## GPU TECHNOLOGY CONFERENCE

## **S7728 - MAGMA Tensors and Batched Computing for Accelerating Applications on GPUs**

**Stan Tomov** - Research Director, UTK **Azzam Haidar** - Research Scientist, UTK

**Abstract**: Learn how to accelerate your machine learning, data mining, and other algorithms through fast matrix and tensor operations on GPUs. There's an increasing demand for accelerated independent computations on tensors and many small matrices. Although common, these workloads cannot be efficiently executed using standard linear algebra libraries. To fill the gap, we developed the MAGMA Batched library that achieves dramatically better performance by repetitively executing the small operations in "batches." We'll describe a methodology on how to develop high-performance BLAS, SVD, factorizations, and solvers for both large- and small-batched matrices. We'll also present the current state-of-the-art implementations and community efforts to standardize an API that extends BLAS for Batched computations.





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# MAGMA Tensors and Batched Computing for Accelerating Applications on GPUs

#### Stan Tomov and Azzam Haidar

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#### In collaboration with:

LLNL, Livermore, CA, USA University of Manchester, Manchester, UK University of Paris-Sud, France

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#### **Outline**

- Introduction
- MAGMA library
  - Numerical Linear Algebra (NLA) for large problems
  - NLA for applications that need small problems
- MAGMA Tensor contraction computations
- MAGMA Batched Computing
- MAGMA-DNN NLA backend for DNN
- Algorithms and optimization techniques
- Conclusions





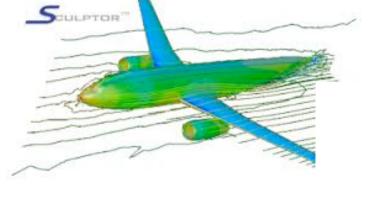


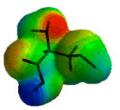


# Wide range of Applications depend on Numerical Linear Algebra (NLA) Libraries

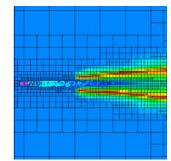
- Airplane wing design,
- Quantum chemistry,
- Geophysical flows,
- Stealth aircraft,
- Diffusion of solid bodies in a liquid,
- Adaptive mesh refinement,
- Computational materials research,
- Deep learning in neural networks,
- Stochastic simulation,
- Massively parallel data mining,



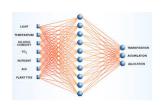


















**NLA is the backend** that accelerates a wide variety of science and engineering applications:

#### Linear system

Solve Ax = b

 Computational electromagnetics, material science, applications using boundary integral equations, airflow past wings, fluid flow around ship and other offshore constructions, and many more

#### Least squares:

Find x to minimize | Ax - b |

 Convex optimization, Computational statistics (e.g., linear least squares or ordinary least squares), econometrics, control theory, signal processing, curve fitting, and many more

#### Eigenproblems:

Solve  $Ax = \lambda x$ 

• Computational chemistry, quantum mechanics, material science, face recognition, PCA, data-mining, marketing, Google Page Rank, spectral clustering, vibrational analysis, compression, and many more

#### • Singular Value Decomposition (SVD):

 $A = U \Sigma V^*$ 

• Information retrieval, web search, signal processing, big data analytics, low rank matrix approximation, total least squares minimization, pseudo-inverse, and many more

#### Many variations depending on structure of A

• A can be symmetric, positive definite, tridiagonal, Hessenberg, banded, sparse with dense blocks, etc.

LA is crucial to the development of sparse solvers









**NLA is the backend** that accelerates a wide variety of science and engineering applications:

For big NLA problems
 (BLAS, convolutions, SVD, linear system solvers, etc.)



In contemporary libraries:
BLAS
LAPACK
ScaLAPACK

MAGMA (for GPUs)









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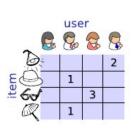


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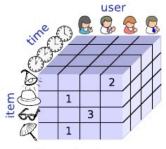
MAGMA (for GPUs)

- Numerous important applications need NLA for small problems
  - Machine learning / DNNs
  - Data mining / analytics
  - · High-order FEM,
  - · Graph analysis,
  - Neuroscience,
  - Astrophysics,
  - Quantum chemistry,
  - Signal processing, and more

Where data can be multidimensional / relational



















**NLA is the backend** that accelerates a wide variety of science and engineering applications:

For big NLA problems
 (BLAS, convolutions, SVD, linear system solvers, etc.)



In contemporary libraries:
BLAS
LAPACK
ScaLAPACK

MAGMA (for GPUs)

- Adding in MAGMA application backends for small problems
  - Machine learning / DNNs
  - Data mining / analytics
  - High-order FEM,
  - · Graph analysis,
  - Neuroscience,
  - · Astrophysics,
  - Quantum chemistry,
  - Signal processing, and more

#### **Small matrices / tensors**



Fixed-size batches



Variable-size batches



Dynamic batches















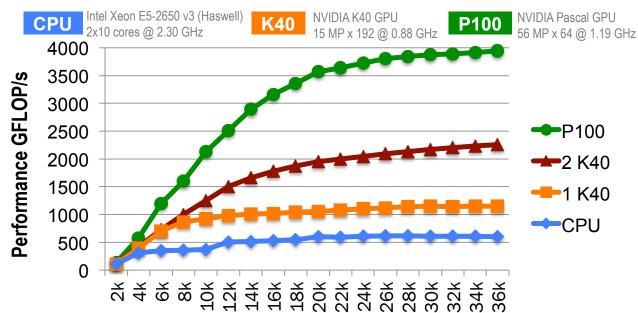
#### **Key Features of MAGMA 2.2**

#### TASK-BASED ALGORITHMS

MAGMA uses task-based algorithms where the computation is split into tasks of varying granularity and their execution scheduled over the hardware components. Scheduling can be static or dynamic. In either case, small non-parallelizable tasks, often on the critical path, are scheduled on the CPU, and larger more parallelizable ones, often Level 3 BLAS, are scheduled on the GPUs.

