Tensor computations: A fragmented landscape

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About me

HPAC High Performance and Automatic Computing

HPC2N

High-Performance Computing Center North

- Taxonomy of contractions: Can you GEMM? — E. Di Napoli, D. Traver-Fabregat

  "Towards an Efficient Use of the BLAS Library for Multilinear Tensor Contractions", AMC 235, 2014

- Performance prediction — E. Peise

  "On the Performance Prediction of BLAS-based Tensor Contractions", PMBS, SC'14

- Density Functional Theory: FLAPW methods — E. Di Napoli, E. Peise

  "High-Performance Generation of the Hamiltonian and Overlap Matrices in FLAPW Methods", CPC 2017

- High-performance kernels — P. Springer

  "TTC: A high-performance Compiler for Tensor Transpositions", ACM TOMS 44(2), 2017
  "Design of a High-Performance GEMM-like Tensor-Tensor Multiplication", ACM TOMS 44(3), 2018
  "Spin Summations: A High-Performance Perspective", ACM TOMS 45(1), 2019

- High-intensity kernels — C. Psarras, L. Karsson

  "Concurrent Alternating Least Squares for multiple simultaneous Canonical Polyadic Decompositions", 2020

Outline

- Part 1: (Dense) Linear Algebra – historical overview
- Part 2: Tensor Operations

Dense Linear Algebra – 1973

"[..] a fairly small number of basic operations which are generally responsible for a significant percentage of the total execution time" – Hanson, Krogh, Lawson

- `DOT`: $\boldsymbol{w} := \boldsymbol{x}^T \boldsymbol{y}$
- `ELVOP`: $\boldsymbol{y} := \alpha \boldsymbol{x} + \boldsymbol{y}$
- `NRM`: $\eta := (\boldsymbol{x}^T \boldsymbol{x})^{1/2}$

1973 – 1979

- 1973: *"A proposal for standard linear algebra subprograms"* – Hanson, Krogh, Lawson
  Class I: DOT, ELVOP, G2, MG2 – Assembly
  Class II: NRM, XDOT, COPY, SWAP, SCALE, SUM, MAX – Fortran
- 1974: *"Standardization of FORTRAN callable subprograms for basic linear algebra"* – Lawson
- 1975–: LINPACK
- 1977: *"Basic Linear Algebra Subprograms for FORTRAN usage—an extended report"* – Hanson, Krogh, Kinkaid, Lawson
- 1977: *"Fortran BLAS timing"* – Dongarra
  Tests on 24 different computers

1979: BLAS 1

"Basic Linear Algebra Subprograms for FORTRAN usage"
— Hanson, Krogh, Kinkaid, Lawson (ACM TOMS)

"38 subprograms for basic operations of linear algebra"

- "aid in **design** and **coding** stages"
- "self-**documenting** quality of code"
- "a reduction of the execution time spent in these operations might be reflected in **cost savings** in the running of programs"
- "the programming of some of these low level operations involves **algorithmic and implementation subtleties** that are likely to be ignored"

- 1988: BLAS 2 *“with some modern machine architectures, the use of the BLAS is not the best way to improve the efficiency of higher level codes. [..] the use of BLAS inhibits this optimization.”*

  Matrix-vector operations **NOT** built on top of BLAS 1

- 1990: BLAS 3 *“Unfortunately, [BLAS 2] is often not well suited to computers with a hierarchy of memory”*

  Matrix-matrix operations **NOT** built on top of BLAS 1 & 2

- Immediate, widespread adoption: LAPACK, ScaLAPACK, PETSc, PLAPACK, ...

- Specialization, optimization, auto-tuning, high-level notation, automation, ...

But ...

But ...

- Rigid interface
- Inflexible black-box nature
- (Often) Sub-optimal at small scale
- . . .

