    - ICL, University of Tennessee
    - Parallel runtime scheduling and execution control
  - StarPU
    - INRIA, Bordeaux
    - Unified runtime system for heterogeneous multicore architecture
Tile Low Rank (TLR) is a compromise between optimality and implementation complexity.

**TLR Cholesky factorization**

\[ T = \frac{N}{B} \quad \# \text{B is block size; } T \text{ is tiles per dimension} \]

for \( k = 1 \) to \( T \) do

- **POTRF**\((D(k,k))\)

  for \( i = k+1 \) to \( T \) do

    - **TRSM**\((V(i,k), D(k,k))\)

      for \( j = k+1 \) to \( T \)

        - **LR_SYRK**\((D(j,j), U(j,k), V(j,k))\)

      for \( i = j+1 \) to \( T \)

        - **LR_GEMM**\((U(i,k), V(i,k), U(j,k), V(j,k), U(i,j), V(i,j), \text{acc})\)

Swapping out a \( B \) for a rank, where \( \text{rank} \ll B \), provides an easy win.

However, one must pay the cost of initial compression and of recompression after updates.

<table>
<thead>
<tr>
<th>Kernel</th>
<th>Dense Cholesky</th>
<th>TLR Cholesky</th>
</tr>
</thead>
<tbody>
<tr>
<td>POTRF</td>
<td>( \frac{1}{3} \times B^3 )</td>
<td>( \frac{1}{3} \times B^3 )</td>
</tr>
<tr>
<td>TRSM</td>
<td>( B^3 )</td>
<td>( B^2 \times \text{rank} )</td>
</tr>
<tr>
<td>SYRK/LR_SYRK</td>
<td>( B^3 )</td>
<td>( 2 \times B^2 \times \text{rank} + 4 \times B \times \text{rank}^2 )</td>
</tr>
<tr>
<td>GEMM/LR_GEMM</td>
<td>( 2 \times B^3 )</td>
<td>( 36 \times B \times \text{rank}^2 + 157 \times \text{rank}^3 )</td>
</tr>
<tr>
<td>Total</td>
<td>( O(N^3) )</td>
<td>( O(N^2 \times \text{rank}) )</td>
</tr>
</tbody>
</table>
Low rank approximation for off-diag tiles

There are several means of forming data sparse representations of the amenable off-diagonal blocks

- **standard SVD:** $O(n^3)$, too expensive for initial and especially for repeated compressions after 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

* RSVD and ACA routines offered in KBLAS at github.com/ecrc/kblas-gpu
Jacobi-SVD also offered in KBLAS for small matrices in batched mode
Geospatial statistics motivation

“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
Geospatial statistics applications

Synthetic test matrix: random coordinate generation within the unit square or unit cube with Matérn kernel decay, each pair of points connected by

- linear exp to square exp decay, $a_{ij} \sim \exp(-c|x_i - x_j|^p)$, $p = 1, 2$
Large dense symmetric systems arise as covariance matrices in 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 the log-likelihood function involving a large dense (but data sparse) covariance

\[
\ell(\theta) = -\frac{1}{2} Z^T \Sigma^{-1}(\theta) Z - \frac{1}{2} \log |\Sigma(\theta)|
\]

• Solve \( \Sigma^{-1} \) and determinant \( |\Sigma| \) and depend upon Cholesky, dominated by DPOTRF factorization routine (next slides)
TLR vs. Intel MKL on shared memory

Geospatial statistics (Gaussian kernel) to accuracy 1.0e-8

- Three generations of Intel manycore (Sandy Bridge, Haswell, Skylake)
- Two generations of linear algebra (classical dense and tile low rank)

Red arrows: speedups from hardware, same algorithm

Green arrows: speedups from algorithm, same hardware

Blue arrow: from both

Akbudak, Ltaief, Mikhalev, Charara & K., *Exploiting Data Sparsity for Large-scale Matrix Computations*, Euro-Par 2018
Memory footprint for DP matrix of size 1M

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

NB: log scale

Akbudak, Ltaief, Mikhalev, Charara & K., *Exploiting Data Sparsity for Large-scale Matrix Computations*, EuroPar 2018
Nearly 2 orders of magnitude for 0.5M size matrix on 16 nodes

HiCMA 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
**TLR tour de force**

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

- would require 14.1 PetaBytes in dense DP
- would require 77 days by ScaLAPACK (at the TLR rate of 3.7 Pflop/s)

