

PPAM 17

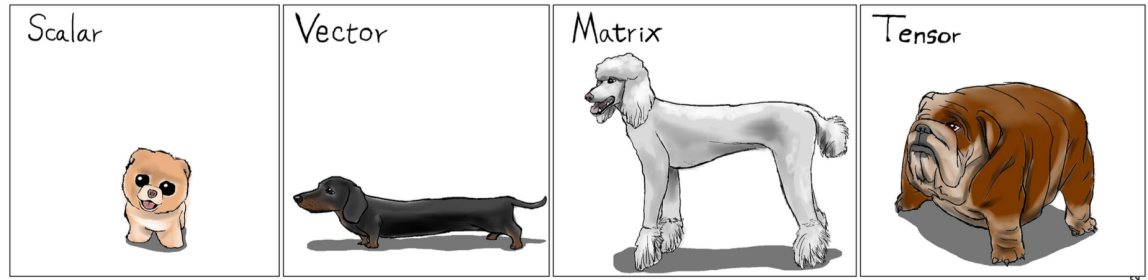
Tensor Contractions and Low-Communication FFT

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TENSOR CONTRACTIONS



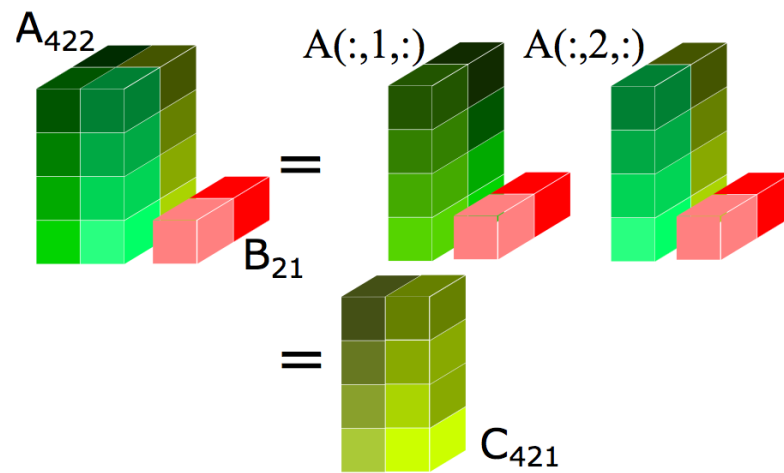
Modern data is inherently multi-dimensional.

NVIDIA especially interested due to ML.

Portability, BLAS spec, efficiency.

TENSOR CONTRACTIONS

$$C_C = A_A B_B$$



e.g. $C_{mnp} = A_{mnk} B_{kp}$

- Core primitive of multilinear algebra
- BLAS level 3 – unbounded compute intensity.

What do we have?

Tensor computation libraries

- ① Arbitrary/restricted tensor operation of any order and dimension
 - ① Tensortoolbox (Matlab)
 - ② FTensor (C++)
 - ③ Cyclops (C++)
 - ④ BTAS (C++)
 - ⑤ All the Python...

Efficient computing frame

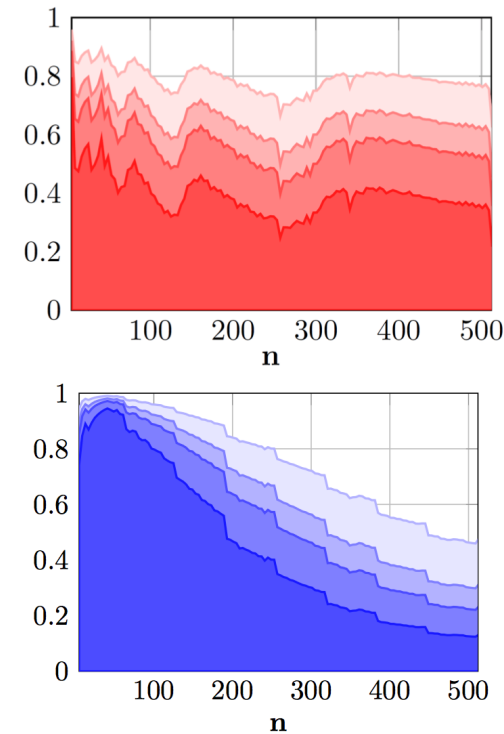
- ① Static analysis solutions
 - ① PPCG [ISL] (polyhedral)
 - ② TCE (DSL)
- ② Parallel and distributed primitives
 - ① BLAS, cuBLAS
 - ② BLIS, BLASX, cuBLASXT

TENSOR LIBRARIES

Explicit permutation dominates.

Consider $C_{mnp} = A_{km} B_{pkn}$.

- ① $A_{km} \rightarrow A_{mk}$
- ② $B_{pkn} \rightarrow B_{kpn}$
- ③ $C_{mnp} \rightarrow C_{mpn}$
- ④ $C_{m(pn)} = A_{mk} B_{k(pn)}$
- ⑤ $C_{mpn} \rightarrow C_{mnp}$



(Top) CPU. (Bottom) GPU. The fraction of time spent in copies/transpositions. Lines are shown with 1, 2, 3, and 6 transpositions.

EXISTING PRIMITIVES

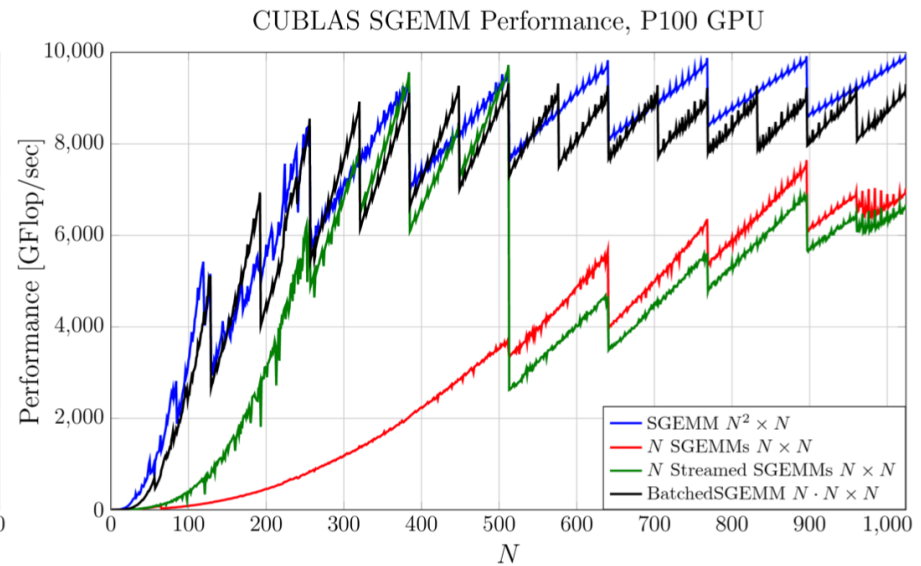
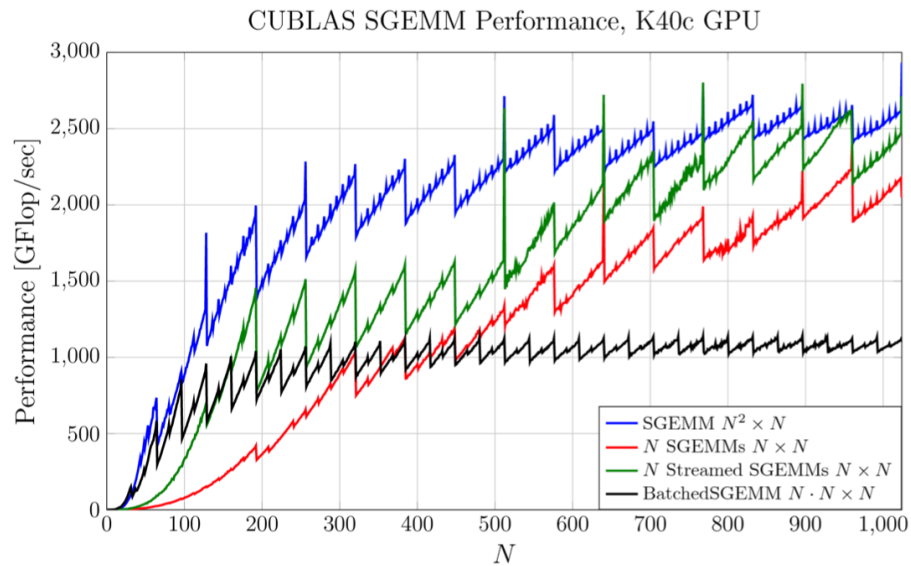
- GEMM
 - Suboptimal for many small matrices
- Pointer-to-pointer BatchedGEMM
 - Available since MKL 13.1b and cuBLAS 4.0

$$C[p] = \alpha \text{op}(A[p]) \text{op}(B[p]) + \beta C[p]$$

```
cublas<T>gemmBatched(cublasHandle_t handle,  
                     cublasOperation_t transA, cublasOperation_t transB,  
                     int M, int N, int K,  
                     const T* alpha,  
                     const T** A, int ldA,  
                     const T** B, int ldB,  
                     const T* beta,  
                     T** C, int ldC,  
                     int batchSize)
```

EXISTING PRIMITIVES

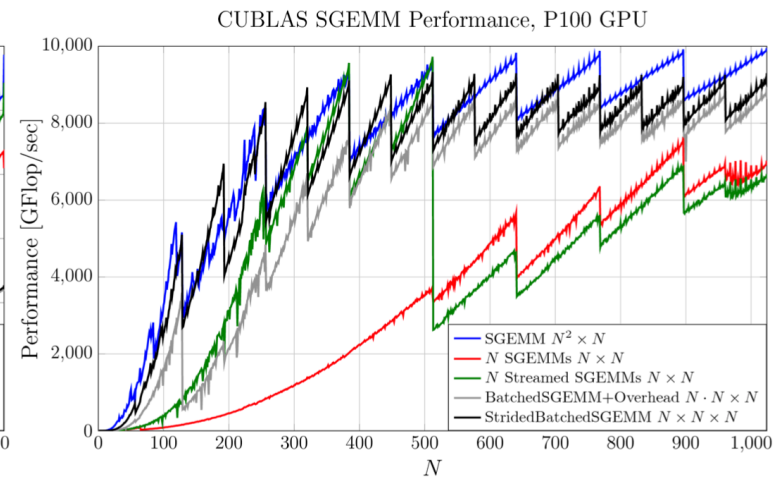
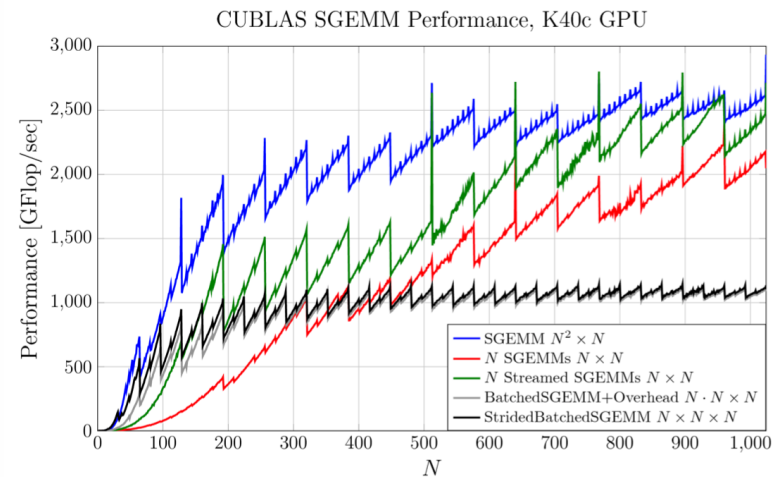
Pointer-to-Pointer BatchedGEMM



EXISTING PRIMITIVES

Pointer-to-Pointer BatchedGEMM

Except actually...



