Using CUDA Libraries with OpenACC

3 Ways to Accelerate Applications

Applications

Libraries

OpenACC Directives

Programming Languages

CUDA Libraries are interoperable with OpenACC

"Drop-in" Acceleration

Easily Accelerate Applications

Maximum Flexibility

3 Ways to Accelerate Applications

Applications

Libraries

OpenACC Directives

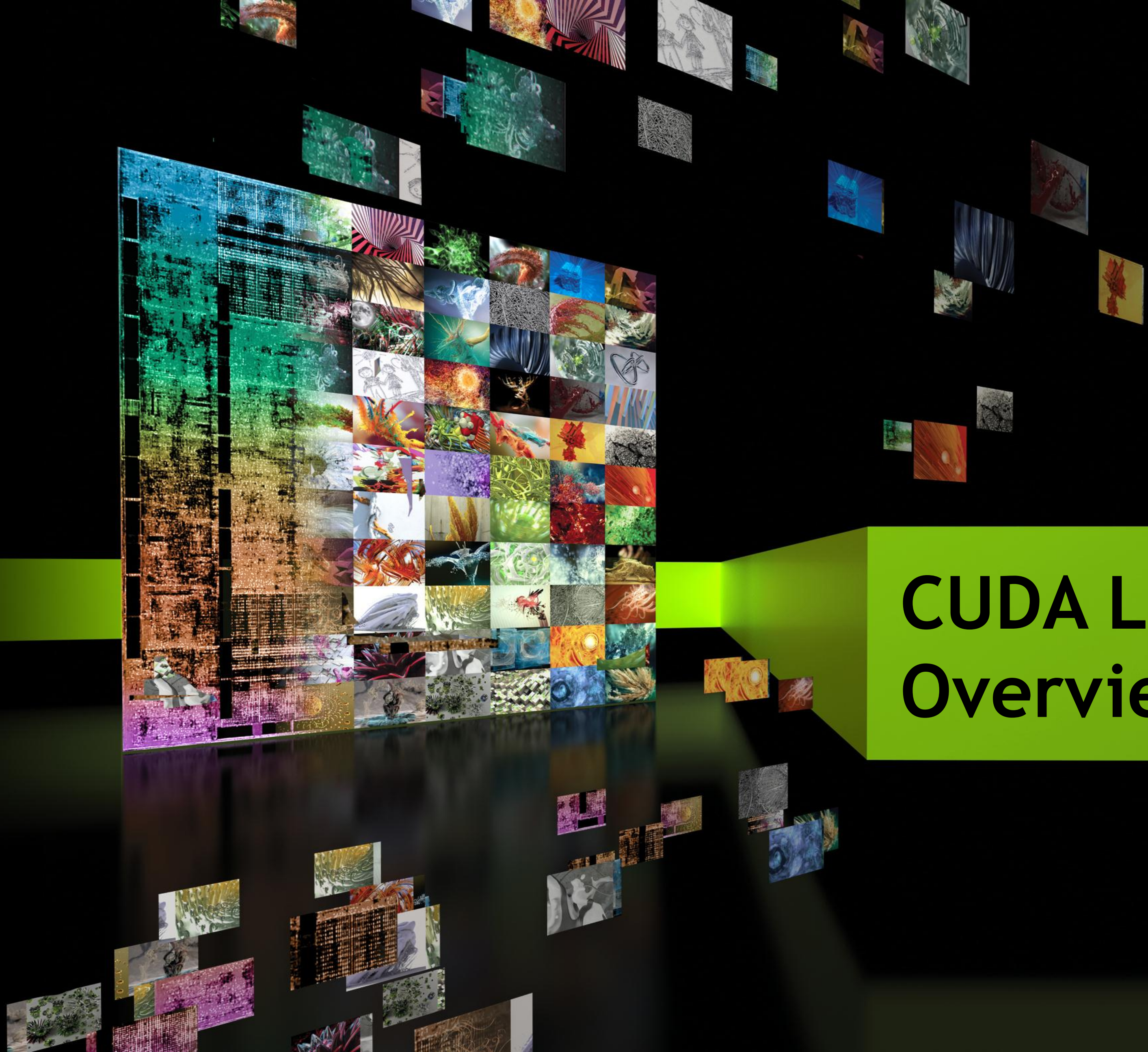
Programming Languages

CUDA Languages are interoperable with OpenACC, too!