In practice:

Signal Processing	$x := \left(A^{-T}B^TBA^{-1} + R^TLR\right)^{-1} A^{-T}B^TBA^{-1}y$	$R \in \mathbb{R}^{n-1\times n}$, UT; $L \in \mathbb{R}^{n-1\times n-1}$, DI
Kalman Filter	$K_k := P_k^bH^T(HP_k^bH^T + R)^{-1};\ x_k^a := x_k^b + K_k(z_k - Hx_k^b);\ P_k^a := (I - K_KH)\, P_k^b$	
Ensemble Kalman Filter	$X^a := X^b + \left(B^{-1} + H^TR^{-1}H\right)^{-1}\left(Y - HX^b\right)$	$B \in \mathbb{R}^{N\times N}$ SSPD; $R \in \mathbb{R}^{m\times m}$, SSPD
Image Restoration	$x_k := (H^TH + \lambda\sigma^2 I_n)^{-1}(H^Ty + \lambda\sigma^2(v_{k-1} - u_{k-1}))$	
Rand. Matrix Inversion	$\Lambda := S(S^TAWAS)^{-1}S^T;\ \Theta := \Lambda AW;\ M_k := X_kA - I$ $X_{k+1} := X_k - M_k\Theta - (M_k\Theta)^T + \Theta^T(AX_kA - A)\Theta$	
Generalized Least Squares	$b := (X^TM^{-1}X)^{-1}X^TM^{-1}y$	$n > m$; $M \in \mathbb{R}^{n\times n}$, SPD; $X \in \mathbb{R}^{n\times m}$; $y \in \mathbb{R}^n$
Stochastic Newton	$B_k := \frac{k}{k-1}B_{k-1}(I_n - A^TW_k((k-1)I_l + W_k^TAB_{k-1}A^TW_k)^{-1}W_k^TAB_{k-1})$	
Optimization	$x_f := WA^T(AWA^T)^{-1}(b - Ax);\ \ x_o := W(A^T(AWA^T)^{-1}Ax - c)$	
Tikhonov Regularization	$x := (A^TA + \Gamma^T\Gamma)^{-1}A^Tb$	$A \in \mathbb{R}^{n\times m}$; $\Gamma \in \mathbb{R}^{m\times m}$; $b \in \mathbb{R}^{n\times 1}$
Gen. Tikhonov Reg.	$x := (A^TPA + Q)^{-1}(A^TPb + Qx_0)$	$P \in \mathbb{R}^{n\times n}$, SSPD; $Q \in \mathbb{R}^{m\times m}$, SSPD; $x_0 \in \mathbb{R}$
LMMSE estimator	$K_{t+1} := C_tA^T(AC_tA^T + C_z)^{-1};\ x_{t+1} := x_t + K_{t+1}(y - Ax_t);\ C_{t+1} := (I - K_{t+1}A)C_t$	

. . .

$$K_k := P_k^b H^T (H P_k^b H^T + R)^{-1}; \quad x_k^a := x_k^b + K_k(z_k - H x_k^b); \quad P_k^a := (I - K_K H)\, P_k^b$$

$$\begin{cases} C_\dagger := PCP^T + Q \\ K := C_\dagger H^T (H C_\dagger H^T)^{-1} \end{cases}$$

$$\Lambda := S(S^T AWAS)^{-1} S^T; \; \Theta := \Lambda AW; \; M_k := X_k A - I$$
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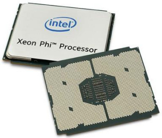

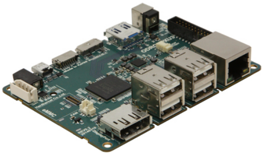

MUL ADD MOV

MOVAPD

VFMADDPD ...

$$K_k := P_k^b H^T (H P_k^b H^T + R)^{-1}; \quad x_k^a := x_k^b + K_k(z_k - H x_k^b); \quad P_k^a := (I - K_K H)\, P_k^b$$

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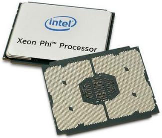
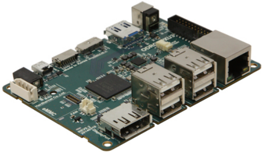
$y := \alpha x + y$ | $LU = A$ | $\cdots$ | $C := \alpha AB + \beta C$

$X := A^{-1} B$ | $C := AB^T + BA^T + C$ | $X := L^{-1} M L^{-T}$ | $QR = A$

... **BLAS** **LAPACK** ...





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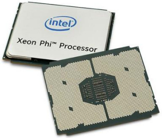
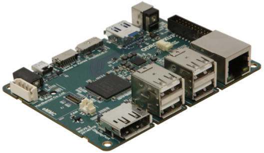
... BLAS LAPACK ...