Solution: StridedBatchedGEMM

STRIDED BATCHED GEMM

```
cublas<T>gemmStridedBatched(cublasHandle_t handle,  
                             cublasOperation_t transA, cublasOperation_t transB,  
                             int M, int N, int K,  
                             const T* alpha,  
                             const T* A, int ldA1, int strideA,  
                             const T* B, int ldB1, int strideB,  
                             const T* beta,  
                             T* C, int ldC1, int strideC,  
                             int batchSize)
```

- Common use case for pointer-to-pointer batched GEMM
- No pointer-to-pointer data structure or overhead
- Performance on par with pure GEMM (P100 and beyond)

CONTRACTIONS

$$C_{mnp} = A_{**} \times B_{***}$$

$$C_{mnp} \equiv C[m + n \cdot \text{ldC1} + p \cdot \text{ldC2}]$$

Case	Contraction	Kernel1	Kernel2	Case	Contraction	Kernel1	Kernel2
1.1	$A_{mk}B_{knp}$	$C_{m(np)} = A_{mk}B_{k(np)}$	$C_{mn[p]} = A_{mk}B_{kn[p]}$	4.1	$A_{kn}B_{kmp}$	$C_{mn[p]} = B_{km[p]}^\top A_{kn}$	
1.2	$A_{mk}B_{kpn}$	$C_{mn[p]} = A_{mk}B_{k[p]n}$	$C_{m[n]p} = A_{mk}B_{kp[n]}$	4.2	$A_{kn}B_{kpm}$	$C_{mn[p]} = B_{k[p]m}^\top A_{kn}$	
1.3	$A_{mk}B_{nkp}$	$C_{mn[p]} = A_{mk}B_{nk[p]}^\top$		4.3	$A_{kn}B_{mkp}$	$C_{mn[p]} = B_{mk[p]} A_{kn}$	
1.4	$A_{mk}B_{pkn}$	$C_{m[n]p} = A_{mk}B_{pk[n]}^\top$		4.4	$A_{kn}B_{pkm}$		
1.5	$A_{mk}B_{npk}$	$C_{m(np)} = A_{mk}B_{(np)k}^\top$	$C_{mn[p]} = A_{mk}B_{n[p]k}^\top$	4.5	$A_{kn}B_{mpk}$	$C_{mn[p]} = B_{m[p]k} A_{kn}$	
1.6	$A_{mk}B_{pnk}$	$C_{m[n]p} = A_{mk}B_{p[n]k}^\top$		4.6	$A_{kn}B_{pmk}$		
2.1	$A_{km}B_{knp}$	$C_{m(np)} = A_{km}^\top B_{k(np)}$	$C_{mn[p]} = A_{km}^\top B_{kn[p]}$	5.1	$A_{pk}B_{kmn}$	$C_{(mn)p} = B_{k(mn)}^\top A_{pk}^\top$	$C_{m[n]p} = B_{km[n]}^\top A_{pk}^\top$
2.2	$A_{km}B_{kpn}$	$C_{mn[p]} = A_{km}^\top B_{k[p]n}$	$C_{m[n]p} = A_{km}^\top B_{kp[n]}$	5.2	$A_{pk}B_{knm}$	$C_{m[n]p} = B_{k[n]m}^\top A_{pk}^\top$	
2.3	$A_{km}B_{nkp}$	$C_{mn[p]} = A_{km}^\top B_{nk[p]}^\top$		5.3	$A_{pk}B_{mkn}$	$C_{m[n]p} = B_{mk[n]} A_{pk}^\top$	
2.4	$A_{km}B_{pkn}$	$C_{m[n]p} = A_{km}^\top B_{pk[n]}^\top$		5.4	$A_{pk}B_{nkm}$		
2.5	$A_{km}B_{npk}$	$C_{m(np)} = A_{km}^\top B_{(np)k}^\top$	$C_{mn[p]} = A_{km}^\top B_{n[p]k}^\top$	5.5	$A_{pk}B_{mnk}$	$C_{(mn)p} = B_{(mn)k} A_{pk}^\top$	$C_{m[n]p} = B_{m[n]k} A_{pk}^\top$
2.6	$A_{km}B_{pnk}$	$C_{m[n]p} = A_{km}^\top B_{p[n]k}^\top$		5.6	$A_{pk}B_{nmk}$		
3.1	$A_{nk}B_{kmp}$	$C_{mn[p]} = B_{km[p]}^\top A_{nk}^\top$		6.1	$A_{kp}B_{kmn}$	$C_{(mn)p} = B_{k(mn)}^\top A_{kp}$	$C_{m[n]p} = B_{km[n]}^\top A_{kp}$
3.2	$A_{nk}B_{kpm}$	$C_{mn[p]} = B_{k[p]m}^\top A_{nk}^\top$		6.2	$A_{kp}B_{knm}$	$C_{m[n]p} = B_{k[n]m}^\top A_{kp}$	
3.3	$A_{nk}B_{mkp}$	$C_{mn[p]} = B_{mk[p]} A_{nk}^\top$		6.3	$A_{kp}B_{mkn}$	$C_{m[n]p} = B_{mk[n]} A_{kp}$	
3.4	$A_{nk}B_{pkm}$			6.4	$A_{kp}B_{nkm}$		
3.5	$A_{nk}B_{mpk}$	$C_{mn[p]} = B_{m[p]k} A_{nk}^\top$		6.5	$A_{kp}B_{mnk}$	$C_{(mn)p} = B_{(mn)k} A_{kp}$	$C_{m[n]p} = B_{m[n]k} A_{kp}$
3.6	$A_{nk}B_{pmk}$			6.6	$A_{kp}B_{nmk}$		

 : Single GEMM
(Provided compact layout)

CONTRACTIONS

$$C_{mnp} = A_{**} \times B_{***}$$

$$C_{mnp} \equiv C[m + n \cdot \text{ldC1} + p \cdot \text{ldC2}]$$

 : Single SB-GEMM
(Any layout)

Case	Contraction	Kernel1	Kernel2	Case	Contraction	Kernel1	Kernel2
1.1	$A_{mk}B_{knp}$	$C_{m(np)} = A_{mk}B_{k(np)}$	$C_{mn[p]} = A_{mk}B_{kn[p]}$	4.1	$A_{kn}B_{kmp}$	$C_{mn[p]} = B_{km[p]}^T A_{kn}$	
1.2	$A_{mk}B_{kpn}$	$C_{mn[p]} = A_{mk}B_{k[p]n}$	$C_{m[n]p} = A_{mk}B_{kp[n]}$	4.2	$A_{kn}B_{kpm}$	$C_{mn[p]} = B_{k[p]m}^T A_{kn}$	
1.3	$A_{mk}B_{nkp}$	$C_{mn[p]} = A_{mk}B_{nk[p]}^T$		4.3	$A_{kn}B_{mkp}$	$C_{mn[p]} = B_{mk[p]} A_{kn}$	
1.4	$A_{mk}B_{pkn}$	$C_{m[n]p} = A_{mk}B_{pk[n]}^T$		4.4	$A_{kn}B_{pkm}$		
1.5	$A_{mk}B_{npk}$	$C_{m(np)} = A_{mk}B_{(np)k}^T$	$C_{mn[p]} = A_{mk}B_{n[p]k}^T$	4.5	$A_{kn}B_{mpk}$	$C_{mn[p]} = B_{m[p]k} A_{kn}$	
1.6	$A_{mk}B_{pnk}$	$C_{m[n]p} = A_{mk}B_{p[n]k}^T$		4.6	$A_{kn}B_{pmk}$		
2.1	$A_{km}B_{knp}$	$C_{m(np)} = A_{km}^T B_{k(np)}$	$C_{mn[p]} = A_{km}^T B_{kn[p]}$	5.1	$A_{pk}B_{kmn}$	$C_{(mn)p} = B_{k(mn)}^T A_{pk}^T$	$C_{m[n]p} = B_{km[n]}^T A_{pk}^T$
2.2	$A_{km}B_{kpn}$	$C_{mn[p]} = A_{km}^T B_{k[p]n}$	$C_{m[n]p} = A_{km}^T B_{kp[n]}$	5.2	$A_{pk}B_{knm}$	$C_{m[n]p} = B_{k[n]m}^T A_{pk}^T$	
2.3	$A_{km}B_{nkp}$	$C_{mn[p]} = A_{km}^T B_{nk[p]}^T$		5.3	$A_{pk}B_{mkn}$	$C_{m[n]p} = B_{mk[n]} A_{pk}^T$	
2.4	$A_{km}B_{pkn}$	$C_{m[n]p} = A_{km}^T B_{pk[n]}^T$		5.4	$A_{pk}B_{nkm}$		
2.5	$A_{km}B_{npk}$	$C_{m(np)} = A_{km}^T B_{(np)k}^T$	$C_{mn[p]} = A_{km}^T B_{n[p]k}^T$	5.5	$A_{pk}B_{mnk}$	$C_{(mn)p} = B_{(mn)k} A_{pk}^T$	$C_{m[n]p} = B_{m[n]k} A_{pk}^T$
2.6	$A_{km}B_{pnk}$	$C_{m[n]p} = A_{km}^T B_{p[n]k}^T$		5.6	$A_{pk}B_{nmk}$		
3.1	$A_{nk}B_{kmp}$	$C_{mn[p]} = B_{km[p]}^T A_{nk}^T$		6.1	$A_{kp}B_{kmn}$	$C_{(mn)p} = B_{k(mn)}^T A_{kp}$	$C_{m[n]p} = B_{km[n]}^T A_{kp}$
3.2	$A_{nk}B_{kpm}$	$C_{mn[p]} = B_{k[p]m}^T A_{nk}^T$		6.2	$A_{kp}B_{knm}$	$C_{m[n]p} = B_{k[n]m}^T A_{kp}$	
3.3	$A_{nk}B_{mkp}$	$C_{mn[p]} = B_{mk[p]} A_{nk}^T$		6.3	$A_{kp}B_{mkn}$	$C_{m[n]p} = B_{mk[n]} A_{kp}$	
3.4	$A_{nk}B_{pkm}$			6.4	$A_{kp}B_{nkm}$		
3.5	$A_{nk}B_{mpk}$	$C_{mn[p]} = B_{m[p]k} A_{nk}^T$		6.5	$A_{kp}B_{mnk}$	$C_{(mn)p} = B_{(mn)k} A_{kp}$	$C_{m[n]p} = B_{m[n]k} A_{kp}$
3.6	$A_{nk}B_{pmk}$			6.6	$A_{kp}B_{nmk}$		