"Drop-in" Acceleration

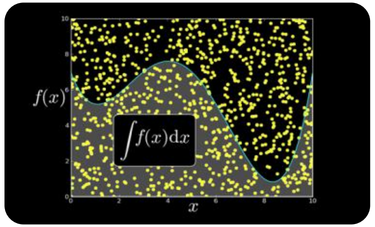
Easily Ac
Applications

imum
Flexibility

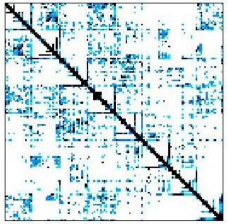


CUDA Libraries Overview

NVIDIA cuBLAS



NVIDIA cuRAND



NVIDIA cuSPARSE

NVIDIA NPP

GPU VSIPL

Vector Signal Image Processing

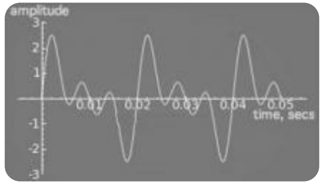
CULA tools

GPU Accelerated Linear Algebra

MAGMA

Matrix Algebra on GPU and Multicore

open source initiative



NVIDIA cuFFT

ROGUE WAVE SOFTWARE

IMSL Library

libjacket

Building-block Algorithms for CUDA

CUSP

Sparse Linear Algebra

open source initiative

Thrust

C++ STL Features for CUDA

open source initiative

GPU Accelerated Libraries

"Drop-in" Acceleration for Your Applications

CUDA Math Libraries

High performance math routines for your applications:

- cuFFT - Fast Fourier Transforms Library
- cuBLAS - Complete BLAS Library
- cuSPARSE - Sparse Matrix Library
- cuRAND - Random Number Generation (RNG) Library
- NPP - Performance Primitives for Image & Video Processing
- Thrust - Templated C++ Parallel Algorithms & Data Structures
- math.h - C99 floating-point Library

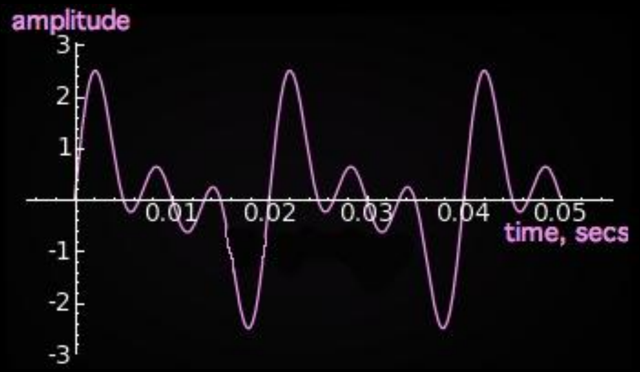
Included in the CUDA Toolkit Free download @ www.nvidia.com/getcuda

More information on CUDA libraries:

http://www.nvidia.com/object/gtc2010-presentation-archive.html#session2216

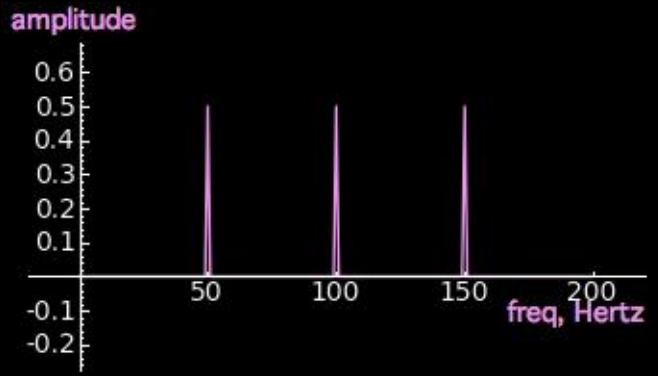
cuFFT: Multi-dimensional FFTs

- New in CUDA 4.1
  - Flexible input & output data layouts for all transform types
    - Similar to the FFTW "Advanced Interface"
    - Eliminates extra data transposes and copies
  - API is now thread-safe & callable from multiple host threads
  - Restructured documentation to clarify data layouts



