The fragmented landscape of tensor computations

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About me

About me: Background in linear algebra

- Parallel eigensolvers
- Automatic generation of algorithms
- Stability analysis
- Performance modeling & prediction
- Compilers for matrix operations
- Applications
  - Covariance matrix
  - Genome-Wide Association Studies (GWAS)
- ...

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Everything relies on linear algebra libraries

Hierarchy of linear algebra libraries

PETSc, ...

ScaLAPACK, PLAPACK, ...

LAPACK

BLAS-1, BLAS-2, BLAS-3

More libraries ... (and many more iterative ones)

PETSc, Trilinos, ...

ScaLAPACK, PLAPACK, Elemental, ...

LAPACK, Plasma, SuperMatrix, Magma, ...

BLAS-1, BLAS-2, BLAS-3, ATLAS, BTO-BLAS, BLIS, ...

Applications

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

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

$$\Lambda := S(S^T A W A S)^{-1} S^T; \ \Theta := \Lambda A W; \ M_k := X_k A - I$$
$$X_{k+1} := X_k - M_k \Theta - (M_k \Theta)^T + \Theta^T (A X_k A - A)\Theta$$

$$x := A(B^T B + A^T R^T \Lambda R A)^{-1} B^T B A^{-1} y \quad \ldots \quad E := Q^{-1} U (I + U^T Q^{-1} U)^{-1} U^T$$

Applications $\longrightarrow$ libraries

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$$\boxed{y := \alpha x + y} \quad \boxed{LU = A} \quad \cdots \quad \boxed{C := \alpha AB + \beta C}$$
$$\boxed{X := A^{-1} B} \quad \boxed{C := AB^T + BA^T + C} \quad \boxed{X := L^{-1} M L^{-T}} \quad \boxed{QR = A}$$

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LINEAR ALGEBRA MAPPING PROBLEM

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LINEAR ALGEBRA MAPPING PROBLEM

"The Linear Algebra Mapping Problem. Current state of linear algebra languages and libraries", ACM TOMS, 2022
C. Psarras, H. Barthels, P. Bientinesi, [arXiv:1911.09421]

"Benchmarking the Linear Algebra Awareness of TensorFlow and PyTorch", iWAPT-22
A. Sankaran, N.A. Alashti, C. Psarras, P. Bientinesi, [arXiv:2202.09888]

"Linnea: Automatic Generation of Efficient Linear Algebra Programs", ACM TOMS, 2021
H. Barthels, C. Psarras, P. Bientinesi, [arXiv:1912.12924]

Tensors

"**Multi**-linear algebra mapping problem" ?

Tensors applications

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t) = \left[\frac{-2\hbar}{2\mu}\nabla^2 + V(\mathbf{r},t)\right]\Psi(\mathbf{r},t)$$

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

Tensor Application #i ... Tensor Application #j

Tensors applications⟶ lin.alg.libs

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

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

- Performance prediction E. Peise, P.B.

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

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

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

Tensor kernels

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t) = \left[\frac{-2\hbar}{2\mu}\nabla^2 + V(\mathbf{r},t)\right]\Psi(\mathbf{r},t)$$

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\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}$$

Tensor Application #i **CHEMOMETRICS** ... Tensor Application #j

Contractions | **???** | $A = U\Sigma W^\star$ | $\cdots$ | $C := \alpha AB + \beta C$ | **Tucker** | **???**

??? | **Transposition** | **???** | **CP** | **ALS** | **???** | **MTTKRP**

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- High-performance kernels P. Springer, P.B.
  - *"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*

Survey

"**The landscape of software for tensor computations**"
C. Psarras, L. Karlsson, J. Li, P.B.

`https://arxiv.org/pdf/2103.13756.pdf`

DatM:	Data Manipulation
EWOps:	Element-Wise Operations
Con:	Contractions
SpecCon:	Specific Contractions
Decomp:	Decompositions

ID	Package Name	Functionality					Type	Platform	Language
		DatM	EWOps	SpecCon	Con	Decomp			
0	Acrotensor	–	–	✓	✓	–	D	C, G	C++
1	AdaTM	–	–	✓	–	✓	S	C	C
2	Boost.uBlas.Tensor	✓	✓	✓	✓	–	D	C	C++
3	BTAS	✓	✓	✓	✓	✓	nan	C	C++
4	COGENT	–	–	✓	✓	–	D	G	Python → CUDA
5	COMET	–	–	✓	✓	–	S	C	C++ → C++
6	CoTenGra	–	–	✓	✓	–	D	C, D, G	Python
7	CP-CALS	–	–	✓	–	✓	D	C, G	C++, Mat^{i}
8	CSTF	–	–	–	–	✓	S	D	Scala
9	CuTensor	✓	✓	✓	✓	–	D	G	C, CUDA
10	cuTT	✓	–	–	–	–	D	G	C++, CUDA
11	Cyclops	✓	✓	✓	✓	–	S, D	C, D, G	C++
12	D-Tucker	–	–	–	–	✓	D	C	Matlab
13	DFacTo	–	–	–	–	✓	S	C, D	C++
14	Eigen Tensor	✓	✓	✓	✓	–	D	C, G	C++
15	ExaTN	✓	✓	✓	✓	✓	D	C, D, G	C++, Py^{i}
16	Fastor	✓	✓	✓	✓	–	D	C	C++
17	FTensor	✓	✓	✓	✓	–	D	C	C++

