Tensor Computations: Efficiency Or Productivity?

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HPAC High Performance and Automatic Computing

Part I

The HPC perspective

Disclaimer: Talk about awareness, not results

Typical HPC “workflow” – not limited to tensor computations

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⇒ **Caveat**: Gains in the building blocks... often lost at the higher levels

Examples (1/2) Genome-Wide Association Studies (GWAS)

- What is it? Data correlation analysis. 2D grid of generalized least squares problems (GLS)

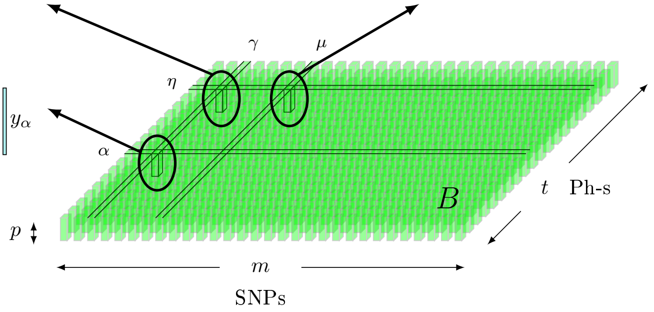
Examples (1/2) Genome-Wide Association Studies (GWAS)

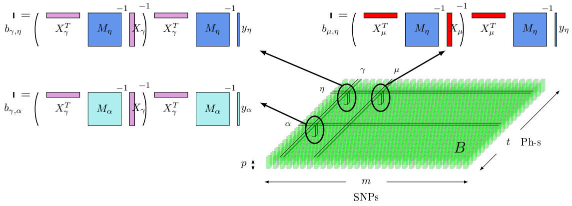
- How is it related to tensors? 1D×1D cartesian product of GLSs, 2D output = 4D data

$$b_{\gamma,\eta} = \left(X_\gamma^T M_\eta^{-1} X_\gamma \right)^{-1} X_\gamma^T M_\eta^{-1} y_\eta$$

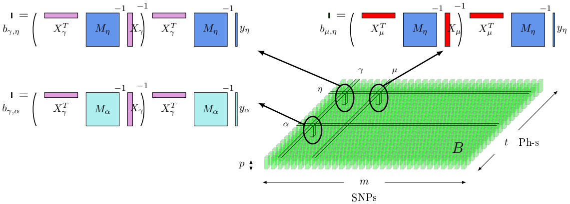
$$b_{\mu,\eta} = \left(X_\mu^T M_\eta^{-1} X_\mu \right)^{-1} X_\mu^T M_\eta^{-1} y_\eta$$

$$b_{\gamma,\alpha} = \left(X_\gamma^T M_\alpha^{-1} X_\gamma \right)^{-1} X_\gamma^T M_\alpha^{-1} y_\alpha$$





- Algorithmic improvement: lower computational complexity
- HPC optimizations: asynch I/O, overlap, BLAS-3, parallelism, ...



Computing Petaflops over Terabytes of Data: The Case of Genome-Wide Association Studies.
ACM TOMS, 2014

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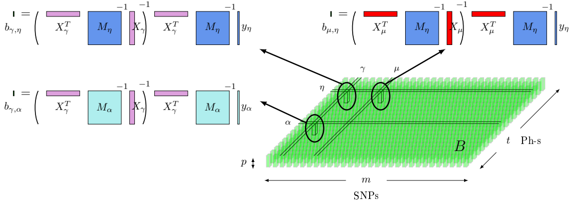

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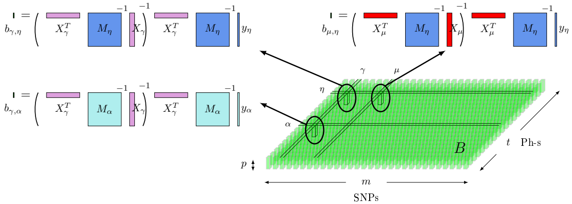

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  - Data management: data formats, overwriting, multiple files
  - Data manipulation: imputation, filtering, selection
  - Workflow not as fixed as first understood: M vs no-M, . . .
  - *“The pre-processing is slower than the analysis”*

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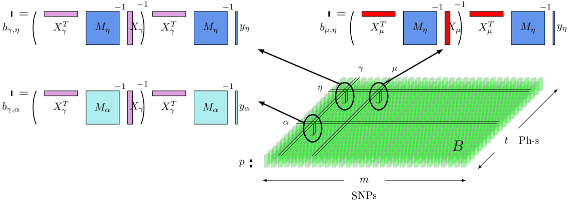

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⇒ Performance is important, but not as much as we like to think

Examples (2/2)

- **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, 2018

  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`

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- Mismatch $\rightarrow$ mapping problem