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LINEAR ALGEBRA MAPPING PROBLEM ("LAMP")

$y := \alpha x + y$ | $LU = A$ | $\cdots$ | $C := \alpha AB + \beta C$

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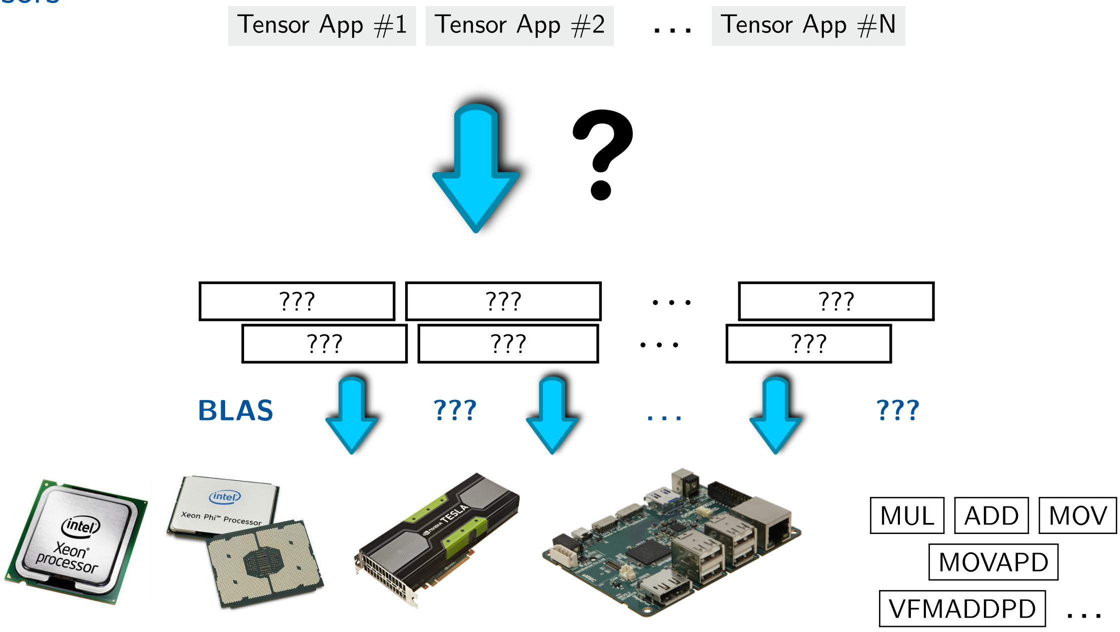
... BLAS LAPACK ...

C. Psarras, H. Barthels, *“The Linear Algebra Mapping Problem. Current state of linear algebra languages and libraries”.* [arXiv:1911.09421]

H. Barthels, C. Psarras, *“Linnea: Automatic Generation of Efficient Linear Algebra Programs”, ACM TOMS, 2021.* [arXiv:1912.12924]

Tensors

Tensors


Tensor App #1
Tensor App #2
...
Tensor App #N
?
???
???
...
???
???
???
...
???
BLAS
???
...
???
intel
Xeon processor
intel
Xeon Phi™ Processor
TESLA
MUL
ADD
MOV
MOVAPD
VFMADDPD
...

Tensors

- No “Tensor BLAS” – collections of building blocks
- No agreement on interface(s)
- Lack of reference implementations
- A jungle of independent libraries and packages, in a variety of languages

Tensor computations

- Two separate worlds
  - Contractions — Computational physics / chemistry
    Tensor = Multi-linear operator
    Generalization of matrix-matrix product

Tensor computations

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  - Contractions — Computational physics / chemistry
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  - Decompositions — Data science
    Tensor = Collection of data
    Generalization of matrix factorizations

Tensor computations

- Two separate worlds
  - Contractions — Computational physics / chemistry
    Tensor = Multi-linear operator
    Generalization of matrix-matrix product
  - Decompositions — Data science
    Tensor = Collection of data
    Generalization of matrix factorizations
- Terminology and notation vary (and conflict) even within one world
- Very few software efforts cut across the boundary

Representative operations

Data layout operations

- Reshape
- Permute / transpose
- Sort (sparse)
- Convert data layout
- Partition
- Distribute
- ...