#### PERFORMANCE & ENERGY EFFICIENCY

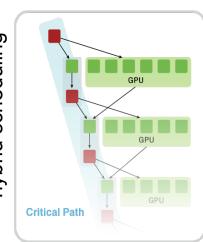
#### MAGMA LU factorization in double precision arithmetic

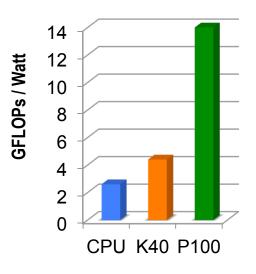


Matrix size N x N



BLAS tasking + hybrid scheduling







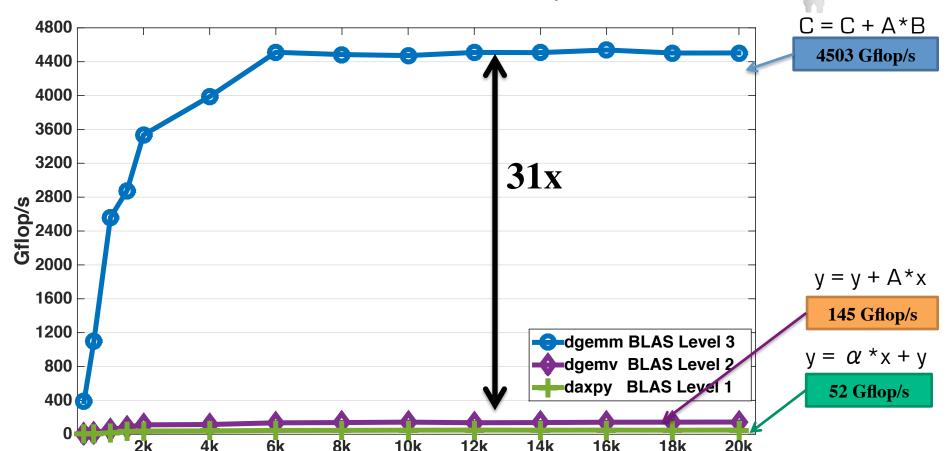






#### MAGMA — designed to use Level 3 BLAS as much as possible

Nvidia **P100**, 1.19 GHz, Peak DP = 4700 Gflop/s



Nvidia P100
The theoretical peak double precision is 4700 Gflop/s CUDA version 8.0



Matrix size (N), vector size (NxN)