2D case: "Right" level of abstraction

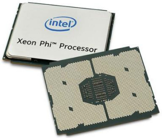
Generalized Least Squares	$b := (X^T M^{-1} X)^{-1} X^T M^{-1} y$	$n > m$; $M \in \mathbb{R}^{n \times n}$, SPD; $X \in \mathbb{R}^{n \times m}$; $y \in \mathbb{R}^{n \times 1}$
Signal Processing	$x := \left(A^{-T} B^T B A^{-1} + R^T L R\right)^{-1} A^{-T} B^T B A^{-1} y$	
Kalman Filter	$K_k := P_k^b H^T (H P_k^b H^T + R)^{-1}$; $x_k^a := x_k^b + K_k (z_k - H x_k^b)$; $P_k^a := (I - K_K H) P_k^b$	
Ensemble Kalman Filter	$X^a := X^b + \left(B^{-1} + H^T R^{-1} H\right)^{-1} \left(Y - H X^b\right)$	
Image Restoration	$x_k := (H^T H + \lambda \sigma^2 I_n)^{-1} (H^T y + \lambda \sigma^2 (v_{k-1} - u_{k-1}))$	
Rand. Matrix Inversion	$X_{k+1} := S(S^T A S)^{-1} S^T + (I_n - S(S^T A S)^{-1} S^T A) X_k (I_n - A S (S^T A S)^{-1} S^T)$	
Stochastic Newton	$B_k := \frac{k}{k-1} B_{k-1} (I_n - A^T W_k ((k-1) I_l + W_k^T A B_{k-1} A^T W_k)^{-1} W_k^T A B_{k-1})$	
Optimization	$x_f := W A^T (A W A^T)^{-1} (b - Ax)$; $x_o := W (A^T (A W A^T)^{-1} A x - c)$	
Tikhonov Regularization	$x := (A^T A + \Gamma^T \Gamma)^{-1} A^T b$	$A \in \mathbb{R}^{n \times m}$; $\Gamma \in \mathbb{R}^{m \times m}$; $b \in \mathbb{R}^{n \times 1}$
Gen. Tikhonov Reg.	$x := (A^T P A + Q)^{-1} (A^T P b + Q x_0)$	$P \in \mathbb{R}^{n \times n}$, SSPD; $Q \in \mathbb{R}^{m \times m}$, SSPD; $x_0 \in \mathbb{R}^{m \times 1}$
LMMSE estimator	$K_{t+1} := C_t A^T (A C_t A^T + C_z)^{-1}$; $x_{t+1} := x_t + K_{t+1} (y - A x_t)$; $C_{t+1} := (I - K_{t+1} A) C_t$	

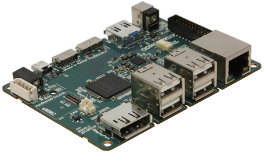
$$x := A(B^TB + A^TR^T\Lambda RA)^{-1}B^TBA^{-1}y$$

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

$$E := Q^{-1}U(I + U^TQ^{-1}U)^{-1}U^T \quad \ldots$$

?





MUL | ADD | MOV

MOVAPD

VFMADDPD ...

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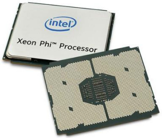
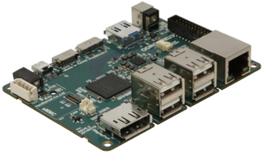
$\boxed{y := \alpha x + y}$ $\boxed{LU = A}$ $\cdots$ $\boxed{C := \alpha AB + \beta C}$

$\boxed{X := A^{-1}B}$ $\boxed{C := AB^T + BA^T + C}$ $\boxed{X := L^{-1}ML^{-T}}$ $\boxed{QR = A}$

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





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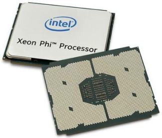

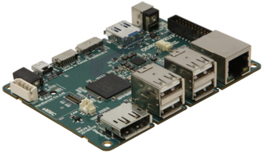

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...

LINEAR ALGEBRA MAPPING PROBLEM (LAMP)

$y := \alpha x + y$

$:= \alpha AB + \beta C$

$X := A^{-1}B$

$C := A$

$^{-1}ML^{-T}$

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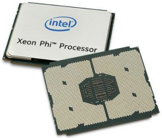

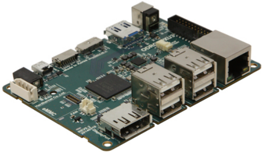

MUL ADD MOV

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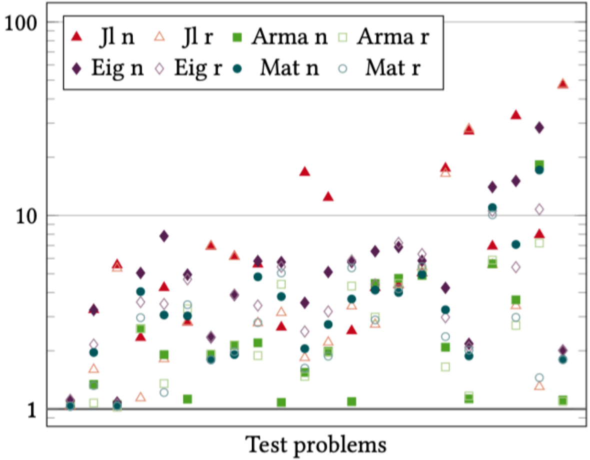
LAMP: A problem often ignored