FAST FOURIER TRANSFORM

$$[\mathbf{F}_N]_{ij} = e^{-2\pi i j / N}$$

Ubiquitous primitive in computational sciences

Arguably one of the oldest and most well-studied

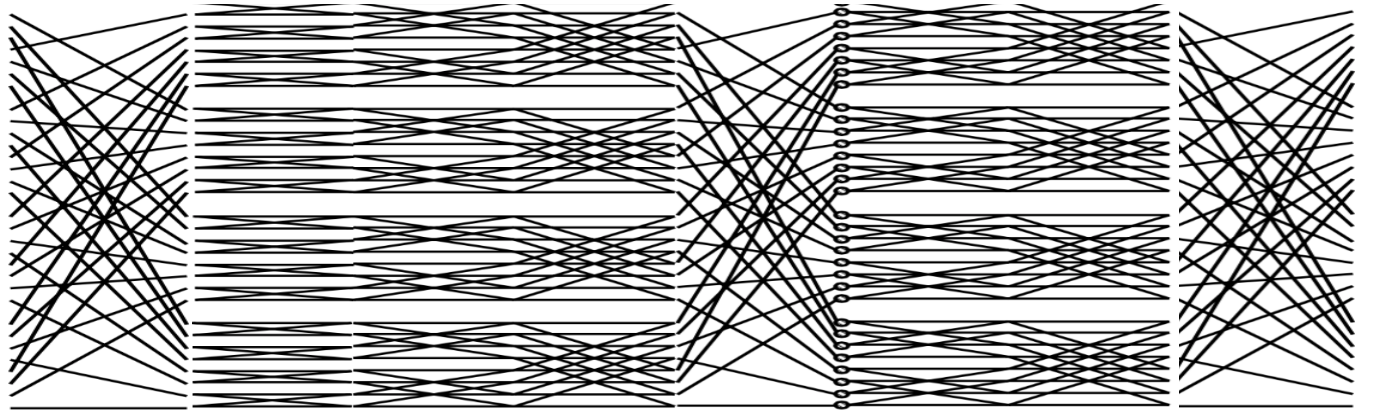
Performance on modern architectures...

SPLIT-RADIX FFT

Algorithm

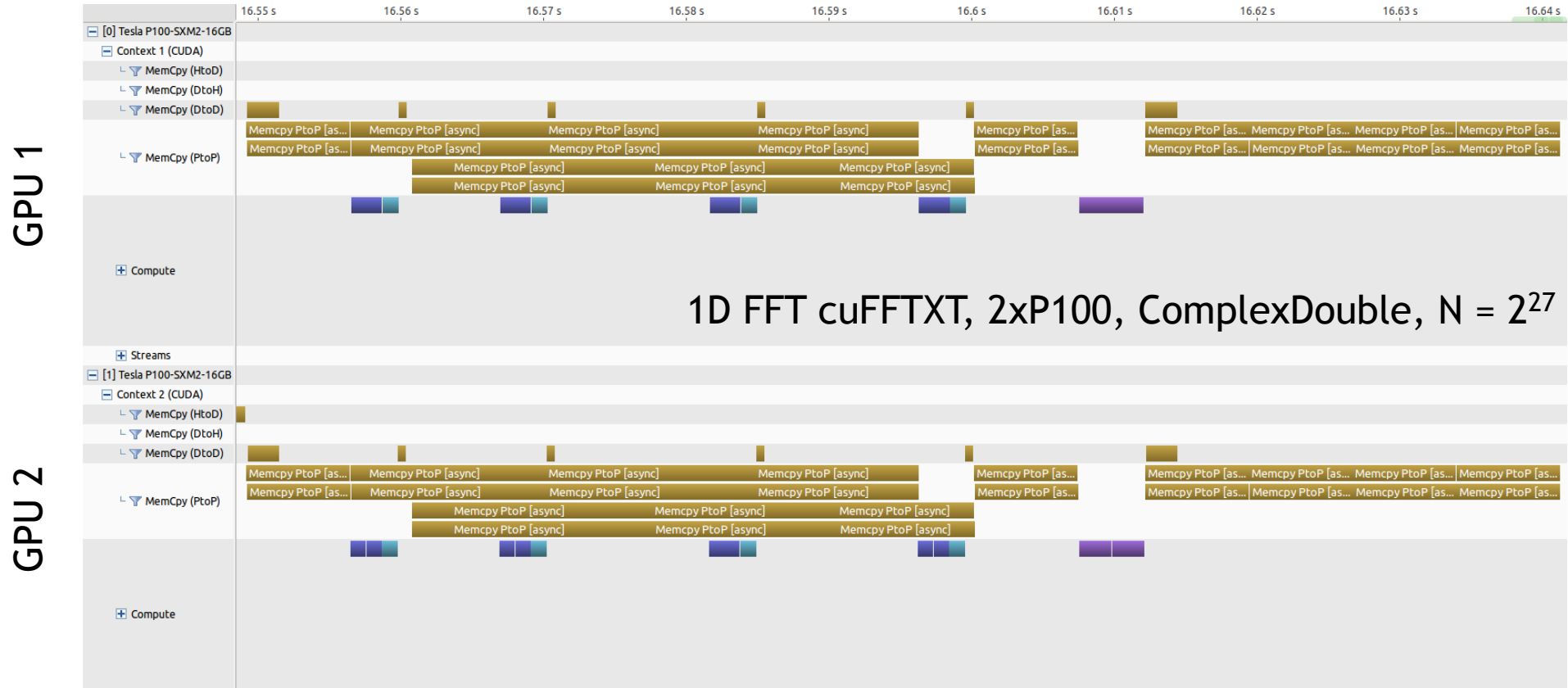
$$\mathbf{F}_N = \mathbf{\Pi}_{M,P} (\mathbf{I}_M \otimes \mathbf{F}_P) \mathbf{\Pi}_{P,M} \mathbf{T}_{M,P} (\mathbf{I}_P \otimes \mathbf{F}_M) \mathbf{\Pi}_{M,P}$$

1. Transpose $P \rightarrow M$.
2. P local FFTs of size M .
3. Twiddle factors $\mathbf{T}$.
4. Transpose $M \rightarrow P$.
5. M local FFTs of size P .
6. Transpose $P \rightarrow M$.



SPLIT-RADIX FFT

Profile

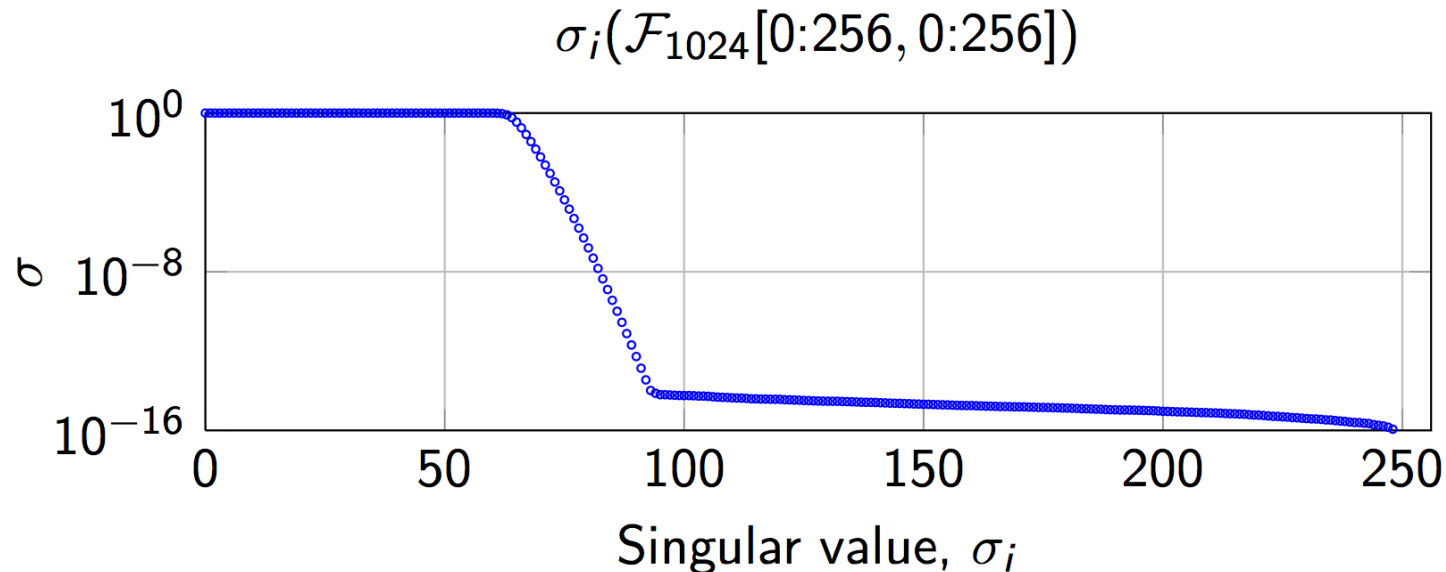


FMM-FFT

Edelman et al. 1999

$$F_N = \begin{pmatrix} F_{N|P} & \cdots & D^{P-1}F_{N|P} \\ F_{N|P}D & \cdots & D^{P-1}F_{N|P}D \\ \vdots & & \vdots \\ F_{N|P}D^{P-1} & \cdots & D^{P-1}F_{N|P}D^{P-1} \end{pmatrix}$$

Low-rank structure



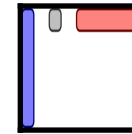
STRUCTURED DENSE MATRICES AND FMM

- SVD:

$$A = U D V^*$$

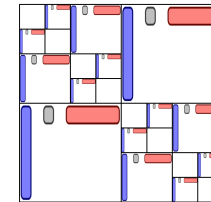
- Low-Rank:

$$K = U \tilde{K}_{r \times r} V^*$$

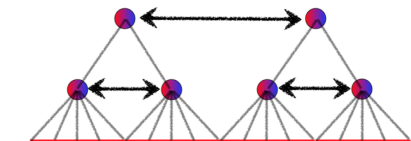
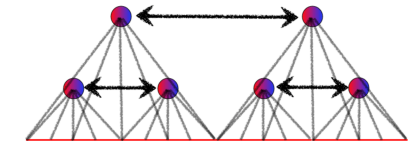
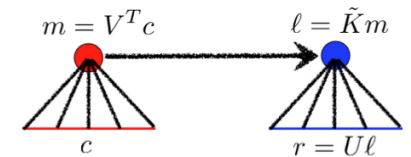


- Hierarchically LR:

$$K_{\mathcal{IJ}} = U_{\mathcal{I}} \tilde{K}_{\mathcal{IJ}} V_{\mathcal{J}}^*$$



- H-Semi-Separable: $K_{\mathcal{IJ}} = U_{\mathcal{I}} \tilde{U}_{\tilde{\mathcal{I}}} \tilde{K}_{\tilde{\mathcal{I}}\tilde{\mathcal{J}}} \tilde{V}_{\tilde{\mathcal{J}}}^* V_{\mathcal{J}}^*$



- H²-Matrix/FMM

FMM-FFT

Edelman et al. 1999 Algorithm

$$\mathbf{F}_N = (\mathbf{I}_P \otimes \mathbf{F}_M) \mathbf{\Pi}_{M,P} (\mathbf{I}_M \otimes \mathbf{F}_P) \mathbf{M}_{M,P}$$

$$\mathbf{M}_{M,P} = \mathbf{\Pi}_{P,M} \text{diag}(\mathbf{I}_M, \mathbf{C}_1, \mathbf{C}_2, \dots, \mathbf{C}_p) \mathbf{\Pi}_{M,P}$$

Block diagonal matrix with P blocks of M x M.