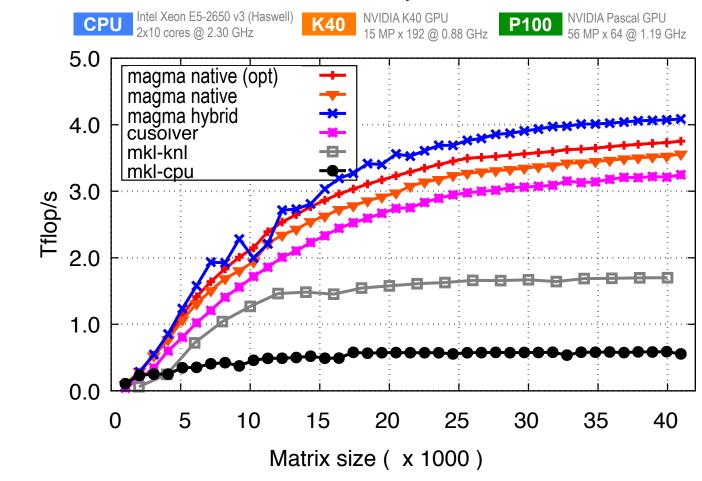






# MAGMA Algorithms (influenced by hardware trend) Hybrid (using CPU + GPUs) and/vs. GPU-only

#### MAGMA LU factorization in double precision arithmetic







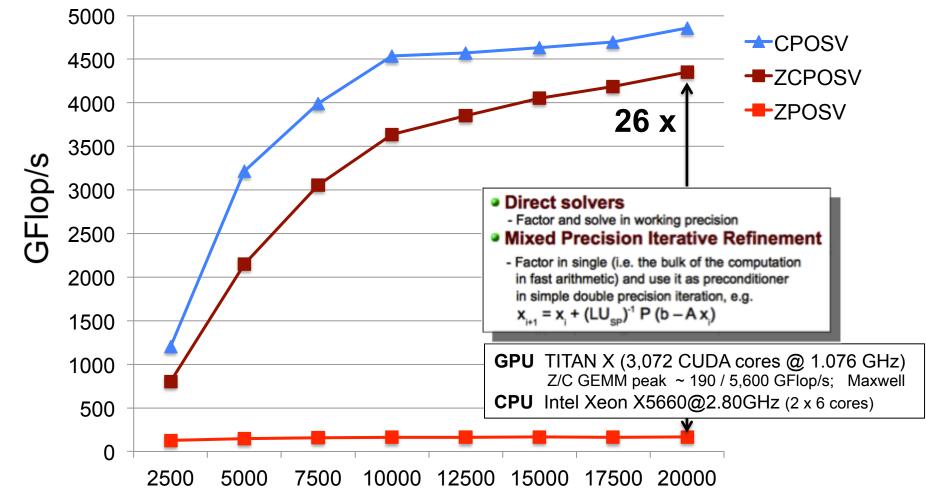




#### MAGMA Algorithms (influenced by hardware trend)

#### **Mixed-precision iterative refinement**

Solving general dense linear systems using mixed precision iterative refinement



Matrix size

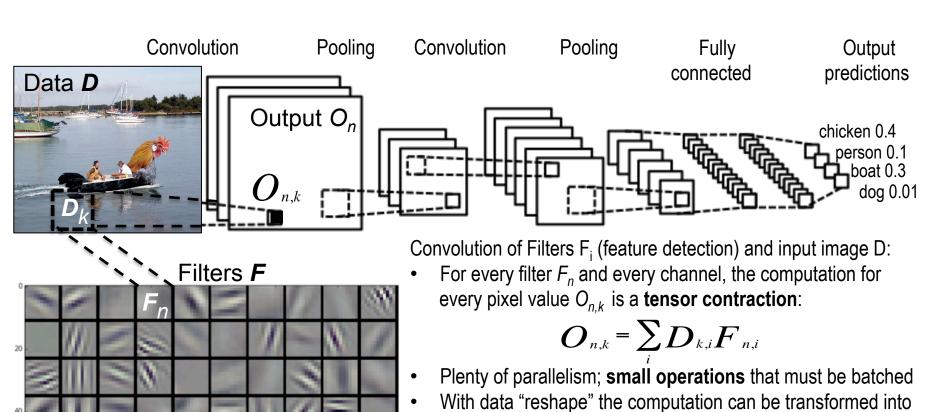




#### **Backend for DNN and Data Analytics**

#### Support for various **Batched and/or Tensor contraction** routines

e.g., Convolutional Neural Networks (CNNs) used in computer vision Key computation is convolution of Filter Fi (feature detector) and input image D (data):









a **batched GEMM** (for efficiency; among other approaches)



## **Tensor contractions for high-order FEM**

#### Lagrangian Hydrodynamics in the BLAST code<sup>[1]</sup>

On semi-discrete level our method can be written as

Momentum Conservation:  $\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = -\mathbf{M}_{\mathbf{v}}^{-1}\mathbf{F}\cdot\mathbf{1}$ 

Energy Conservation:  $\frac{\mathrm{d}\mathbf{e}}{\mathrm{d}t} = \mathbf{M}_{\mathbf{e}}^{-1}\mathbf{F}^{\mathbf{T}} \cdot \mathbf{v}$ 

Equation of Motion:  $\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = \mathbf{v}$ 

where v, e, and x are the unknown velocity, specific internal energy, and grid position, respectively;  $M_v$  and  $M_e$  are independent of time velocity and energy mass matrices; and F is the generalized corner force matrix depending on (v,e,x) that needs to be evaluated at every time step.

#### Reference:

V. Dobrev, Tz. Kolev, R. Rieben, *High-order curvilinear finite element methods for Lagrangian hydrodynamics*, SIAM J. Sci. Comp., B606-B641. (36 pages)

 Contractions can often be implemented as index reordering plus batched GEMM (and hence, be highly efficient)

#### TENSOR KERNELS FOR ASSEMBLY/EVALUATION

stored components	FLOPs for assembly	amount of storage	FLOPs for matvec	numerical kernels				
	full assembly							
M	$M \hspace{1cm} O(p^{3d}) \hspace{1cm} O(p^{2d}) \hspace{1cm} O(p^{2d}) \hspace{1cm} B, D \mapsto B^TDB, x \mapsto Mx$							
			decomposed	evaluation				
B, D	$O(p^{2d})$	$O(p^{2d})$	$O(p^{2d})$	$x\mapsto Bx, x\mapsto B^Tx, x\mapsto Dx$				
		near-optin	nal assembly	equations (1) and (2)				
$M_{i_1,\cdots,j_d}$	$O(p^{2d+1})$	$O(p^{2d})$	$O(p^{2d})$	$A_{i_1,k_2,j_1} = \sum_{k_1} B^{1d}_{k_1,i_1} B^{1d}_{k_1,j_1} D_{k_1,k_2}$	(1a)			
				$A_{i_1,i_2,j_1,j_2} = \sum_{k_2} B^{1d}_{k_2,i_2} B^{1d}_{k_2,j_2} C_{i_1,k_2,j_1}$	(1b)			
				$A_{i_1,k_2,k_3,j_1} = \sum_{k_1} B^{1d}_{k_1,i_1} B^{1d}_{k_1,j_1} D_{k_1,k_2,k_3}$	(2a)			
				$A_{i_1,i_2,k_3,j_1,j_2} = \sum_{k_2} B^{1d}_{k_2,i_2} B^{1d}_{k_2,j_2} C_{i_1,k_2,k_3,j_1}$	(2b)			
				$A_{i_1,i_2,i_3,j_1,j_2,j_3} = \sum_{k_3} B^{1d}_{k_3,i_3} B^{1d}_{k_3,j_3} C_{i_1,i_2,k_3,j_1,j_2}$	(2c)			
	near-op	timal evaluat	tion (partial a	ssembly) – equations (3) and (4)				
$B^{1d}, D$	$O(p^d)$	$O(p^d)$	$O(p^{d+1})$	$A_{j_1,k_2} = \sum_{j_2} B^{1d}_{k_2,j_2} V_{j_1,j_2}$	(3a)			
				$A_{k_1,k_2} = \sum_{j_1} B^{1d}_{k_1,j_1} C_{j_1,k_2}$	(3b)			
				$A_{k_1,i_2} = \sum_{k_2} B^{1d}_{k_2,i_2} C_{k_1,k_2}$	(3c)			
				$A_{i_1,i_2} = \sum_{k_1} B^{1d}_{k_1,i_1} C_{k_1,i_2}$	(3d)			
				$A_{j_1,j_2,k_3} = \sum_{j_3} B^{1d}_{k_3,j_3} V_{j_1,j_2,j_3}$	(4a)			
				$A_{j_1,k_2,k_3} = \sum_{j_2} B^{1d}_{k_2,j_2} C_{j_1,j_2,k_3}$	(4b)			
				$A_{k_1,k_2,k_3} = \sum_{j_1} B^{1d}_{k_1,j_1} C_{j_1,k_2,k_3}$	(4c)			
				$A_{k_1,k_2,i_3} = \sum_{k_3} B^{1d}_{k_3,i_3} C_{k_1,k_2,k_3}$	(4d)			
				$A_{k_1,i_2,i_3} = \sum_{k_2} B^{1d}_{k_2,i_2} C_{k_1,k_2,i_3}$	(4e)			
				$A_{i_1,i_2,i_3} = \sum_{k_1} B^{1d}_{k_1,i_1} C_{k_1,i_2,i_3}$	(4f)			
matrix-free evaluation								