Arithmetic operations

- Add, subtract, scale
- Inner product
- Norms
- Element-wise operations
- Tensor-times-vector (TTV)
- Tensor-times-matrix (TTM)
- MTTKRP
- Contractions
- ...

Decompositions

- CP (CANDECOMP/PARAFAC)
- Tucker
- INDSCAL
- PARAFAC2
- CANDELINC
- DEDICOM
- PARATUCK2
- ...

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In setting up a library, where to draw the boundaries?

Contractions

Contractions

- **Tensor Transpositions**

$$\mathcal{B}_{i_1 i_2 \ldots i_N} \leftarrow \alpha \cdot \mathcal{A}_{\pi(i_1 i_2 \ldots i_N)} + \beta \cdot \mathcal{B}_{i_1 i_2 \ldots i_N}$$

- **Summations** — linear summation over tensor transpositions

$$\mathcal{B}_{i_0 i_1 i_2} \leftarrow 2\mathcal{A}_{i_0 i_1 i_2} - \mathcal{A}_{i_2 i_1 i_0} - \mathcal{A}_{i_0 i_2 i_1}$$

$$\mathcal{B}_{i_0 i_1 i_2} \leftarrow 4\mathcal{A}_{i_0 i_1 i_2} - 2\mathcal{A}_{i_1 i_0 i_2} - 2\mathcal{A}_{i_2 i_1 i_0} + \mathcal{A}_{i_1 i_2 i_0} - 2\mathcal{A}_{i_0 i_2 i_1} + \mathcal{A}_{i_2 i_0 i_1}$$

$$\mathcal{B}_{i_0 i_1 i_2 i_3} \leftarrow 2\mathcal{A}_{i_0 i_1 i_2 i_3} - \mathcal{A}_{i_2 i_1 i_0 i_3} - \mathcal{A}_{i_0 i_2 i_1 i_3} - \mathcal{A}_{i_0 i_1 i_3 i_2}$$

- **Tensor Contractions**

$$\mathcal{C}_{\pi_{\mathcal{C}}(I_m \cup I_n)} \leftarrow \alpha \cdot \mathcal{A}_{\pi_{\mathcal{A}}(I_m \cup I_k)} \times \mathcal{B}_{\pi_{\mathcal{B}}(I_n \cup I_k)} + \beta \cdot \mathcal{C}_{\pi_{\mathcal{C}}(I_m \cup I_n)}$$

- **Tensor Transpositions**

  TTC: A high-performance Compiler for Tensor Transpositions. ACM TOMS, 2017

  Compiler: `https://github.com/HPAC/TTC` **Library**: `https://github.com/HPAC/hptt`

- **Summations** — linear summation over tensor transpositions

  Spin Summations: A High-Performance Perspective. ACM TOMS, 2019

  Generator: `https://github.com/springer13/spin-summations`

- **Tensor Contractions**

  Design of a high-performance GEMM-like Tensor-Tensor Multiplication. ACM TOMS, 2018

  Compiler: `https://github.com/HPAC/tccg` **Library**: `https://github.com/springer13/tcl`

But . . .

But . . .

Coupled-Cluster methods

$$
\begin{aligned}
\tau_{ij}^{ab} &= t_{ij}^{ab} + \frac{1}{2} P_b^a P_j^i t_i^a t_j^b, \\
\tilde{F}_e^m &= f_e^m + \sum_{fn} v_{ef}^{mn} t_n^f, \\
\tilde{F}_e^a &= (1-\delta_{ae}) f_e^a - \sum_{m} \tilde{F}_e^m t_m^a - \frac{1}{2} \sum_{mnf} v_{ef}^{mn} t_{mn}^{af} + \sum_{fn} v_{ef}^{an} t_n^f, \\
\tilde{F}_i^m &= (1-\delta_{mi}) f_i^m + \sum_{e} \tilde{F}_e^m t_i^e + \frac{1}{2} \sum_{nef} v_{ef}^{mn} t_{in}^{ef} + \sum_{fn} v_{if}^{mn} t_n^f,
\end{aligned}
$$