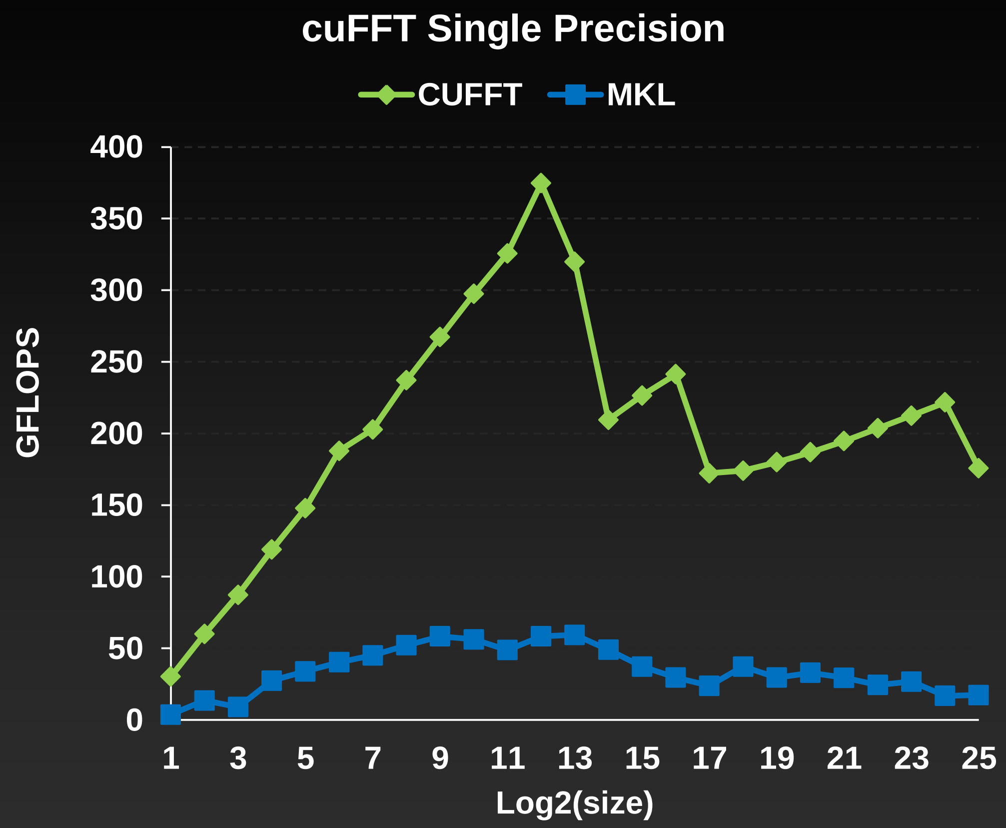
$$F(x) = \sum_{n=0}^{N-1} f(n) e^{-j2\pi(x\frac{n}{N})}$$

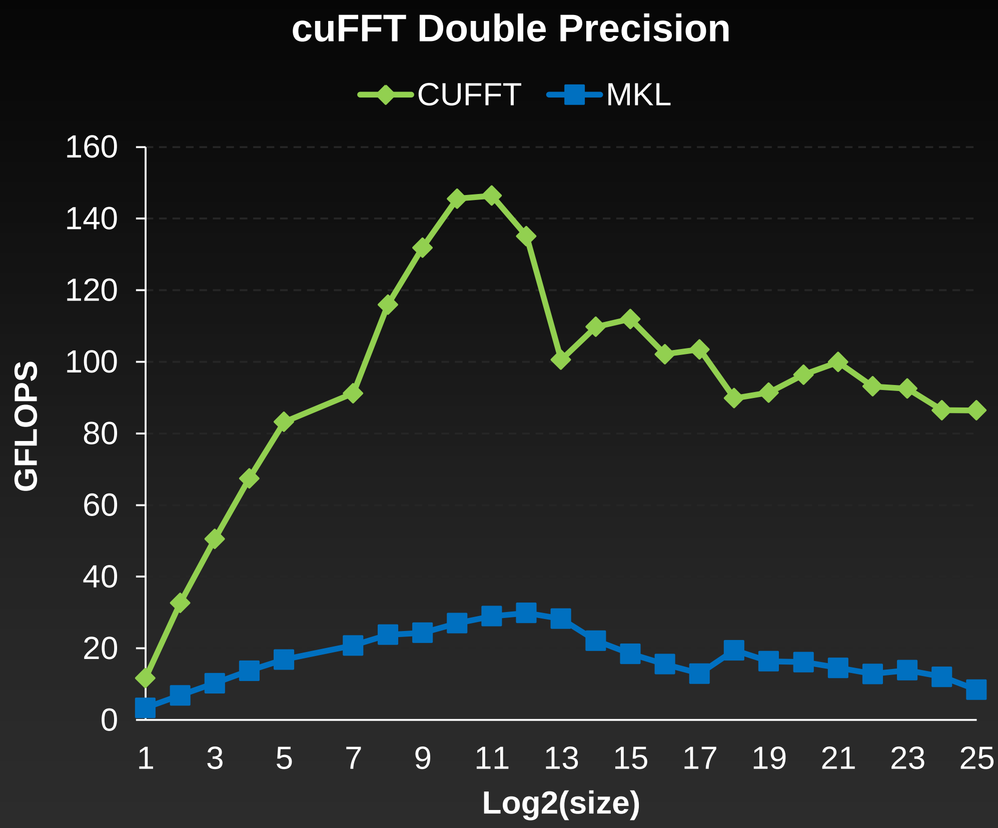
$$f(n) = \frac{1}{N} \sum_{n=0} F(x) e^{j2\pi(x\frac{n}{N})}$$