#### Reference:

A. Abdelfattah, M. Baboulin, V. Dobrev, J. Dongarra, C. Earl, J. Falcou, A. Haidar, I. Karlin, Tz. Kolev, I. Masliah, S. Tomov, *High-Performance Tensor Contractions for GPUs*, ICCS 2016, San Diego, CA, June 6—8, 2016.









evaluating entries of  $B^{1d}$ , D, (3a)–(4f) sums

#### **Batched routines released in MAGMA**

#### **MAGMA BATCHED**

#### BATCHED FACTORIZATION OF A SET OF SMALL MATRICES IN PARALLEL

Numerous applications require factorization of many small matrices

- Deep learning
- Structural mechanics High-order FEM
- Astrophysics

- Sparse direct solvers
- High-order FEM simulations

# Vers MAGMA Batched Framework & Abstractions Autotuning Inlining & Code Generation CPUs GPUs Coprocessors KNC/KNL

**DEVICES** 

#### **ROUTINES**

LU, QR, and Cholesky

Solvers and matrix inversion

All BLAS 3 (fixed + variable)

SYMV, GEMV (fixed + variable)

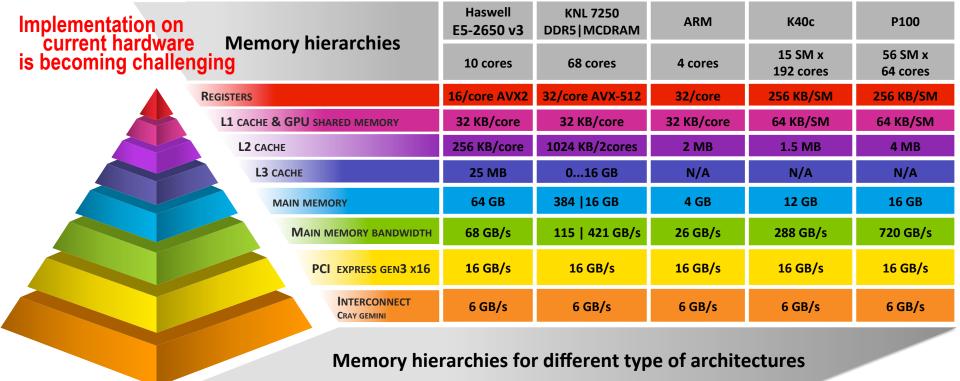












Workshop on Batched, Reproducible, and Reduced Precision BLAS

Georgia Tech
Computational Science and Engineering
Atlanta, GA
February 23—25, 2017

http://bit.ly/Batch-BLAS-2017

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Draft Reports
Batched BLAS Draft Reports:

https://www.dropbox.com/s/olocmipyxfvcaui/batched api 03 30 2016.pdf?dl=0

**Batched BLAS Poster:** 

https://www.dropbox.com/s/ddkym76fapddf5c/Batched%20BLAS%20Poster%2012.pdf?dl=0

**Batched BLAS Slides:** 

https://www.dropbox.com/s/kz4fhcipz3e56ju/BatchedBLAS-1.pptx?dl=0

Webpage on ReproBLAS:

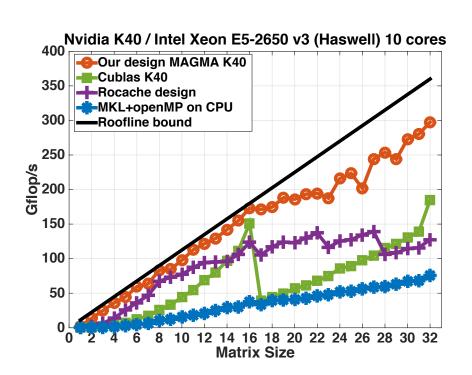
http://bebop.cs.berkeley.edu/reproblas/

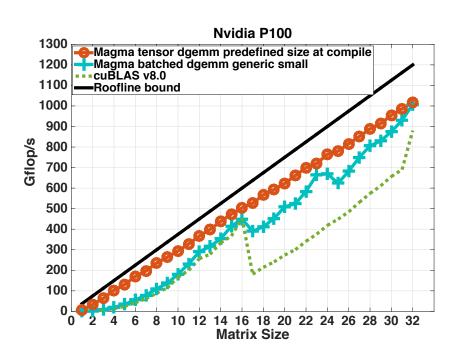
**Efficient Reproducible Floating Point Summation and BLAS:** 

http://www.eecs.berkeley.edu/Pubs/TechRpts/2015/EECS-2015-229.pdf

## **Tensor contractions – performance**

Performance comparison of tensor contraction versions using batched C =  $\alpha$ AB +  $\beta$ C on 100,000 square matrices of size n on a **K40c GPU** and 16 cores of Intel Xeon E5-2670, 2.60 GHz CPUs.





#### Reference:

I. Masliah, A. Abdelfattah, A. Haidar, S. Tomov, M. Baboulin, J. Falcou, and J. Dongarra, *High-performance matrix-matrix multiplications of very small matrices*, Euro-Par'16, Grenoble, France, August 22-26, 2016.









#### **Motivation**

- Deep learning architectures show promising results in abstract tasks like image classifications
- They inherently consist of same old neural networks as before except
  - The size of the networks has increased drastically, more compute power,
  - Training dataset is huge, but fast
- Any improvement in the core modules of such networks will greatly influences the training and increases performance, also helps in understanding the network well
- Spatial convolution in convnets takes up to 70% of the total execution.
- We optimize spatial convolution module specifically for convnets.

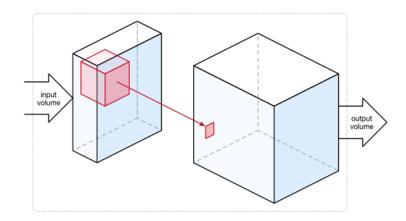


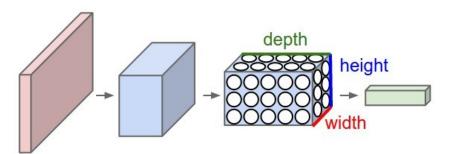






## **Introduction to Spatial Convolution:**





- Input and weights are 3D tensors
- As the filter traverses across the input volume horizontally and vertically it generates a 2D activation map
- Multiple filters generate multiple 2D output frames
- These output frames are stacked to form a 3D output tensor

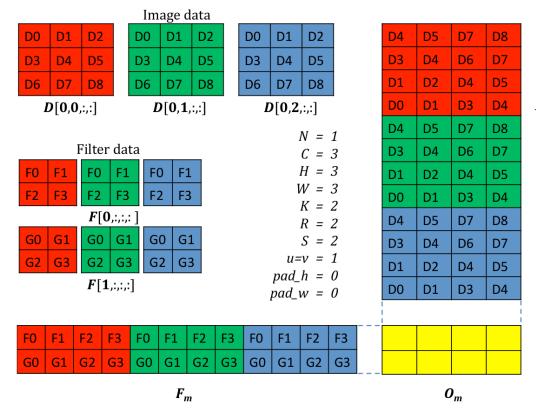








## Background or existing technique: Unfold and GEMM



#### VGG-16 D conv modules

Conv	Weight Matrix	Data Matrix
1	64x27	27x50176
2	64x576	$576 \times 50176$
3	128x576	576x12544
4	128x1152	1152 x 12544
5-7	256x2304	2304x3136
8	512x2304	2304x784
9-10	512x4608	4608x784
10-13	512x4608	4608x196











## Background or existing technique: Unfold and GEMM

#### **Advantages:**

- Unfold involves streaming memcpy and can be made parallel by having many threads working on many sections of the input
- Many BLAS libraries contain fine tuned GEMM routines that can be used
- The output format is consistent with the actual convolution output

#### **Disadvantages:**

- Unfold operation requires extra memory
- Matrix shapes can be greatly skewed









## Convolution using transformation techniques

#### FFT method:

- Convolution becomes elementwise product in frequency domain
- Complexity in 2D is O(RS log(HW)), better than O(RSHW) in direct convolution
- Caution !! filter dimension should be similar to image dimension but in convnets that are used widely RS << HW</li>

#### Winograd Minimal filtering:

- Best suited for small filters, RS << HW</li>
- Reduces the arithmetic operations by constant factor thus improves the asymptotic timing



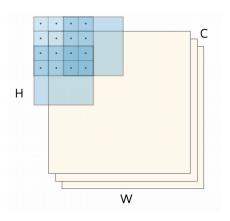






## Winograd algorithm

$$2. \quad \boxed{ \begin{bmatrix} \frac{1}{k_1} & 0 & 0 \\ \frac{k_2}{k_2} & \frac{k_2}{k_2} & \frac{k_2}{k_2} \\ 0 & 0 & 1 \end{bmatrix}} \bullet \quad \boxed{ \begin{bmatrix} \frac{1}{k_1} & 0 & 0 \\ \frac{k_2}{k_2} & -\frac{k_2}{k_2} & \frac{k_2}{k_2} \\ 0 & 0 & 1 \end{bmatrix}}^T$$