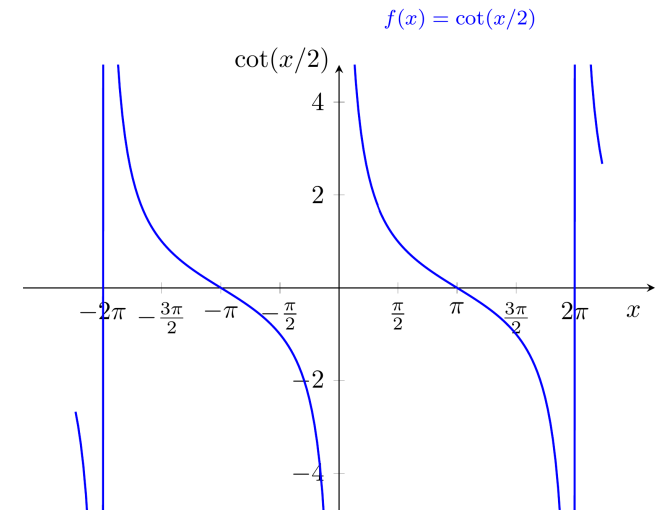
Direct application would destroy asymptotic complexity of the FFT and not effect communication.

However, each C is a *dense kernel matrix*.

COTANGENT FMM

$$[\mathbf{C}_p]_{mn} = \rho_p \left[\cot \left(\frac{\pi}{M} \left(n - m + \frac{p}{P} \right) \right) + \imath \right]$$

- One dimensional
- Uniform — source/target are the integers
- Periodic
- Distributed
- Size M-by-M
- P of them!
 - Interleaved



FMM-FFT

Edelman et al. 1999 Algorithm

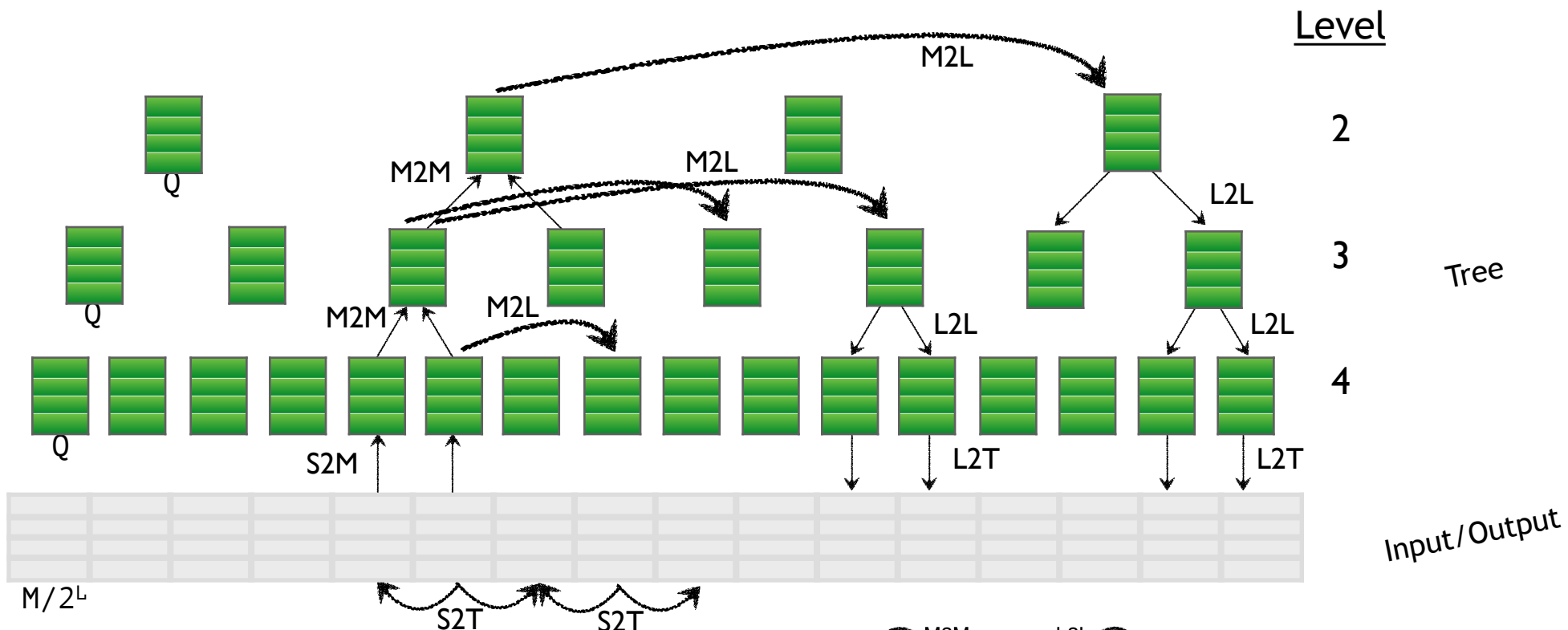
$$\mathbf{F}_N = (\mathbf{I}_P \otimes \mathbf{F}_M) \mathbf{\Pi}_{M,P} (\mathbf{I}_M \otimes \mathbf{F}_P) \mathbf{M}_{M,P}$$

$$\mathbf{M}_{M,P} = \mathbf{\Pi}_{P,M} \text{diag}(\mathbf{I}_M, \mathbf{C}_1, \mathbf{C}_2, \dots, \mathbf{C}_p) \mathbf{\Pi}_{M,P}$$

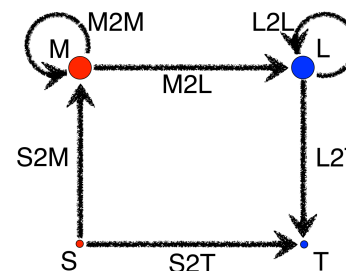
1. Compute $P - 1$ distributed FMMs of size $M \times M$.
 2. M local FFTs of size P .
 3. Transpose $P \rightarrow M$.
 4. P local FFTs of size M .
- } 2D $M \times P$ FFT

FMM OPERATORS

- S: "Source"
- T: "Target"
- M: "Multipole"
- L: "Local"



Each operator is an (implicit) matrix.



PARAMETERS OF THE FMM-FFT

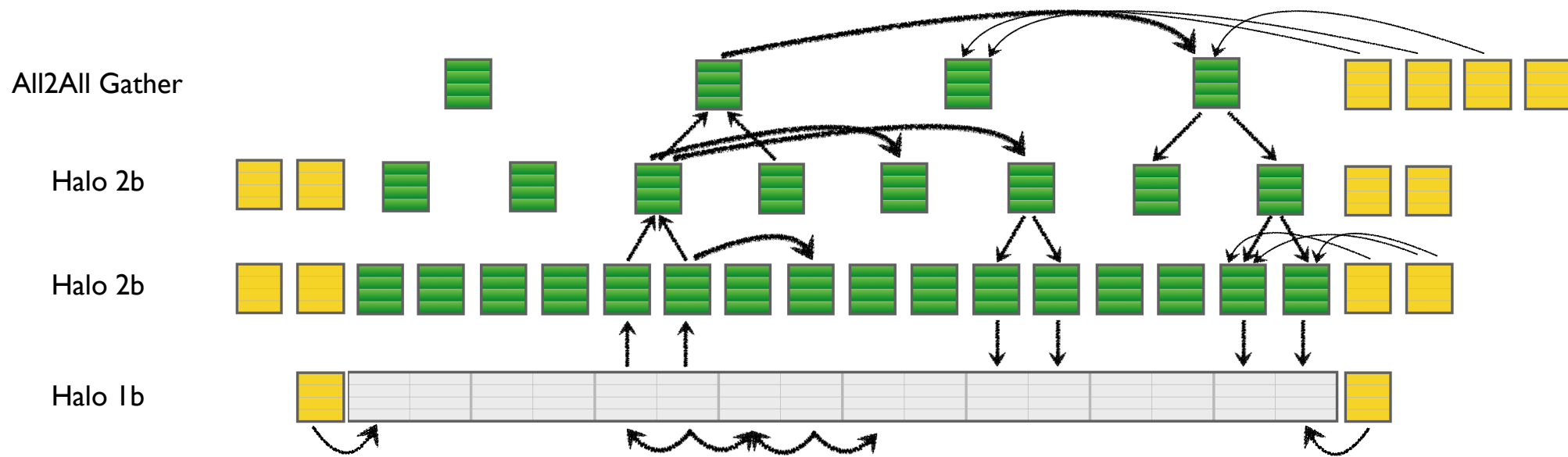
- FFT $N = M P$

P FMMs to perform of size $M \times M$

- FMM

- Rank Q
- Leaf box size M_L
- Base level B
- Leaf level $L = \log_2(M/M_L)$

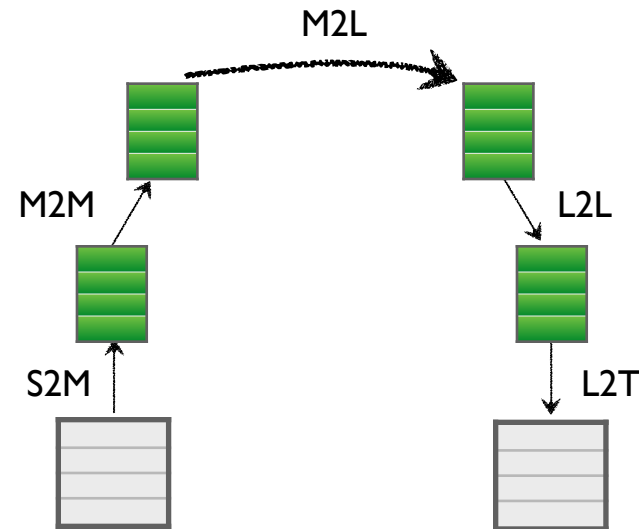
DISTRIBUTED FMM



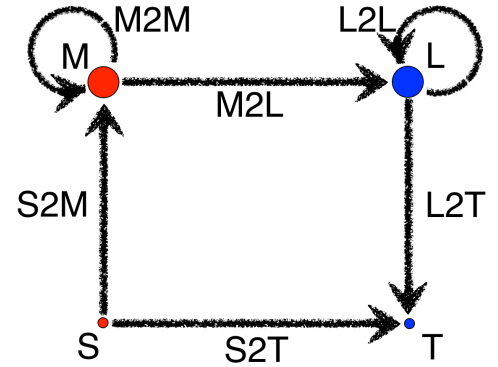
INTERPOLATIVE FMM

Chebyshev interpolations

- Use Chebyshev interpolations as the intermediate data
 - Same operators across all boxes
 - Same operators across all levels
 - Almost same operators across all FMMs
- Express as tensors and efficiently compute.