$$
\begin{aligned}
\tilde{W}_{ei}^{mn} &= v_{ei}^{mn} + \sum_{f} v_{ef}^{mn} t_i^f, \\
\tilde{W}_{ij}^{mn} &= v_{ij}^{mn} + P_j^i \sum_{e} v_{ie}^{mn} t_j^e + \frac{1}{2} \sum_{ef} v_{ef}^{mn} \tau_{ij}^{ef}, \\
\tilde{W}_{ie}^{am} &= v_{ie}^{am} - \sum_{n} \tilde{W}_{ei}^{mn} t_n^a + \sum_{f} v_{ef}^{ma} t_i^f + \frac{1}{2} \sum_{nf} v_{ef}^{mn} t_{in}^{af}, \\
\tilde{W}_{ij}^{am} &= v_{ij}^{am} + P_j^i \sum_{e} v_{ie}^{am} t_j^e + \frac{1}{2} \sum_{ef} v_{ef}^{am} \tau_{ij}^{ef}, \\
z_i^a &= f_i^a - \sum_{m} \tilde{F}_i^m t_m^a + \sum_{e} f_e^a t_i^e + \sum_{em} v_{ei}^{ma} t_m^e + \sum_{em} v_{im}^{ae} \tilde{F}_e^m + \frac{1}{2} \sum_{efm} \\
z_{ij}^{ab} &= v_{ij}^{ab} + P_j^i \sum_{e} v_{ie}^{ab} t_j^e + P_b^a P_j^i \sum_{me} \tilde{W}_{ie}^{am} t_{mj}^{eb} - P_b^a \sum_{m} \tilde{W}_{ij}^{am} t_m^b + P
\end{aligned}
$$

credits to D. Matthews, E. Solomonik, J. Stanton, and J. Gauss

But . . .

Coupled-Cluster methods

$$\tau_{ij}^{ab} = t_{ij}^{ab} + \frac{1}{2} P_b^a P_j^i t_i^a t_j^b,$$

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$$\tilde{W}_{ei}^{mn} = v_{ei}^{mn} + \sum_f v_{ef}^{mn} t_i^f,$$

$$\tilde{W}_{ij}^{mn} = v_{ij}^{mn} + P_j^i \sum_e v_{ie}^{mn} t_j^e + \frac{1}{2} \sum_{ef} v_{ef}^{mn} \tau_{ij}^{ef},$$

$$\tilde{W}_{ie}^{am} = v_{ie}^{am} - \sum_n \tilde{W}_{ei}^{mn} t_n^a + \sum_f v_{ef}^{ma} t_i^f + \frac{1}{2} \sum_{nf} v_{ef}^{mn} t_{in}^{af},$$

$$\tilde{W}_{ij}^{am} = v_{ij}^{am} + P_j^i \sum_e v_{ie}^{am} t_j^e + \frac{1}{2} \sum_{ef} v_{ef}^{am} \tau_{ij}^{ef},$$

$$z_i^a = f_i^a - \sum_m \tilde{F}_i^m t_m^a + \sum_e f_e^a t_i^e + \sum_{em} v_{ei}^{ma} t_m^e + \sum_{em} v_{im}^{ae} \tilde{F}_e^m + \frac{1}{2} \sum_{efm}$$

$$z_{ij}^{ab} = v_{ij}^{ab} + P_j^i \sum_e v_{ie}^{ab} t_j^e + P_b^a P_j^i \sum_{me} \tilde{W}_{ie}^{am} t_{mj}^{eb} - P_b^a \sum_m \tilde{W}_{ij}^{am} t_m^b + P$$