#### Steps:

- Transform a 4x4 image tile
- Transform a 3x3 filter
- Perform element wise product between the transformed tiles
- Inverse transform on the product tile

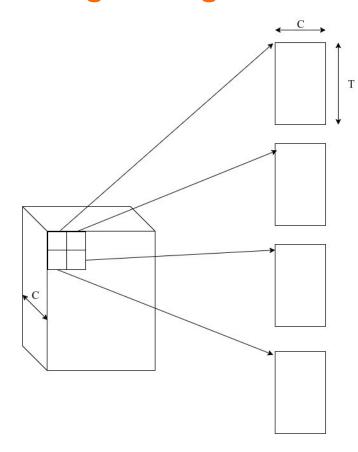








## Winograd algorithm: reduction to GEMM's



- Each Image tensor has 16 matrices of size TxC
- The K filters are reduced to 16 CxK matrices
- For a batch size of N there are 16N GEMMs, for example N=64 gives 1024 GEMMs.
- 16 filter matrices are common for all the GEMMs, so better last level cache efficiency
- Once GEMM are performed, "Gather" the elements from the 16 output matrices to form a 4x4 output tile
- Apply inverse transform on the output tile to obtain 2x2 convolution output











## Winograd algorithm: Advantage of GEMM's

- Each transformed image tile is reused with K filters. Similarly, each filter tile is reused with all the input tiles across the batch of N
- If N and K are large enough, the transformation cost is amortized because of max re- usage of transformed tiles
- Instead of applying inverse across C and then accumulating, the natural form of GEMM accumulates the result across C and then inverse can be applied once to the GEMM output tile.
- This is possible because of the linearity property for Winograd convolution Fine tuned GEMM APIs are available
- Good cache efficiency Good arithmetic intensity









## Winograd algorithm

l I	Fast Cor	ivolut	ion	
Layer	$\overline{m}$	$\overline{n}$	k	M
1	12544	64	3	1
2	12544	64	64	1
3	12544	128	64	4
4	12544	128	128	4
5	6272	256	128	8
6	6272	256	256	8
7	6272	256	256	8
8	3136	512	256	16
9	3136	512	512	16
10	3136	512	512	16
11	784	512	512	16
12	784	512	512	16
13	784	512	512	16

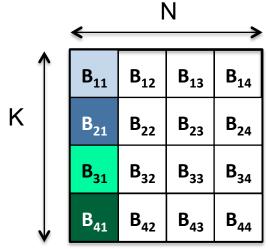




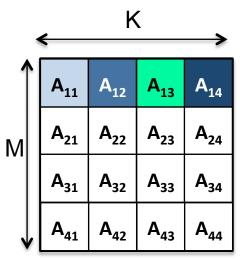




## **Optimizing GEMM's: Kernel design**



$$C = \beta C + \alpha AB$$



C <sub>11</sub>	C <sub>12</sub>	C <sub>13</sub>	C <sub>14</sub>
C <sub>21</sub>	C <sub>22</sub>	C <sub>23</sub>	C <sub>24</sub>
C <sub>31</sub>	C <sub>32</sub>	C <sub>33</sub>	C <sub>34</sub>
C <sub>41</sub>	C <sub>42</sub>	C <sub>43</sub>	C <sub>44</sub>

$T_1 = \alpha A_{11}$	]
$T_2 = \alpha A_{12}$	
$T_3 = \alpha A_{13}$	ſ
$T_{\star} = \alpha A_{\star \star}$	

 $C_{11} = \beta C_{11} + \Sigma T_k$ 

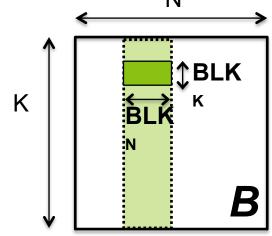


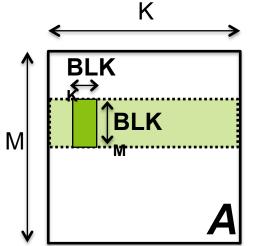






## **Optimizing GEMM's: Kernel design**





C <sub>11</sub>	C <sub>12</sub>	C <sub>13</sub>	C <sub>14</sub>
C <sub>21</sub>	C <sub>22</sub>	C <sub>23</sub>	C <sub>24</sub>
C <sub>31</sub>	C <sub>32</sub>	C <sub>33</sub>	C <sub>34</sub>
C <sub>41</sub>	C <sub>42</sub>	C <sub>43</sub>	C <sub>44</sub>



- Assign every block of C<sub>ii</sub> to a TB
- Hold the block C<sub>ii</sub> in register/sm
- Slide the green tile of A and B and compute C = βC + αAB
- This design guarantee reproducibility of results
- The kernel is parameterized to allow tuning and optimization