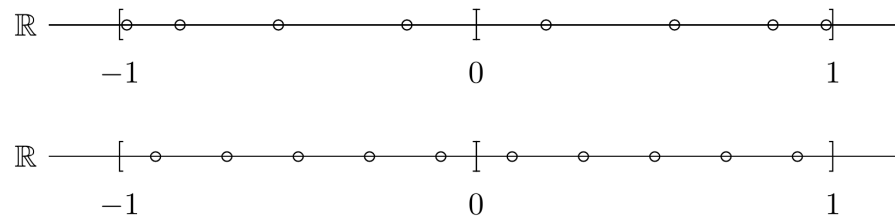


S2M/L2T



$$\mathcal{M}_{(p-1)qb}^L = S2M_{qm} \mathcal{S}_{pmb}$$

$$\mathcal{T}_{pmb} = L2T_{mq} \mathcal{L}_{(p-1)qb} + \mathcal{T}_{pmb}$$



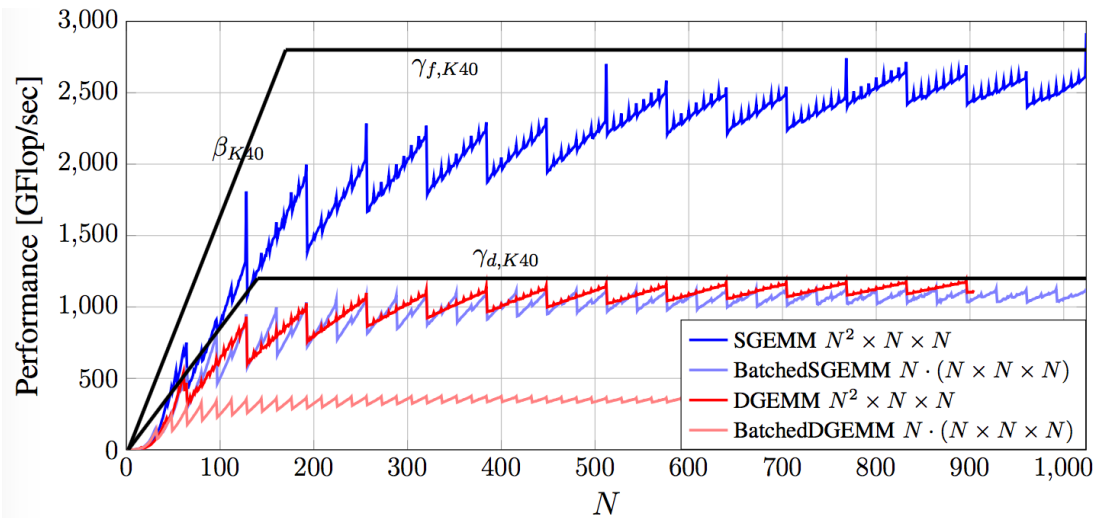
Tree Leaf (M)

Sources (S)

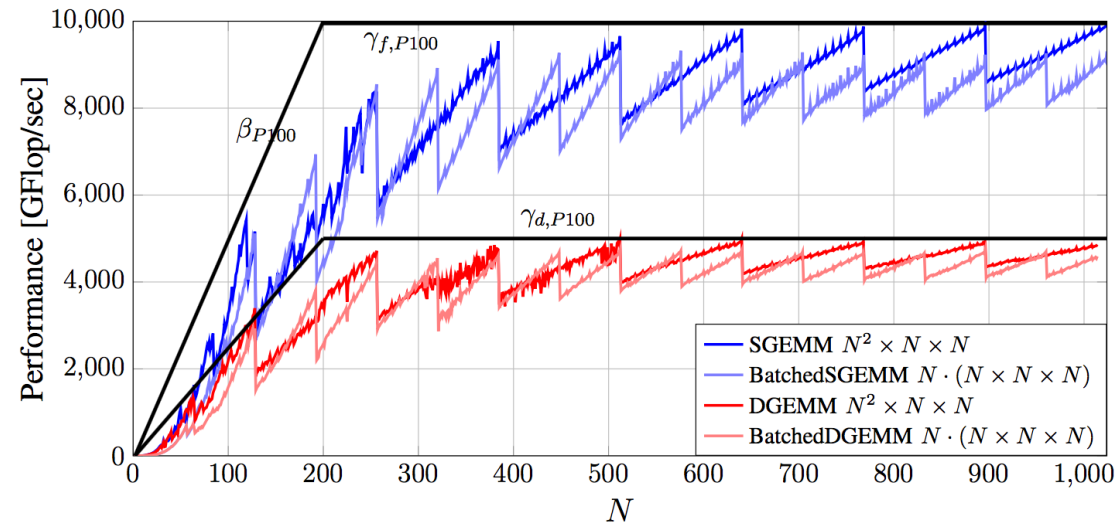
Computed with *single BatchedGEMM*

BATCHED MATRIX-MATRIX MULTIPLY

cublas<T>gemmStridedBatched
in cuBLAS 8.0

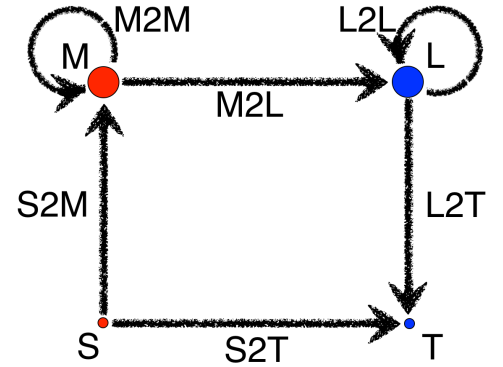


(a) K40c GPU



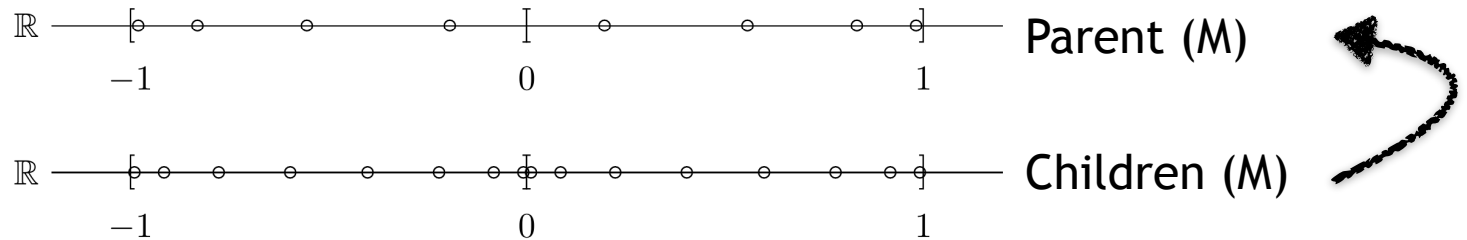
(b) P100 GPU

M2M/L2L



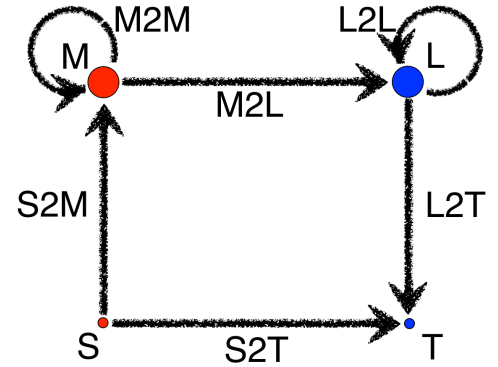
$$\mathcal{M}_{pqb}^{\ell} = M2M_{qk} \mathcal{M}_{pk(2b)}^{\ell+1}$$

$$\mathcal{L}_{pq(2b)}^{\ell+1} = L2L_{qk} \mathcal{L}_{pkb}^{\ell} + \mathcal{L}_{pq(2b)}^{\ell+1}$$



Computed with *single BatchedGEMM*

S2T/M2L



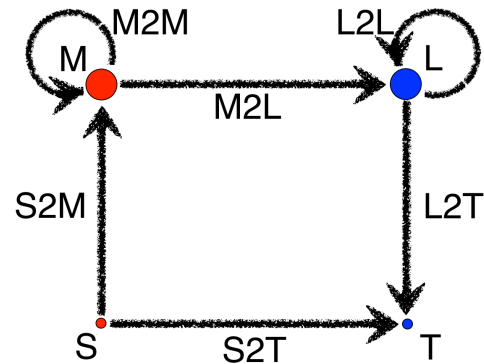
$$\mathcal{T}_{pib} = S2T_{p(j-i)} \mathcal{S}_{pjb}$$

$$S2T_{pk} = \begin{cases} \cot\left(\frac{\pi}{N}(p + Pk)\right) & p > 0 \\ \delta_{k0} & p = 0 \end{cases}$$

$$\mathcal{L}_{pib}^\ell = M2L_{pijs}^\ell \mathcal{M}_{pj(b+s)}^\ell \quad M2L_{pijs}^\ell = \cot\left(\frac{\pi}{2^\ell}\left(\frac{z_j}{2} - \frac{z_i}{2} + s\right) + \frac{\pi}{N}(p+1)\right)$$

- Also Level-3 Linear Algebra computations, but no BLAS primitives.
 - CUSTOM KERNELS

INTERPOLATIVE FMM



Operator

$$S2T_{ij}^{(p)} = \cot \left(\frac{\pi}{M} (j - i) + \frac{\pi}{2L} s + \frac{\pi}{N} p \right)$$

$$S2M_{ij} = \ell_i(s_j) = \begin{cases} 1 & s_j = z_i \\ \frac{\lambda_i \ell(s_j)}{s_j - z_i} & \text{else} \end{cases}$$

$$M2M_{ij}^{\pm} = \ell_i \left(\frac{z_j \pm 1}{2} \right)$$

$$M2L_{ijs}^{(p)} = \cot \left(\frac{\pi}{2L} \left(\frac{z_j}{2} - \frac{z_i}{2} \right) + \frac{\pi}{2L} s + \frac{\pi}{N} p \right)$$

$$L2L_{ij}^{\pm} = \ell_j \left(\frac{z_i \pm 1}{2} \right) = M2M_{ji}^{\pm}$$

$$L2T_{ij} = \ell_j(t_i) = S2M_{ji}$$

Storage

$$P(4M_L - 1)$$

$$QM_L$$

$$2Q^2$$

$$4(L-B)PQ^2$$

$$2Q^2$$

$$QM_L$$

Compute

$$3P2^L M_L^2$$

$$2PMQ$$

$$4(2^L - 2^B)PQ^2$$

$$3(2^L - 2^B)PQ^2$$

$$4(2^L - 2^B)PQ^2$$

$$2PMQ$$

Compute on the fly!