*Cao, Pei, Akbudak, Mikhalev, Bosilca, Ltaief, K. & Dongarra, Extreme-Scale Task-Based Cholesky Factorization Toward Climate and Weather Prediction Applications. PASC ’20 (ACM), 2020*
Execution trace, dense DPOTRF

Chameleon: Dense DPOTRF time 18.1s
4 nodes of Shaheen with a matrix size of 54K using StarPU runtime

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

HiCMA: TLR DPOTRF time **1.8s** (10X faster)
4 nodes of Shaheen with a matrix size of 54K, using StarPU runtime

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

- Tile low rank has a higher percentage of idle time (red), relative to flop-intensive dense tile
- Scales less efficiently relative to itself
- However, for an acceptable accuracy tolerance, it is superior in time and energy

Akbudak, Ltaief, Mikhalev, Charara & K., Exploiting Data Sparsity for Large-scale Matrix Computations, Euro-Par 2018
Algorithm 1. Dense Tile LU factorization of a $N$-by-$N$ matrix $A$ composed of $nb \times nb$ tiles and solve.

1: $p = N / nb$ \hspace{1cm} \triangleright$ number of tiles 
2: for $k = 1$ to $p$ do 
3: \hspace{1cm} ZGETRF($A[k][k]$) 
4: \hspace{1cm} for $m = k+1$ to $p$ do 
5: \hspace{2cm} ZTRSM($U'$, $A[k][k]$, $A[m][k]$) 
6: \hspace{1cm} for $n = k+1$ to $p$ do 
7: \hspace{2cm} ZTRSM($L'$, $A[k][k]$,$A[k][n]$) 
8: \hspace{1cm} for $m = k+1$ to $p$ do 
9: \hspace{2cm} 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.

DAG for 4x4 LU factorization
Compress (once) on the fly, solve many with HLU

Exterior Helmholtz problem: acoustic scattering BIE

Rank distribution challenges with 3D exponential kernels

The simple exponential kernel:

\[ C(r; \ell) = \exp\left( -\frac{r}{\ell} \right) \]

is suited for rough correlations such as the variation of wind speed or temperature with altitude, and leads to wide rank disparities.

Initial ranks following Morton ordering of 3D field with \( N=1.08M \) and \( B=2700 \) for matrix of 400 x 400 tiles:

- Min:18
- Avg:52
- Max:900

Final ranks following Cholesky factorization:

- Min:2
- Avg:64
- Max:1129

Ratio of 500 in rank!

Rank variations before and after factorization:

- Min:-25
- Avg:+13
- Max:+273

Ratio of 50 in rank!

Rank distribution challenges with 3D exponential kernels

Threshold for treating an *individual* data-sparse tile as dense is relatively low (effectively about 15% of tile size)

May be lower considering *distribution* of ranks

Time and annotated flop rates for low rank GEMM and dense GEMM (48 GF/s) for tiles size 2700, with ratios & threshold, as function of rank

Ratio of rank to tile size with matrix size 1.08M; rank is a mathematical object; tile size is an algorithmic parameter

Dynamic data structure adaption:
treat near-diagonal high-rank tiles as fully dense

First, second and third panel factorization & update steps
P - POTRF, T - TRSM, S - SYRK, G – GEMM
Upper color: within tile band adaptively preserved as dense
Lower color: handled as low rank tile

Cao, Pei, Akbudak, Bosilca, Ltaief, K. & Dongarra, Leveraging PaRSEC Runtime Support to Tackle Challenging 3D Data-sparse Matrix Problems. IPDPS (IEEE), 2021
Sensitivity to tile size

Auto-tuning is available based on a starting point for tile size $B = \sqrt{N}$

Cao, Pei, Akbudak, Bosilca, Ltaief, K. & Dongarra, Leveraging PaRSEC Runtime Support to Tackle Challenging 3D Data-sparse Matrix Problems. IPDPS (IEEE), 2021
Dense tile bandsize auto-tuning

Time to Solution

Auto-tuning time on 512 nodes

Boxes indicate bandsize range in which TLR and dense flops for all GEMM and TRSM are within a small range around unity.

Time spent autotuning for bandsize is about 0.1% of cost of solution.

Cao, Pei, Akbudak, Bosilca, Ltaief, K. & Dongarra, Leveraging PaRSEC Runtime Support to Tackle Challenging 3D Data-sparse Matrix Problems. IPDPS (IEEE), 2021
Memory reduction & load imbalance

Even after thresholding high-rank off-diagonal tiles as dense, a wide distribution of smaller ranks remains.