FFTs up to 10x Faster than MKL

1D used in audio processing and as a foundation for 2D and 3D FFTs

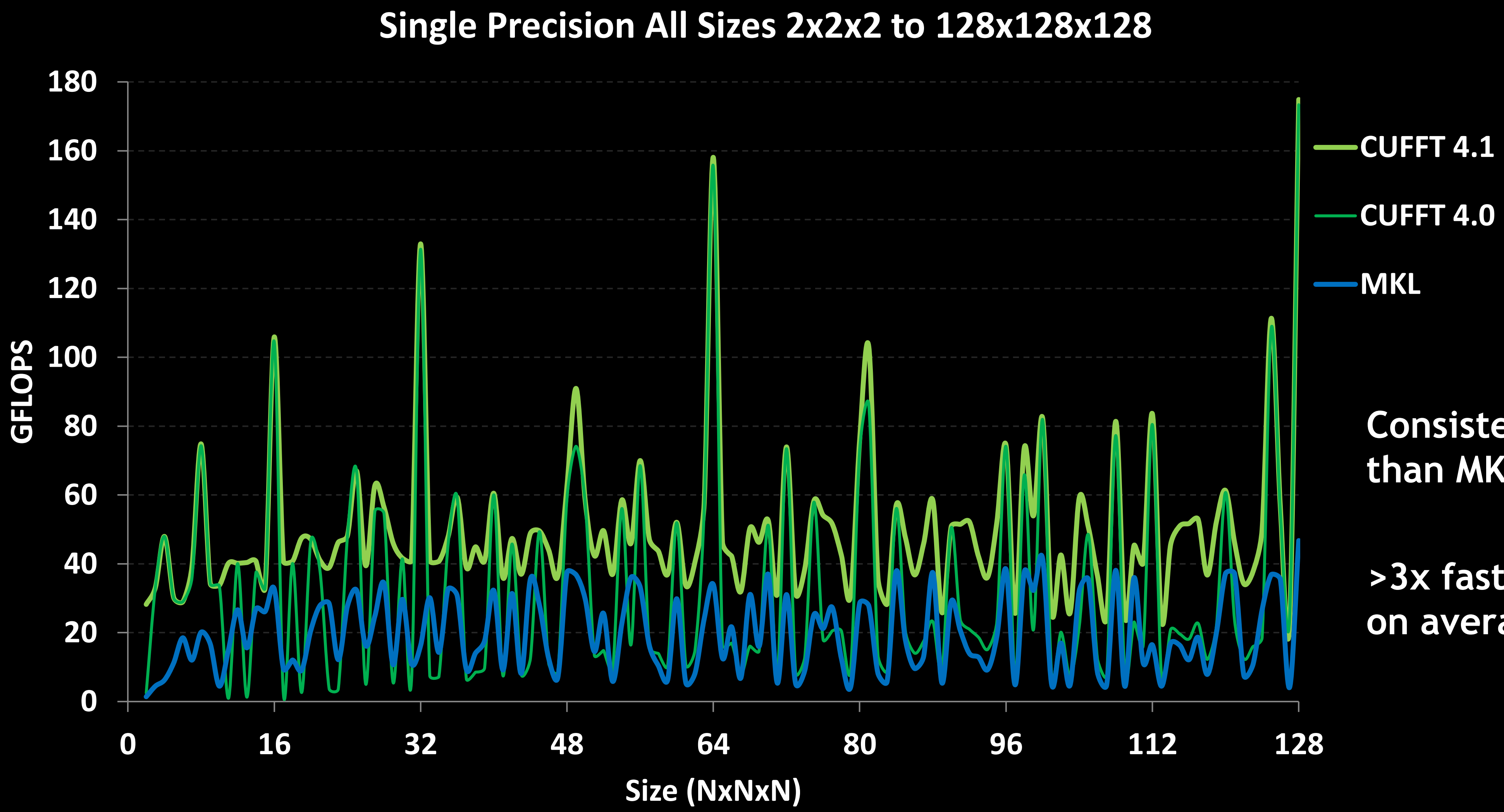




- Measured on sizes that are exactly powers-of-2
- cuFFT 4.1 on Tesla M2090, ECC on
- MKL 10.2.3, TYAN FT72-B7015 Xeon x5680 Six-Core @ 3.33 GHz

Performance may vary based on OS version and motherboard configuration