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18	Genten	–	–	–	–	✓	D, S	C, G	C++
19	GigaTensor	–	–	–	–	✓	S	C, D	Unknown
20	HPTT	✓	–	–	–	–	D	C	C++, Python[i], C[i]
21	ITensor	–	✓	✓	✓	✓	D, BS	C, G[x]	C++, Julia
22	libtensor	–	–	✓	✓	–	D, BS	C	C++
23	Ltensor	–	–	✓	✓	–	D	C	C++
24	MATLAB	✓	✓	✓	✓	–	D	C	Matlab
25	MultiArray	✓	–	–	–	–	D	C	C++
26	multiway	–	–	–	–	✓	D	C	R
27	N-way toolbox	–	–	–	–	✓	D	C	Matlab
28	NCON	–	–	✓	✓	–	D	C	Matlab
29	netcon	–	–	✓	✓	–	D	C	Matlab
30	NumPy	✓	✓	✓	✓	–	D	C	Python
31	Ocean	✓	✓	–	–	–	D	C, G	C, Py[i]
32	ParCube	–	–	–	–	✓	S	C	Matlab
33	ParTensor	–	–	–	–	✓	D	C, G	C++
34	ParTI!	✓	✓	✓	–	✓	S	C, G	C, CUDA, Mat[x]
35	PLANC	–	–	–	–	✓	D	C, D	C++

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36	PLS toolbox	–	–	–	–	✓	D	C	Matlab
37	Pytensor	✓	✓	✓	✓	✓	D, S	C	Python
38	PyTorch	✓	✓	✓	✓	–	D, S	C, G	Python, C++, CUDA
39	quimb	–	–	✓	✓	–	D	C, D, G	Python
40	rTensor	✓	✓	✓	–	✓	D	C	R
41	rTensor (rand.)	–	–	–	–	✓	D	C	Python
42	scikit-tensor	✓	✓	✓	–	✓	D, S	C	Python
43	Scikit-TT	–	–	–	–	✓	D	C	Python
44	SPALS	–	–	–	–	✓	S	C	C++
45	SPARTan	–	–	–	–	✓	S	C	Matlab
46	SPLATT	–	–	✓	–	✓	S	C, D	C, C++, Oct, Mat
47	SuSMoST	–	–	–	–	✓	D	C	Python
48	T3F	✓	✓	–	–	✓	D	C, G	Python
49	TACO	✓	✓	✓	✓	–	D, S	C, G	C++, C++ $\rightarrow$ C++
50	TAL_SH	✓	✓	✓	✓	–	D	C, G	C, C++, Fort
51	TBlis	✓	✓	✓	✓	–	D	C	C++
52	TCCG	–	–	✓	✓	–	D	C	C++
53	TCL	–	–	✓	✓	–	D	C	C++, Python[i]

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54	TDALAB	–	–	–	–	✓	D, S	C	Matlab, GUI
55	TeNPy	–	–	–	–	✓	D	C	Python
56	Tensor Fox	–	–	–	–	✓	D, S	C	Python, Matlab
57	Tensor package	–	–	–	–	✓	D	C	Matlab
58	Tensor Toolbox	✓	✓	✓	✓	✓	D, S	C	Matlab
59	tensor_decompositio	–	–	–	–	✓	D	C, D	Python
60	TensorBox	–	–	–	–	✓	D, S	C	Matlab
61	TensorD	–	–	–	–	✓	D	C, G	Python
62	TensorFlow	✓	✓	✓	✓	–	D, S	C, D, G	C++, Python
63	TensorLab	–	–	–	–	✓	D, S	C	Matlab
64	TensorLab+	–	–	–	–	✓	D, S	C	Matlab
65	TensorLy	✓	✓	✓	✓	✓	D	C, G	Python
66	TensorNetwork	–	–	✓	✓	–	D, S	C, G	Python
67	TensorOperations.	✓	✓	✓	✓	–	D	C, G	Julia
68	TensorTrace	–	–	✓	✓	–	D	C	GUI → Py, Jul, Mat
69	Three-Way	–	–	✓	✓	✓	D	C	R
70	TiledArray	✓	✓	✓	✓	–	D, BS	C, D	C++
71	tncontract	–	–	✓	✓	–	D	C	Python