credits to D. Matthews, E. Solomonik, J. Stanton, and J. Gauss

Finite Element 3D diffusion operator

```
TE.BeginMultiKernelLaunch();
TE("T2_e_i1_i2_k3 = B_k3_i3 X_e_i1_i2_i3", T2, B, X);
TE("T1_e_i1_k2_k3 = B_k2_i2 T2_e_i1_i2_k3", T1, B, T2);
TE("U1_e_k1_k2_k3 = G_k1_i1 T1_e_i1_k2_k3", U1, G, T1);
TE("T1_e_i1_k2_k3 = G_k2_i2 T2_e_i1_i2_k3", T1, G, T2);
TE("U2_e_k1_k2_k3 = B_k1_i1 T1_e_i1_k2_k3", U2, B, T1);
TE("T2_e_i1_i2_k3 = G_k3_i3 X_e_i1_i2_i3", T2, G, X);
TE("T1_e_i1_k2_k3 = B_k2_i2 T2_e_i1_i2_k3", T1, B, T2);
TE("U3_e_k1_k2_k3 = B_k1_i1 T1_e_i1_k2_k3", U3, B, T1);
TE("Z_m_e_k1_k2_k3 = U_n_e_k1_k2_k3 D_e_m_n_k1_k2_k3", Z, U,
TE("T1_e_i3_k1_k2 = B_k3_i3 Z1_e_k1_k2_k3", T1, B, Z1);
TE("T2_e_i2_i3_k1 = B_k2_i2 T1_e_i3_k1_k2", T2, B, T1);
TE("Y_e_i1_i2_i3 = G_k1_i1 T2_e_i2_i3_k1", Y, G, T2);
TE("T1_e_i3_k1_k2 = B_k3_i3 Z2_e_k1_k2_k3", T1, B, Z2);
TE("T2_e_i2_i3_k1 = G_k2_i2 T1_e_i3_k1_k2", T2, G, T1);
TE("Y_e_i1_i2_i3 += B_k1_i1 T2_e_i2_i3_k1", Y, B, T2);
TE("T1_e_i3_k1_k2 = G_k3_i3 Z3_e_k1_k2_k3", T1, G, Z3);
TE("T2_e_i2_i3_k1 = B_k2_i2 T1_e_i3_k1_k2", T2, B, T1);
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TE.EndMultiKernelLaunch();
```

credits to A. Fisher – `https://github.com/LLNL/acrotensor`

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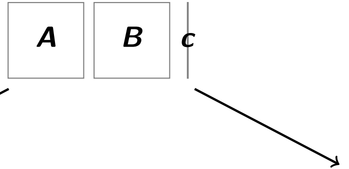

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Product is associative, but its cost is not!

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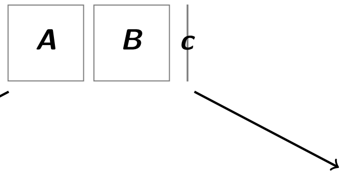

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- Optimal parenthesisation: Polynomial time (matrices), exponential time (tensors)

Decompositions

With L. Karlsson

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- **Survey of the field**
  - From an algorithmic and software perspective

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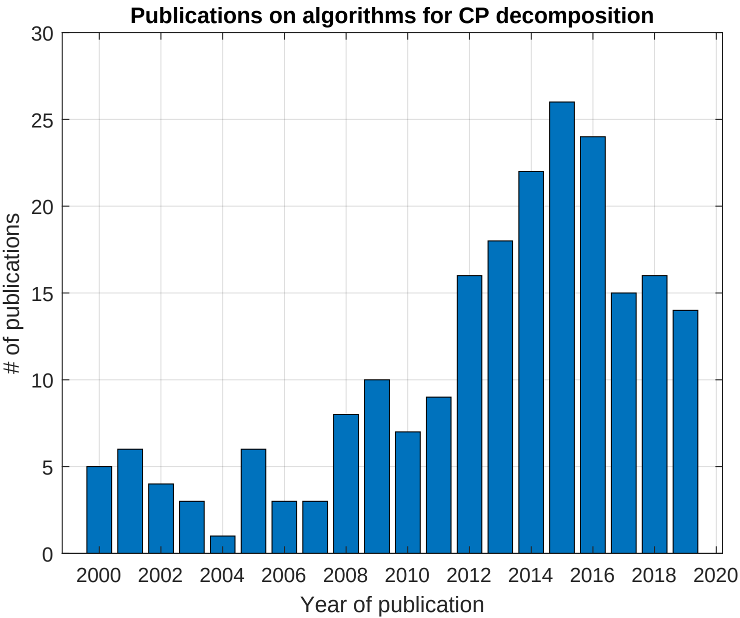
- **Quickly realized there is an abundance of**
  - Decompositions (CP, Tucker, . . .)
  - Variants thereof (non-negative, orthogonal, . . .)
  - Algorithms (alternating, all-at-once, algebraic, . . .)
  - Software packages & languages
  - Papers on software without software