Memory allocations per tile are reduced to those actually needed with major reduction (up to 44x) in band adaptive TLR relative to earlier TLR versions.

Dynamic runtime system deals with tile load variations gracefully.
Comparison with prior state-of-the-art

For exponential kernel matrix of N = 2.16M on 256 nodes, new TLR optimizations to account for rank variation save factor of 5x to 7.5x across a range of relevant sizes for geospatial environmental statistics.

Tile release time to the runtime system (last tile is end of computation)

Sensitivity to accuracy thresholds

Effect of accuracy requirements on 512 nodes
Earlier results were for $10^{-9}$; here are three looser tolerances
Hierarchical Computations on Manycore Architectures: HiCMA*

* appearing one thesis at a time at https://github.com/ecrc
Conclusions, recapped

- With controllable trade-offs, many linear algebra operations adapt well to high performance on emerging architectures through
  - higher residence on the memory hierarchy
  - greater SIMT/SIMD-style concurrency
  - reduced synchronization and communication
- Rank-structured matrices, based on uniform tiles or hierarchical subdivision play a major role
- Rank-structured matrix software is here for shared-memory, distributed-memory, and GPU environments
- Many applications are benefiting
  - by orders of magnitude in memory footprint & runtime
Iconographic conclusion

I ❤️
today

tomorrow
Exploiting Data Sparsity for Large-Scale Matrix Computations

Kadir Akbudak¹, Hatem Ltaief², Aleksandr Mikhailév¹(✉), Ali Charara³, and Anicîlo Esposito⁴

¹ Extreme Computing Research Center, Divison of Computer, Electrical, and Mathematical Sciences and Engineering, King Abdullah University of Science and Technology, Thuwal Jeddah 23955, Kingdom of Saudi Arabia
{kadir.akbudak,hatem.ltaief,aleksandr.mikhailev,ali.charara,david.keyes}@kaust.edu.sa
² Cray EMEA Research Lab, Bristol, UK
esposito@cray.com

Abstract. Exploiting data sparsity in dense matrices is an algorithmic bridge between architectures that are increasingly memory-aware on a per-core basis and extreme-scale applications. In this work, we leverage the Hierarchical Mixed-Data Format (HMDA) library in order to tackle this challenging problem by achieving significant reductions in time to solution and memory footprint, while preserving a specified accuracy requirement of the application. We have extended HMDA to provide a high-performance implementation on distributed-memory systems of one of the most widely used matrix factorization in large-scale scientific applications, i.e., the Cholesky factorization. It employs the tile low-rank data format to compress the dense data-sparse off-diagonal tiles of the matrix. It then decomposes the matrix computations into interdependent tasks and relies on the dynamic runtime system StarPU for asynchronous out-of-order scheduling, while allowing high user productivity. Performance comparisons and memory footprints on matrix dimensions up to eleven million show a performance gain and memory saving of more than an order of magnitude for both matrices on thousands of cores, against state-of-the-art open-source and vendor optimized numerical libraries. This represents an important milestone in enabling large-scale matrix computations toward solving big data problems in geospatial statistics for climate/weather forecasting applications.

1 Introduction

State-of-the-art dense linear algebra libraries are confronting memory capacity limits and/or are not able to produce solutions in reasonable times, when performing large computations (e.g., matrix factorizations and solutions) on large...
Cao, Pei, Akbudak, Mikhalev, Bosilca, Ltaief, K. & Dongarra

Leveraging PaRSEC Runtime Support to Tackle Challenging 3D Data-Sparse Matrix Problems

Qingpei Cao¹, Yu Pei², Kadir Akbudak³, George Bosilca¹, Hatem Ltaief⁶, David Keyes⁷, and Jack Dongarra¹

¹Innovative Computing Laboratory, University of Tennessee, US
²King Abdullah University of Science and Technology, KSA
³AESEL Research Center, Turkey