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72	TNR	–	–	–	–	✓	D	C	Matlab
73	TorchMPS	–	–	✓	✓	–	D	C	Python
74	TT-Toolbox	✓	✓	–	–	✓	D	C, D^x, G^x	Matlab, Python
75	TTC	✓	–	–	–	–	D	C	Python $\rightarrow$ C++
76	TTV	–	–	✓	–	–	D	C	C++
77	TVM	–	✓	–	–	–	D, S	C, G	Python
78	Uni10	✓	✓	✓	✓	–	D	C, G^x	C++
79	xerus	–	–	✓	✓	✓	D, S	C,	C++

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  this is an enormous duplication of effort and functionality!!
  Also, many (severely) suboptimal implementations!

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- 1) Why?!
  2) Is there a way out?

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- Terminology and notation vary (and conflict) even within one world

  "It is pointless to recommend the adoption of a universal tensor notation. However, it would be extremely useful to have a thesaurus that shows how to articulate typical calculations [...]" — **Charles Van Loan**, *2009*

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- Development: application driven — Very few software efforts cut across boundaries

Representative tensor operations / building blocks candidates

Data manipulation

- 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
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Decompositions

- CP (CANDECOMP/PARAFAC)
- Tucker
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- CANDELINC
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How to set the layers?
E.g., where does the "T-BLAS" end and the "T-LAPACK" begin?

Also . . . one vs. many problem instances

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Coupled-Cluster methods

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

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

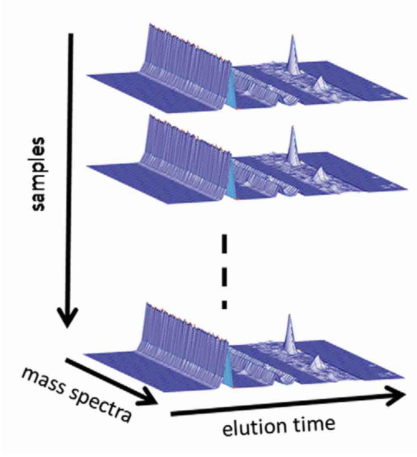
Finite Element 3D diffusion operator

```
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);
TE("Y_e_i1_i2_i3 += B_k1_i1 T2_e_i2_i3_k1", Y, B, T2);
TE.EndMultiKernelLaunch();
```

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

One vs. many problem instances (continued)

Chromatography



Rasmus Bro

Workflow

- ⋮
- **4. Fit model**: 1–20 components;
  PARAFAC — PARAFAC2 — TUCKER
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- **6.** Estimate the sensitivity of the model's parameters

One vs. many problem instances (continued)

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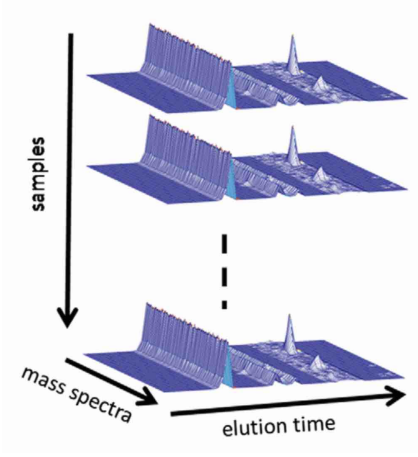

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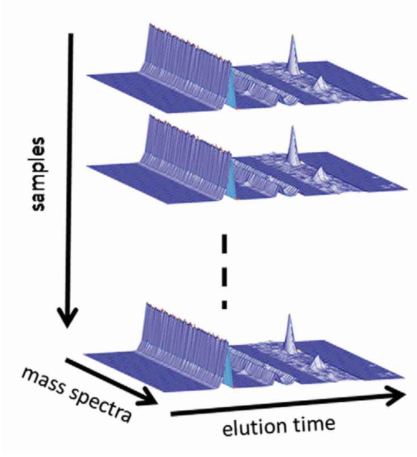

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Huge opportunities for multi-instance & multi-problem optimizations

Antithesis of decomposition into kernels. Here, **high-performance via grouping**!

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

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

- Performance prediction E. Peise, P.B.

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

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

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

- High-performance kernels P. Springer, P.B.
  - *"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, R. Bro, P.B.
  - *"Algorithm 1026: Concurrent Alternating Least Squares for multiple simultaneous Canonical Polyadic Decompositions", ACM TOMS 48(3), 2022*
  - *"Accelerating jackknife resampling for the Canonical Polyadic Decomposition", Frontiers AMS (8), 2022.*

Conclusions

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Thank you!

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