Publications on algorithms for CP decomposition
30
25
20
15
10
5
0
# of publications
2000
2002
2004
2006
2008
2010
2012
2014
2016
2018
2020
Year of publication

Algorithms for CP decomposition

- **Algebraic algorithms**
  - Generalized Rank Annihilation Method
  - Direct TriLinear Decomposition
  - The "algebraic algorithm" by Domanov and De Lathauwer
  - The "simpler algorithm" by Pimentel-Alarcón
  - ...
- **Alternating optimization algorithms**
  - Alternating Least Squares
  - Fast ALS
  - Hierarchical ALS
  - Regularized ALS
  - ...
- **All-at-once optimization algorithms**
  - Gradient descent
  - (Damped) Gauss–Newton
  - Nonlinear CG, GMRES
  - Quasi-Netwon (e.g., L-BFGS)
  - ...
- **Enhancements**
  - Line search
  - Compression
  - Randomization
  - Transient constraints
  - ...

Matlab and R packages with support for CP decomposition (subset)

- **Tensor Toolbox** by Bader, Kolda, & others
  https://www.tensortoolbox.org/
- **Tensorlab** by Vervliet, Debals, Sorber, Van Barel, & De Lathauwer
  https://www.tensorlab.net/index.html
- **The N-way Toolbox** by Bro & Andersson
  http://www.models.life.ku.dk/nwaytoolbox
- **TensorBox** by Phan, Tichavsky, & Cichocki
  https://github.com/phananhhuy/TensorBox
- **Tensor Package** by Comon & others
  http://www.gipsa-lab.fr/~pierre.comon/TensorPackage/tensorPackage.html

- **multiway** by Helwig
  https://cran.r-project.org/package=multiway
- **ThreeWay** by Giordani, Kiers, & Del Ferraro
  https://cran.r-project.org/package=ThreeWay
- **rTensor** by Li, Bien, & Wells
  https://cran.r-project.org/package=rTensor

C/C++ packages with support for CP decomposition (subset)

- **Genten** by SANDIA (Phipps)
  `https://gitlab.com/tensors/genten`
- **SPLATT** by Smith & Karypis
  `https://github.com/ShadenSmith/splatt`
- **ParTI!** by Li, Ma, & Vuduc
  `https://github.com/hpcgarage/ParTI`
- **Cyclops** by Solomonik & others
  `https://github.com/cyclops-community`

And then there's Python, Fortran, ...

Massive redundancy

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- Algorithm versus implementation: Which **algorithm** is fastest?
  - **Runtimes** are measured on **implementations**
  - Different implementations of the same algorithm (on different languages)
  - **Impl. A** faster than **Impl. B** $\not\Rightarrow$ **Alg. A** faster than **Alg. B**

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  2. $\mathbf{9000 \times 300 \times 10}$
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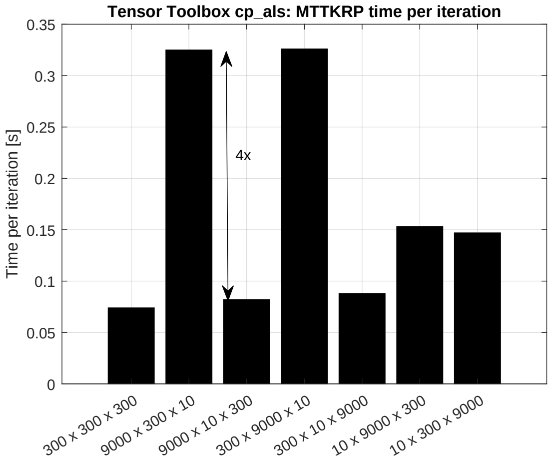
- Building block: "Matricized tensor times Khatri-Rao product" (MTTKRP)