Linnea: A compiler for linear algebra – Henrik Barthels, Christos Psarras

Linnea's speedups



Jl: Julia, **Arma**: Armadillo, **Eig**: Eigen, **Mat**: Matlab. **n**/**r**: naive/recommended implementation

Tensor App #1 | Tensor App #2 | . . . | Tensor App #N

?

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MOVAPD

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Tensor App #1 Tensor App #2 ... Tensor App #N

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Transposition Contraction · · · Alternating LS

Khatri-Rao SpMTTKRP · · · TTV, TTM

HPTT **TCL** **...** **BLAS**

MUL ADD MOV

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nD case: Exemplary applications

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

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\end{aligned}
$$

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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

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Part II

The computational scientists' perspective

"The fastest FLOPS are those that are not executed."
– Lars

Chromatography-MS

PARAFAC | Tucker | PARAFAC2

Transposition | Contraction | · · · | Alternating LS

Khatri-Rao | SpMTTKRP | · · · | TTV, TTM

HPTT | **TCL** | **. . .** | **BLAS**

MUL | ADD | MOV

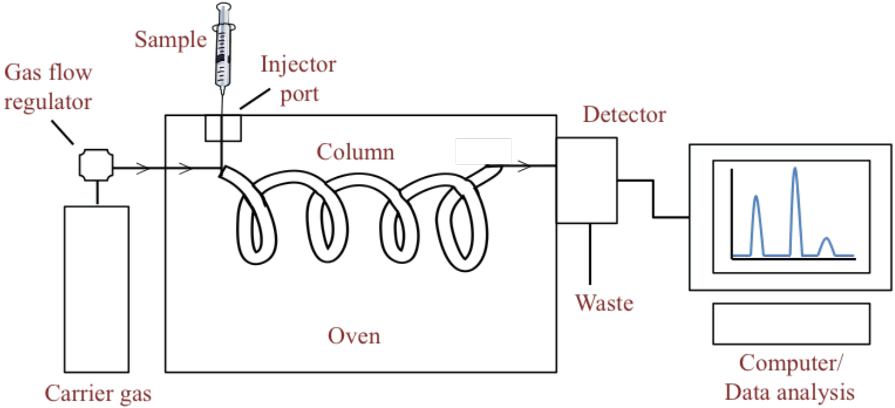
MOVAPD

VFMADDPD . . .

Example application: Untargeted chemical profiling

Chromatography with mass spectrometry detection

- Problem: Identify components in a sample



Jessica Torres – Bitesize Bio

Example application: Untargeted chemical profiling

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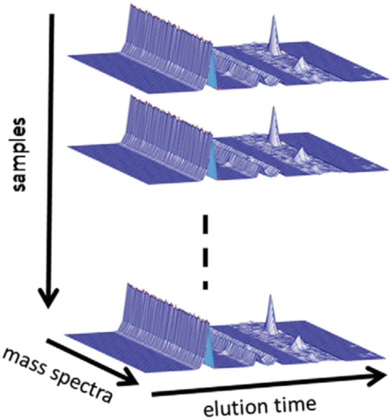
- 3-way data: Mass-spectrum $\times$ elution time $\times$ sample



Rasmus Bro

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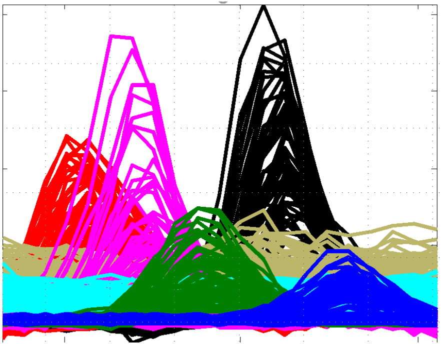
- 3-way tensor $\rightarrow$ Individual components



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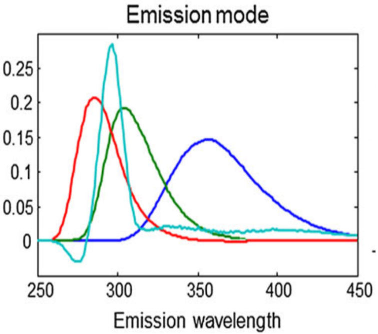
$\rightarrow$



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  PARAFAC — PARAFAC2 — TUCKER
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  - : Determine which of the components represent chemical information
  - : Start over;   add/change constraints, change model

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Thank you

Questions?