Abstract—The task-based programming model associated with dynamic runtime systems has gained popularity for challenging problems because of workload imbalance, heterogeneous resources, or extreme concurrency. During the last decade, low-rank matrix approximations, where the main idea consists of exploiting data sparsity typically by compressing off-diagonal tiles up to an application-specific accuracy threshold, have been adopted to address the curse of dimensionality at extreme scales. In this paper, we create a bridge between the runtime and the linear algebra by communicating knowledge of the data sparsity to the runtime. We design and implement this synergistic approach with high user productivity in mind, in the context of the PaRSEC runtime system and the BLASMA numerical library. This requires to extend PaRSEC with new features to integrate rank information into the dataflow so that proper decisions can be made at runtime. We focus on the low-rank (TLR) Cholesky factorization for solving 3D data-sparse covariance matrix problems arising in environmental applications. In particular, we extend the TLR exponential model of Matérn kernel matrix, which exhibits challenging nonuniform high ranks in off-diagonal tiles. We first provide a dynamic data structure management driven by a performance model to reduce extra floating-point operations. Next, we optimize the memory footprint of the application by utilizing a dynamic memory allocator and supported by a rank-aware data distribution to cope with the workload imbalance. Finally, we expose more parallelism using kernel recursive formulations to shorten the critical path. Our resulting high-performance implementation outperforms existing data-sparse TLR Cholesky factorization by up to 7-fold on a large-scale distributed-memory system, while minimizing the memory footprint up to a 44-fold factor. This interdisciplinary work highlights the need to empower runtime systems beyond their original duty of task scheduling for servicing next-generation low-rank matrix libraries.

Index Terms—Low-rank matrix computations, Task-based programming model, Dynamic runtime system, Asynchronous executions and load balancing, High-performance computing, User productivity, Environmental applications.

I. INTRODUCTION

The HPC community has enjoyed an order of magnitude performance improvement every five years [1] thanks to hardware innovations and technology scaling. At the dawn of exascale, this means systems with tens of millions of concurrent threads. This rapidly evolving hardware landscape requires new software paradigms, and perhaps equivalently important, advanced algorithmic responsibilities [2].

The coupling of task-based programming models with dynamic runtime systems corresponds to one of the most critical paradigms shift embedded in order to replace the traditional bulk synchronous parallel model in favor of the asynchronous execution model [3-5]. This versatile software solution has shown performance superiority by overlapping expensive data movement with fine-grained computations and ultimately achieving higher occupancy on the underlying hardware architecture. Moreover, runtime systems are inherently designed with the abstraction of the hardware complexity. This latter feature enhances user-productivity and permits fast code deployment on massively parallel systems. At the same time, existing numerical methods have displayed limitations in addressing big data problems, due to high algorithmic complexity and large memory footprint. Low-rank matrix approximations may overcome the curse of dimensionality [6]. The main idea consists of approximating off-diagonal tiles up to an application-specific accuracy threshold and carrying out the matrix algorithm on the newly obtained data structures. This compression step may sacrifice numerical accuracy, so it results in a tunable tradeoff. By exploiting the rank structure naturally embedded in the data-sparse operator, lower complexity may be obtained in storage, data motion, and arithmetic operations, compared to traditional dense algorithms.

We propose a synergistic bridge between the runtime and linear algebra communities in the context of dealing with large-scale covariance matrices in geostatistical problems. We employ the ELCGB Tile Low-Rank (TLR) numerical library and the PaRSEC dynamic runtime system to showcase the mutual benefits of this approach. The objective is to propagate the rank information to PaRSEC so that it can take proper runtime decisions before BLASMA operates on the computational kernels. In particular, we focus on the challenging exponential model of Matérn kernel for 3D environmental applications [7]. This model results in heterogeneous rank distribution with high-rank tiles located outside of the diagonal tiles. We extend PaRSEC with new functionality that takes into account the rank information in the task dataflow: (1) a dynamic data structure management driven by a performance model to reduce extra floating-point operations, (2) a dynamic memory allocator to further optimize memory footprint, (3) a rank-aware data distribution to cope with the workload imbalance, and (4) a recursive formulation of computational kernels to expose concurrency during the critical path. We use these features to leverage the performance of the TLR Cholesky factorization at the heart of the Maximum Likelihood Estimation (MLE) [8].
Reference

Al-Harthi, Alomairy, Akbudak, Chen, Ltaief, Bagci & K.

Lecture Notes in Computer Science 12151:209 (2020)
Very special thanks to...

Hatem Ltaief
Principal Research Scientist
Extreme Computing Research Center
KAUST
Closing haiku

Curse of dimension,
Can you be mitigated

By low rank’s blessing?
Thank you!

شكراً

david.keyes@kaust.edu.sa