Algorithm versus implementation



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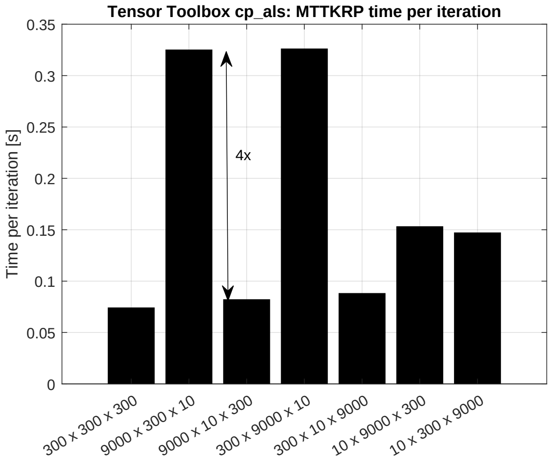

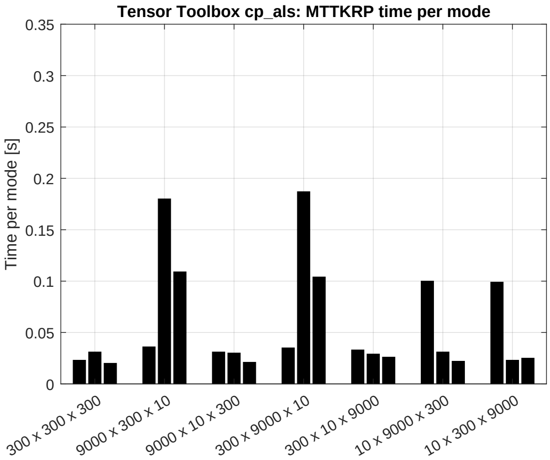

Building blocks for tensor computations

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Workflow

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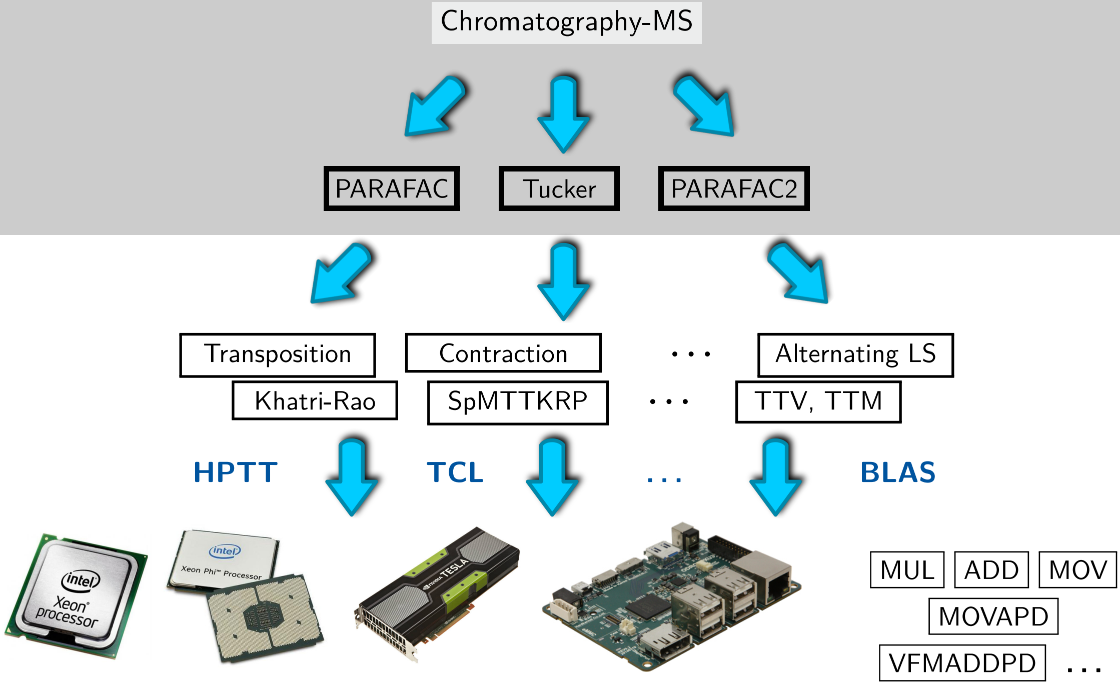
Computation of each individual model: bandwidth bound!

Hence: *"Concurrent Alternating Least Squares for multiple simultaneous Canonical Polyadic Decompositions", with C. Psarras, L. Larsson. (Submitted).*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Transposition
Contraction
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TTV, TTM
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Thank you for the intvitation and for your attention!