Total Precomputation (S2M+M2M):
 $Q^2 M_L + Q^3 \sim 20k$ Flops

Total Overhead (S2M+M2M):
 $QM_L + Q^2 \sim 12k$ Bytes

ALGORITHM

Algorithm 1 The FMM-FFT via tensor contractions.

1: $\mathcal{M}_{(p-1)qb}^L = S2M_{qm} \mathcal{S}_{pmb}$	// S2M
2: SendRecv $\mathcal{S}$ halo.	// COMM $\mathcal{S}$
3: $\mathcal{T}_{pib} = S2T_{p(j-i)} \mathcal{S}_{pjb}$	// S2T
4: for $\ell = L - 1, \dots, B$ do	
5: $\mathcal{M}_{pqb}^\ell = M2M_{qk} \mathcal{M}_{pk(2b)}^{\ell+1}$	// M2M
6: for $\ell = L, \dots, B - 1$ do	
7: SendRecv $\mathcal{M}^\ell$ halo.	// COMM $\mathcal{M}^\ell$
8: $\mathcal{L}_{pib}^\ell = M2L_{pijs}^\ell \mathcal{M}_{pj(b+s)}^\ell$	// M2L ℓ
9: All-to-all gather $\mathcal{M}^B$.	// COMM $\mathcal{M}^B$
10: $\mathcal{L}_{pib}^B = M2L_{pijs}^B \mathcal{M}_{pj(b+s)}^B$	// M2L B
11: $r_p = 1_{qb} \mathcal{M}_{(p-1)qb}^B$	// REDUCE
12: for $\ell = B, \dots, L - 1$ do	
13: $\mathcal{L}_{pq(2b)}^{\ell+1} = L2L_{qk} \mathcal{L}_{pkb}^\ell + \mathcal{L}_{pq(2b)}^{\ell+1}$	// L2L
14: $\mathcal{T}_{pmb} = L2T_{mq} \mathcal{L}_{(p-1)qb}^L + \mathcal{T}_{pmb}$	// L2T
15: $\mathcal{T}_{pmb} = \rho_p(\mathcal{T}_{pmb} + \imath r_p)$	// POST
16: $\mathbf{F}_{M,P} \mathcal{T}$	// 2D FFT

 : Primitive — vendor optimized

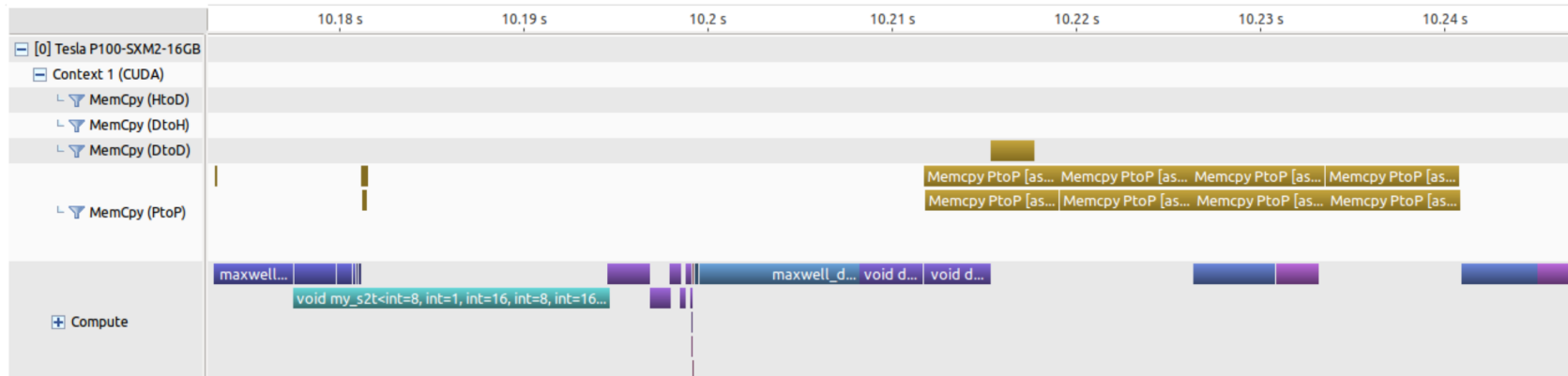
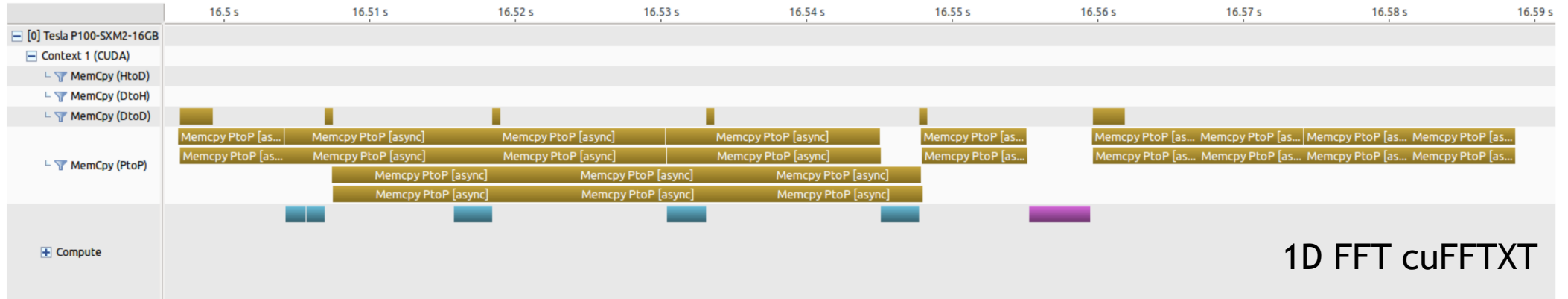
`cublas<T>gemmStridedBatched`

 : Custom kernel

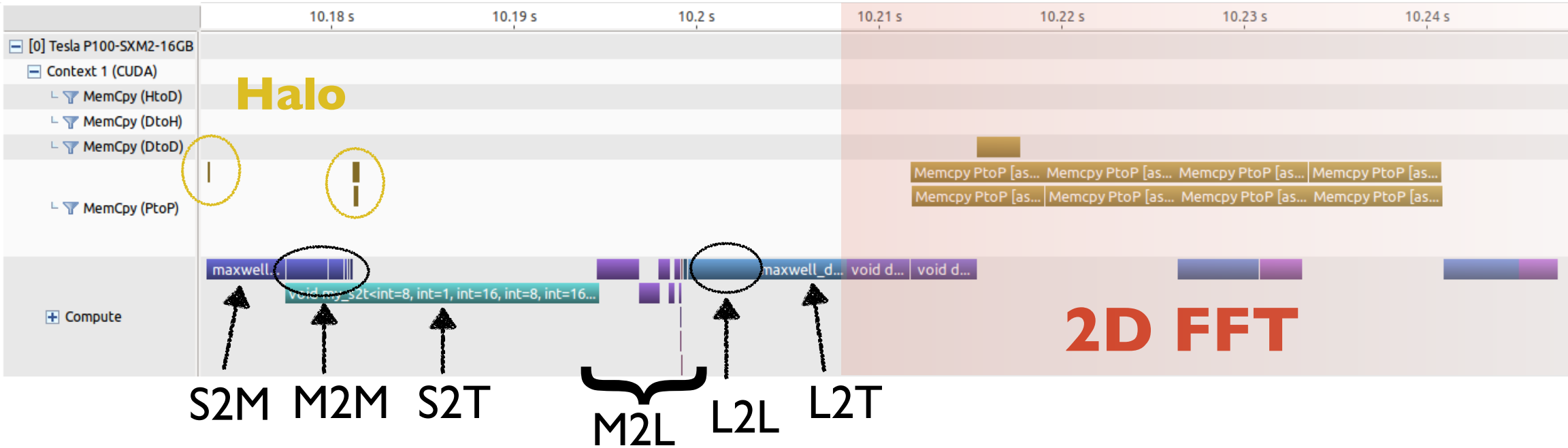
 : FMM Communication

COMPARISON

Profile



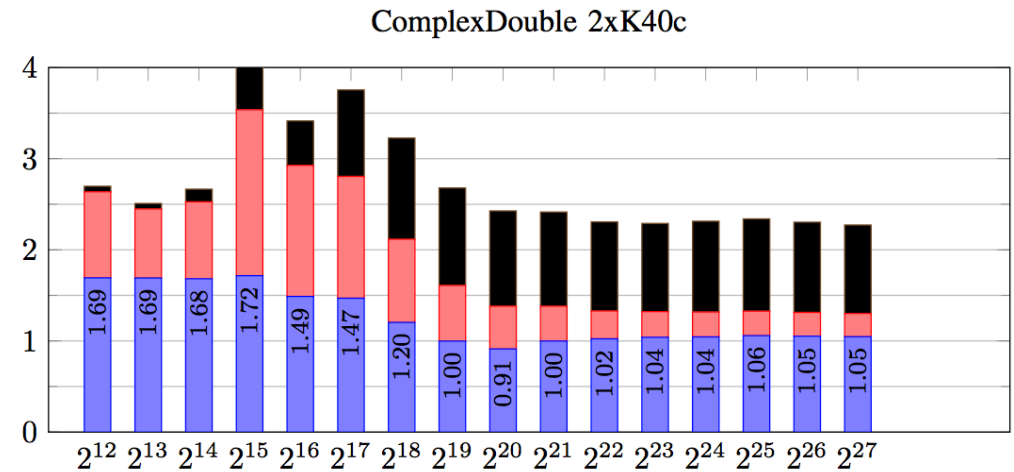
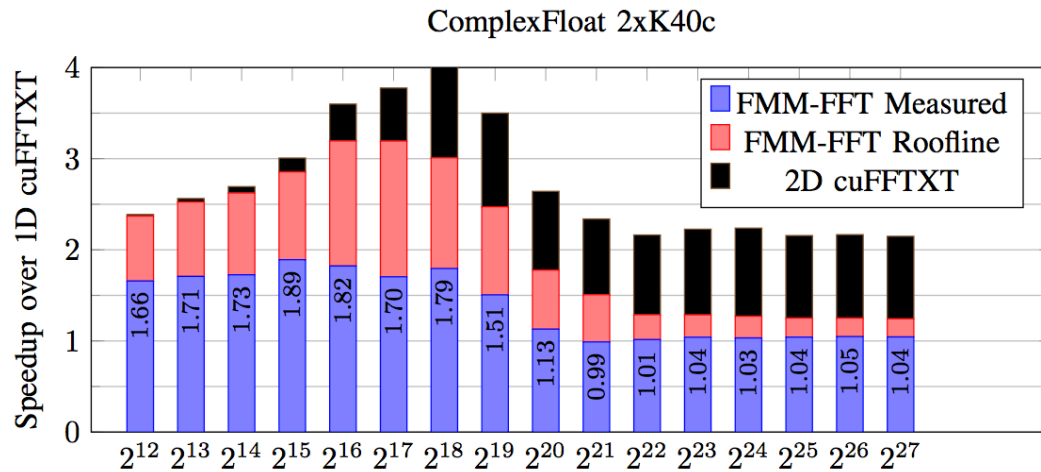
FMM-FFT PROFILE