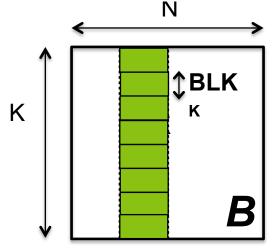




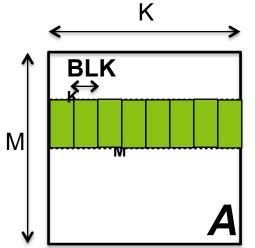


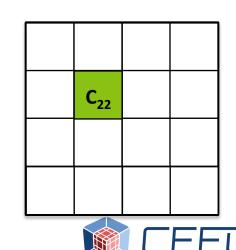


## **Optimizing GEMM's: Kernel design**



$$C = \beta C + \alpha AB$$



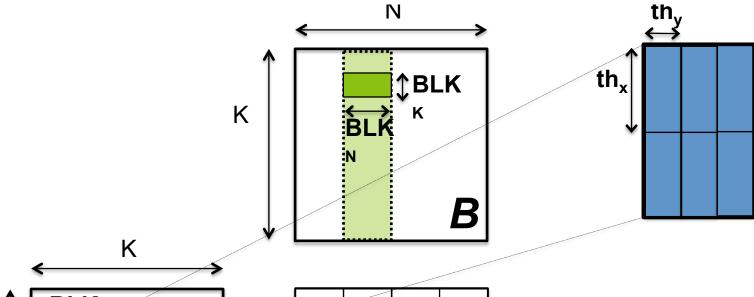


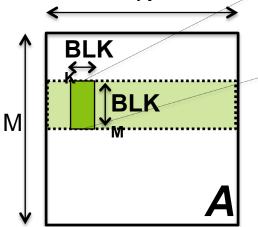
$$T = A_1 B_1$$
 $T += A_2 B_2$ 
 $T += A_3 B_3$ 
 $T += A_4 B_4$ 





## **Optimizing GEMM's: Kernel design**





 $-\epsilon_{_{11}}$	C <sub>12</sub>	C <sub>13</sub>	C <sub>14</sub>
C <sub>21</sub>	C <sub>22</sub>	C <sub>23</sub>	C <sub>24</sub>
C <sub>31</sub>	C <sub>32</sub>	C <sub>33</sub>	C <sub>34</sub>
C <sub>41</sub>	C <sub>42</sub>	C <sub>43</sub>	C <sub>44</sub>

- Reading/writing the elements is based on the TB size (# threads) and so is an extra parameter.
- Also it could be different for A, B and C

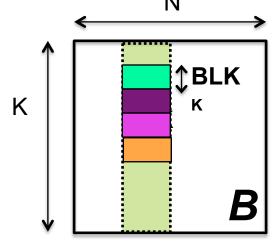


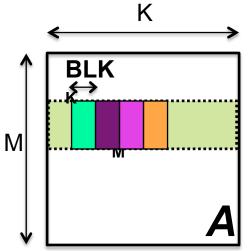






## Optimizing GEMM's: Kernel design





<b>C</b> <sub>11</sub>	C <sub>12</sub>	C <sub>13</sub>	C <sub>14</sub>
C <sub>21</sub>	C <sub>22</sub>	C <sub>23</sub>	C <sub>24</sub>
C <sub>31</sub>	C <sub>32</sub>	C <sub>33</sub>	C <sub>34</sub>
C <sub>41</sub>	C <sub>42</sub>	C <sub>43</sub>	C <sub>44</sub>

Prefetching









## **Optimizing GEMM's: Kernel design**

Are we done, we have our best kernel?

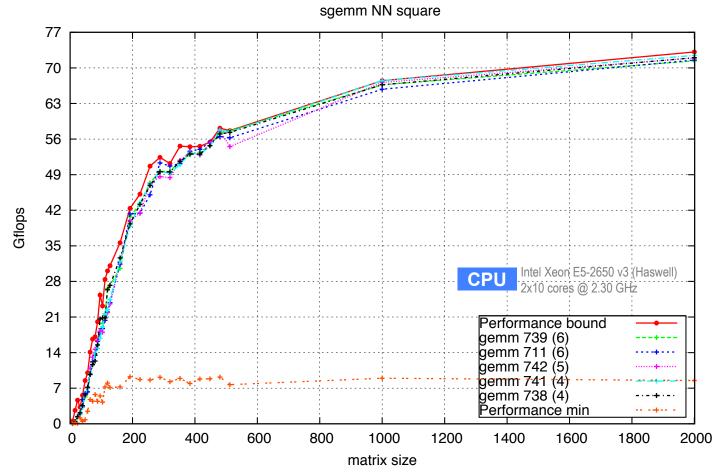
 for most of the case LA algorithms, Deep Learning, etc., the matrices A,B,C are not squares which requires autotunning