Emph: 255 FMMs of size 524k x 524k in 32ms

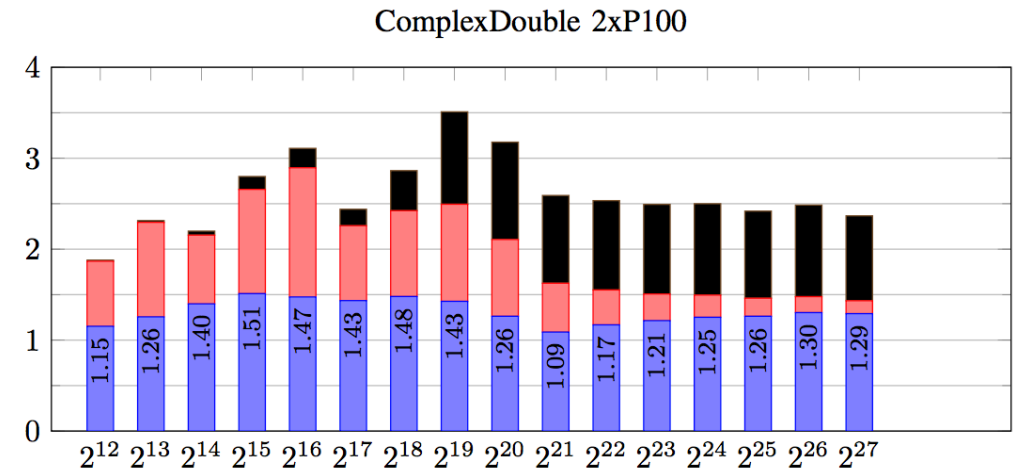
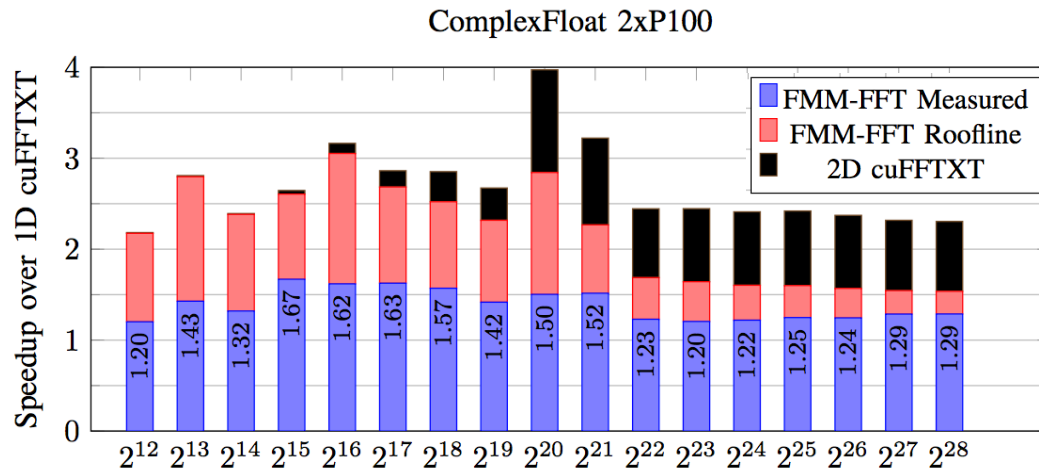
2xK40c, PCIe

FMM-FFT Performance



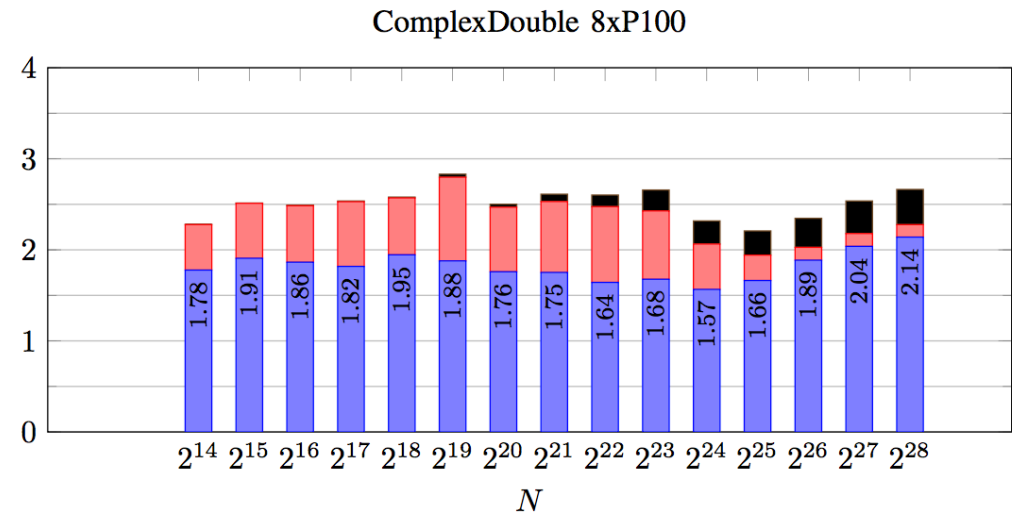
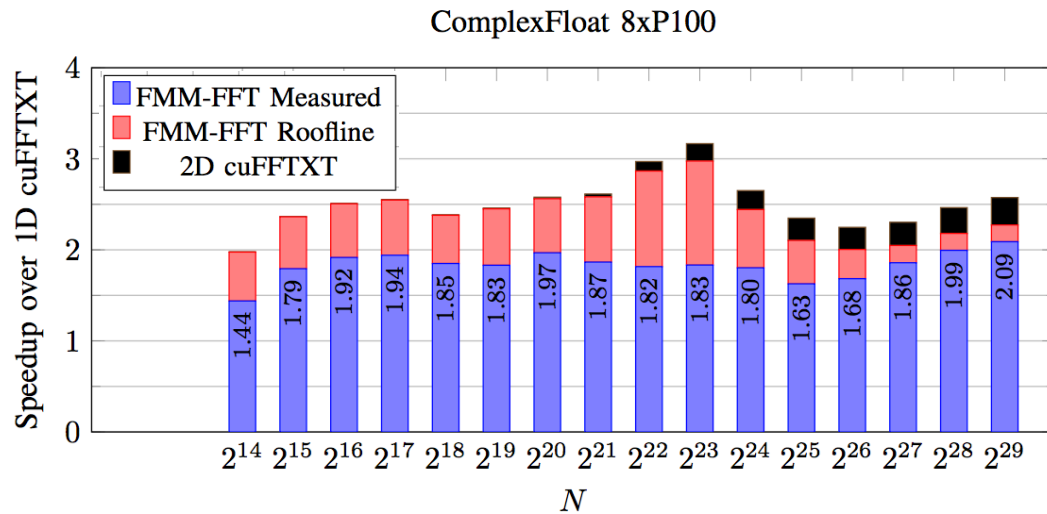
2xP100, NVLINK

FMM-FFT Performance

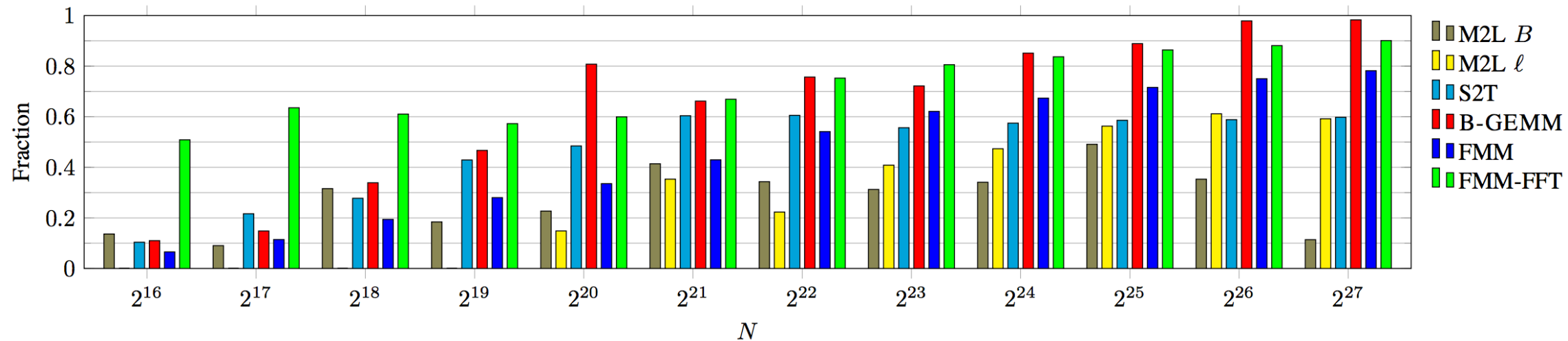


8xP100, NVLINK

FMM-FFT Performance



EFFICIENCY



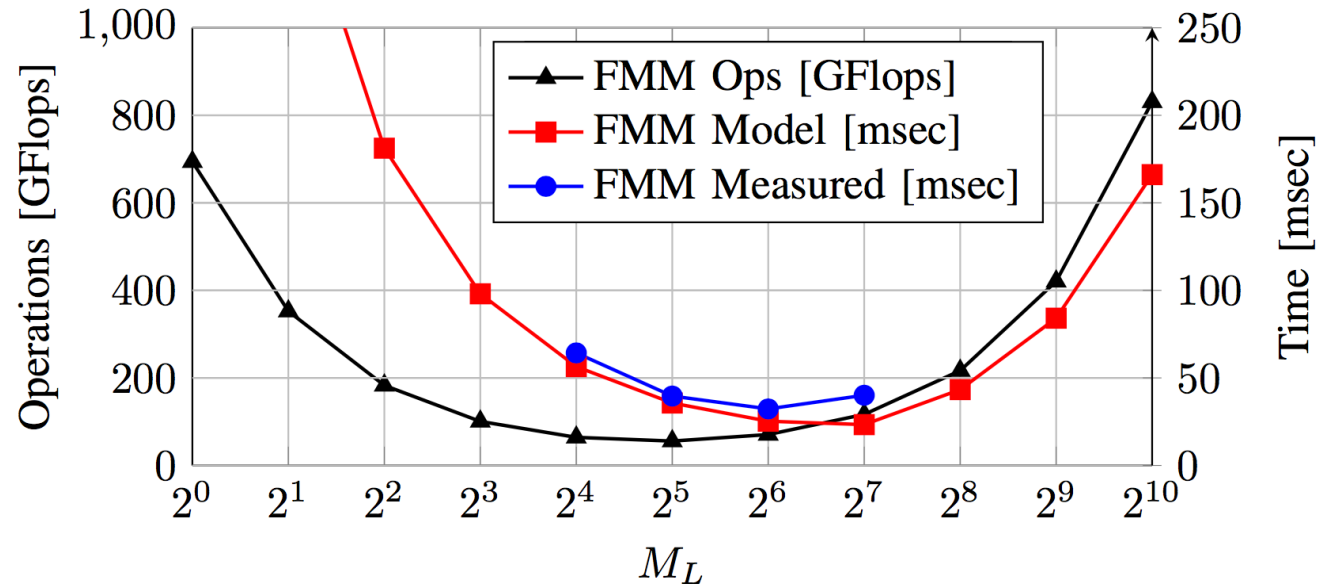
- >95% BatchedGEMM
- 60% S2T/M2L
- >90% FMM-FFT

PARAMETER DEPENDENCE — M_L

Points per leaf box per FMM

ComplexDouble, 2xP100, $N=2^{27}$, $P=256$, $B=3$, $Q=16$

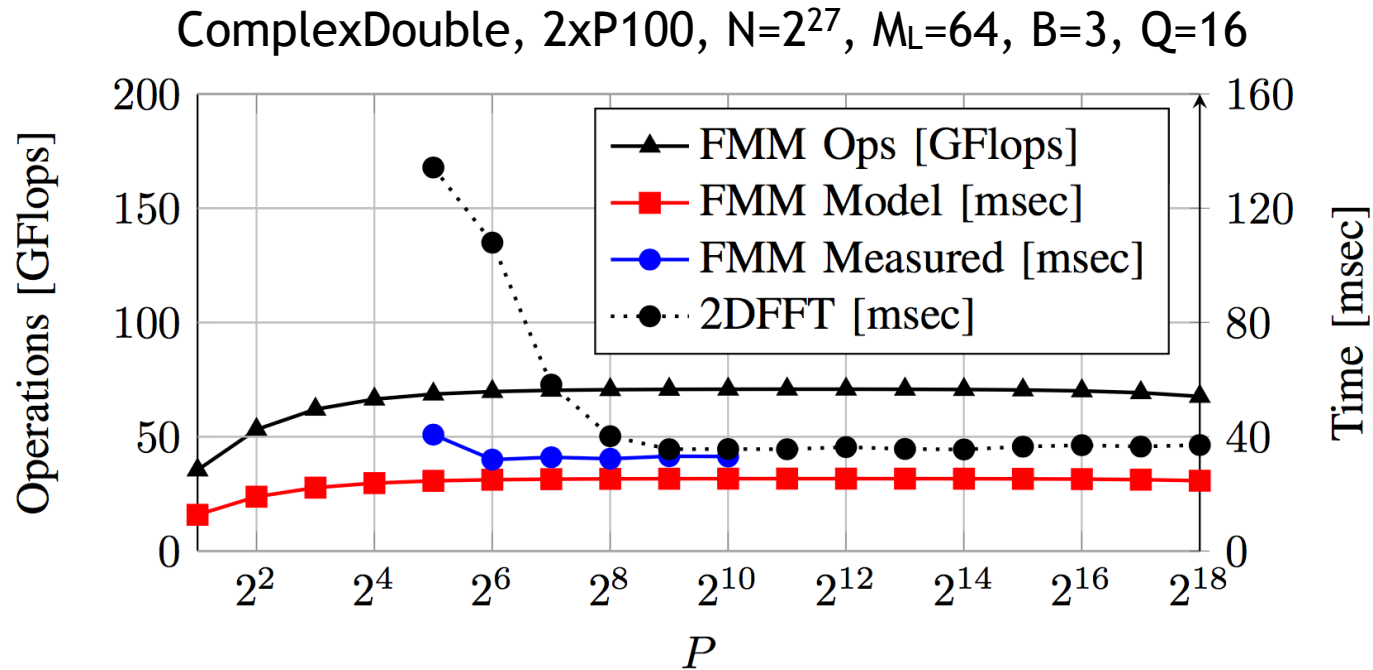
- Trade #levels for S2T comp
- Counting flops not enough
 - Want intensity increase
- Tune performance for $M_L=64$



PARAMETER DEPENDENCE — P

Number of FMMs

- Flops/Intensity approx constant
 - Trade #levels for #FMMs
- Large P good
 - Fill up B-GEMM
 - More square 2D FFT

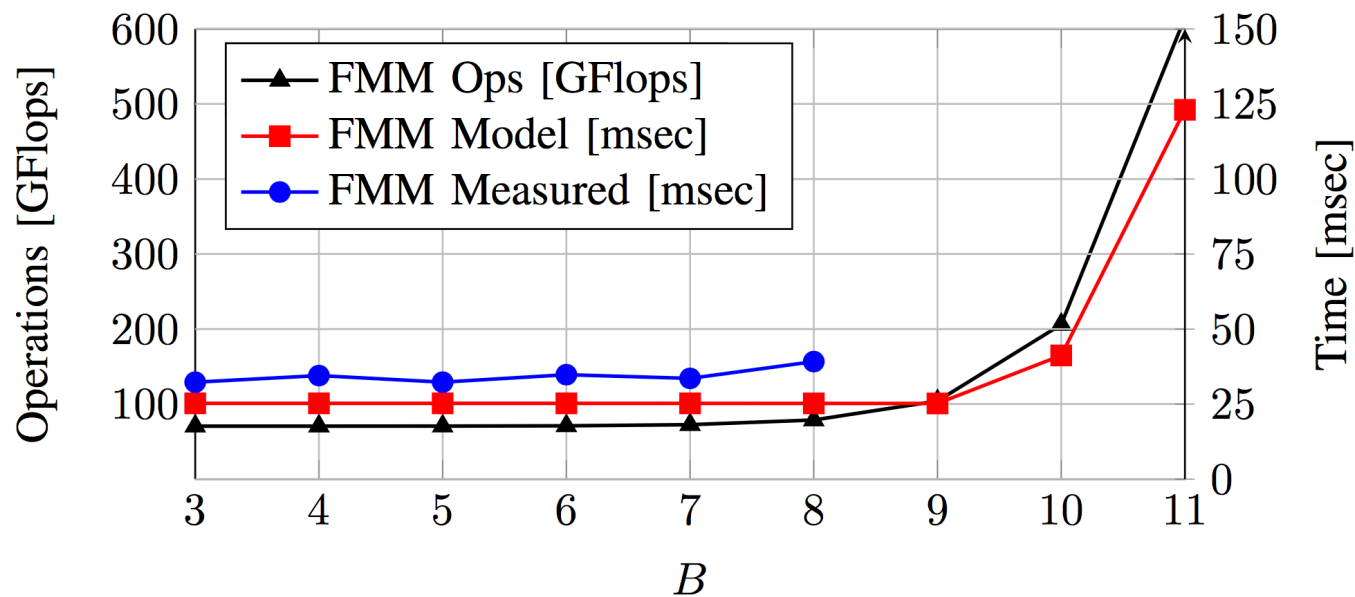


PARAMETER DEPENDENCE — B

Base level of FMM trees

ComplexDouble, 2xP100, $N=2^{27}$, $P=256$, $M_L=64$, $Q=16$

- Not very significant
- Scale to 128 GPUs w/o complications

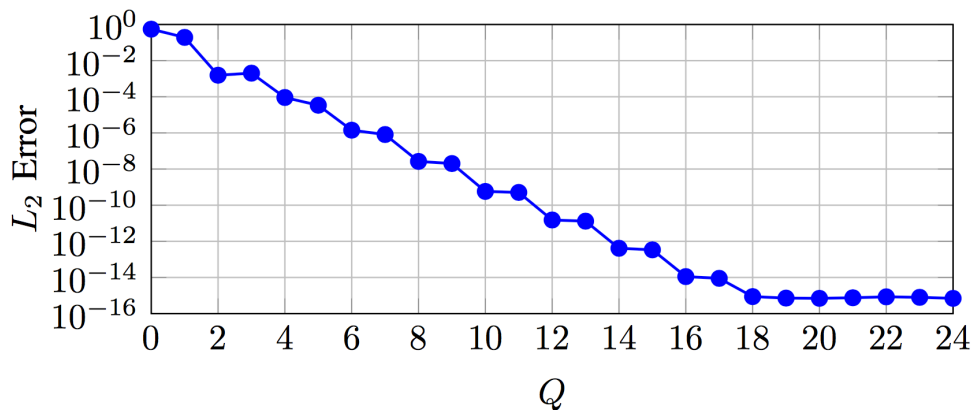
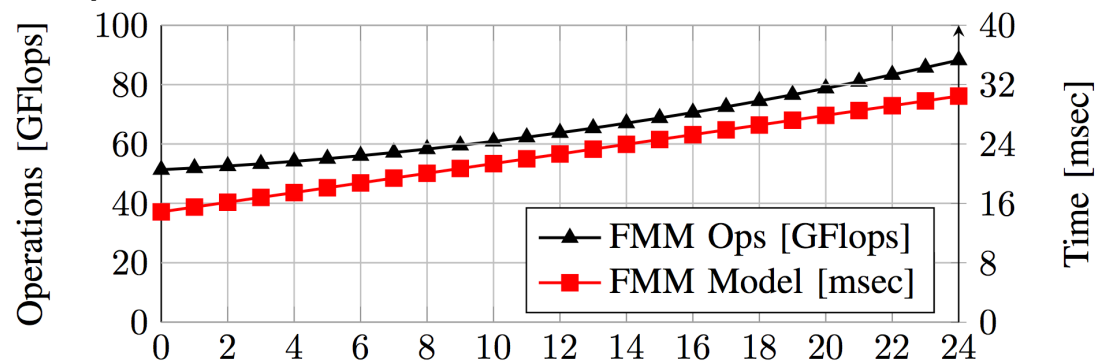


PARAMETER DEPENDENCE – Q

Quadrature order of FMM interpolation

- Accuracy tuning with performance dependence

ComplexDouble, 2xP100, $N=2^{27}$, $P=256$, $M_L=64$, $B=3$



FUTURE

- Integration into cuFFT
- Application to 2D/3D FFTs?
 - Convolutions
- NUFFT, Sparse FFT nearly out-of-the-box
- Volta predictions and measurements
 - Mixed precision (e.g. FP16 far-field) to use Tensor Core?
- Persistent Matrix Batched GEMM (cuBLAS optimization)
 - Staged Persistent Matrix Batched GEMM (cooperative groups, RNNs)

CONCLUSION

- FMM-FFT trades 2/3 communication in 1D FFT for P FMMs
 - Viable on highest comp:comm architecture available
- Detailed implementation that relies heavily on existing primitives
 - Primitives >95% efficient
 - Two custom dense kernels >60% efficient
 - Entire FMM-FFT >90% efficient
- Tunable accuracy-performance tradeoff
- Compute model accurately predicts performance

Cris Cecka, “Low-communication FMM-accelerated FFTs on GPUs” *International Conference for High Performance Computing, Networking, Storage, and Analysis (SC)*, Denver, CO, November 12-17, 2017

Yang Shi, U.N. Niranjan, Animashree Anandkumar, and **Cris Cecka**. “Tensor contractions with extended BLAS kernels on CPU and GPU” In *2016 IEEE 23rd International Conference on High Performance Computing (HiPC)*, pages 193–202, Dec 2016