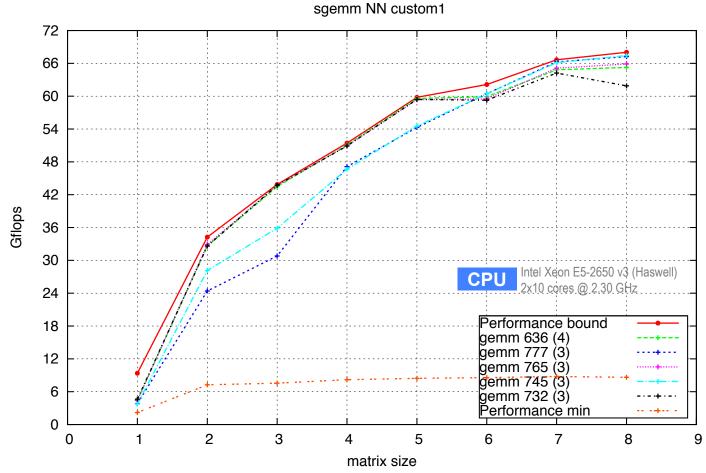










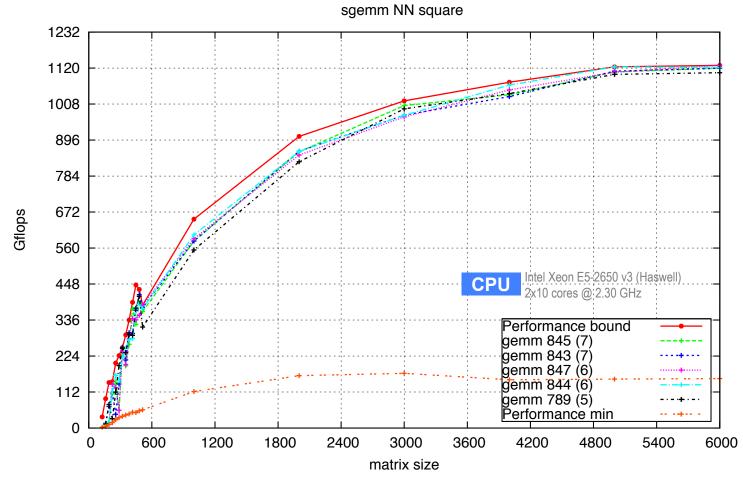










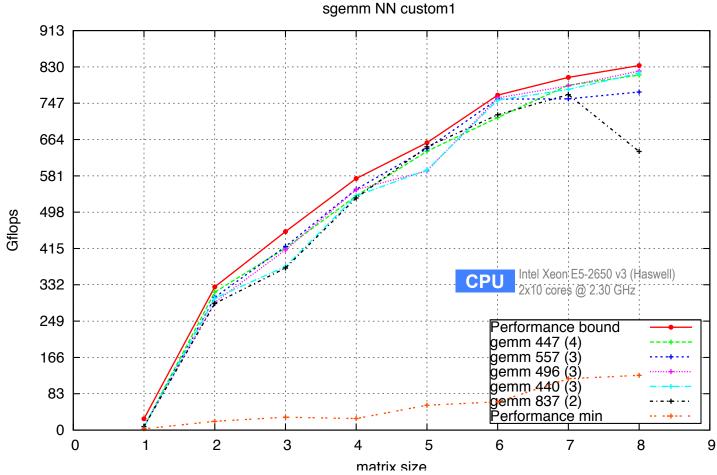










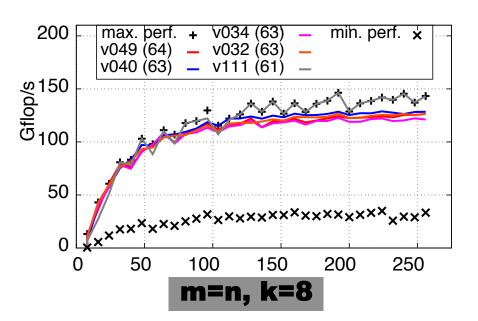


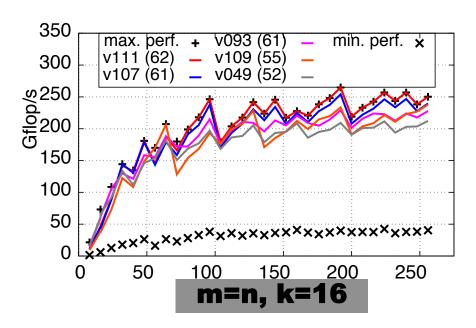


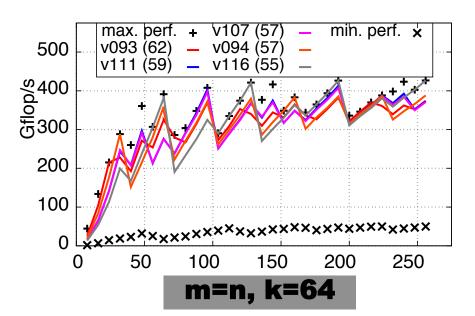


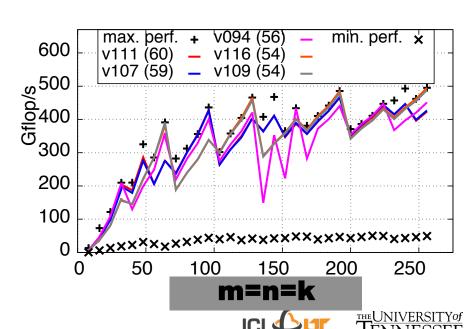












and Computer Science



K40 NVIDIA K40 GPU 15 MP x 192 @ 0.88 GHz

#### **Conclusions and future work**

#### In conclusion:

- Developed a number of NLA in MAGMA targeting applications
  - High-order FEM, DNN, and data analytics;
  - Tensor abstractions and high-performance tensor contractions (for high-order FEM)
- Multidisciplinary effort
- Achieve 90+% of theoretical maximum on GPUs and multicore CPUs
- Use on-the-fly tensor reshaping to cast tensor contractions as small but many GEMMs, executed using batched approaches
- Custom designed GEMM kernels for small matrices and autotuning

#### **Future directions:**

- To release a tensor contractions package through the MAGMA library
- To release NLA backend for DLA and data analytics
- Integrate developments in applications
- Complete autotuning and develop all kernels









## **Collaborators and Support**

#### MAGMA team

http://icl.cs.utk.edu/magma





#### **Collaborating partners**

University of Tennessee, Knoxville **Lawrence Livermore National Laboratory,** Livermore, CA

LLNL led ECP CEED:

Center for Efficient Exascale Discretizations University of Manchester, Manchester, UK

**University of Paris-Sud, France** 

**INRIA**, France













**Rutherford Appleton** Laboratory



University of Manchester