CUDA 4.1 optimizes 3D transforms



Consistently faster than MKL

>3x faster than 4.0 on average

- cuFFT 4.1 on Tesla M2090, ECC on
- MKL 10.2.3, TYAN FT72-B7015 Xeon x5680 Six-Core @ 3.33 GHz

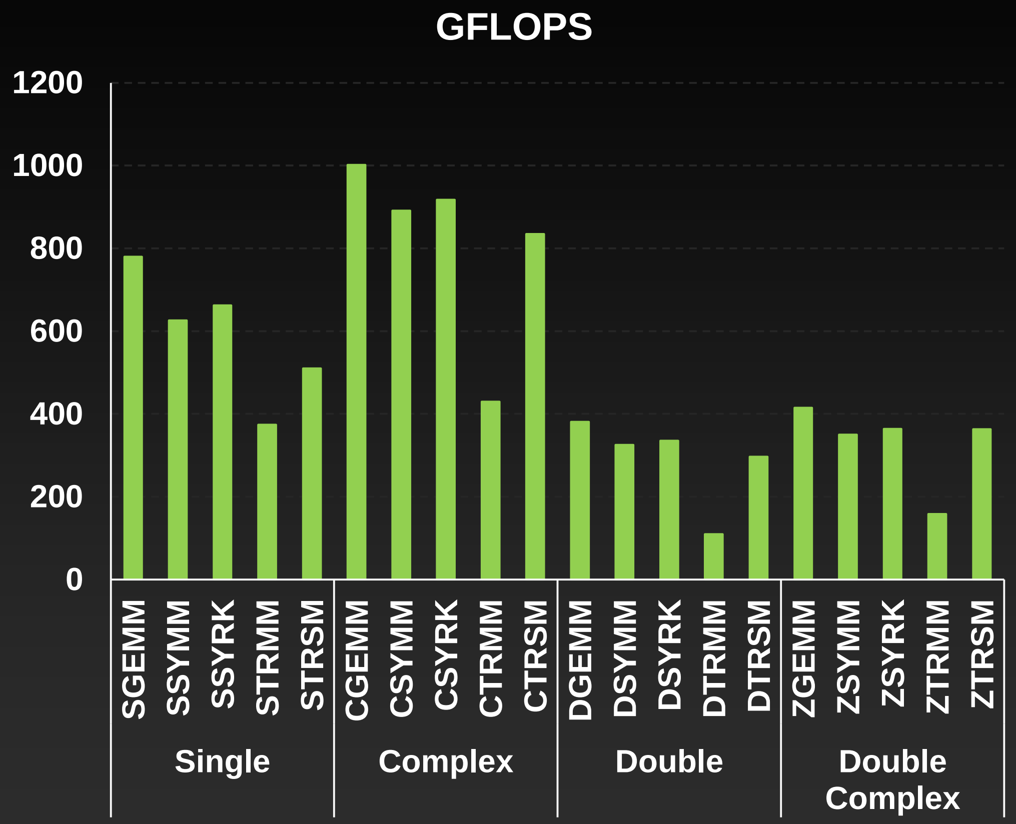
Performance may vary based on OS version and motherboard configuration

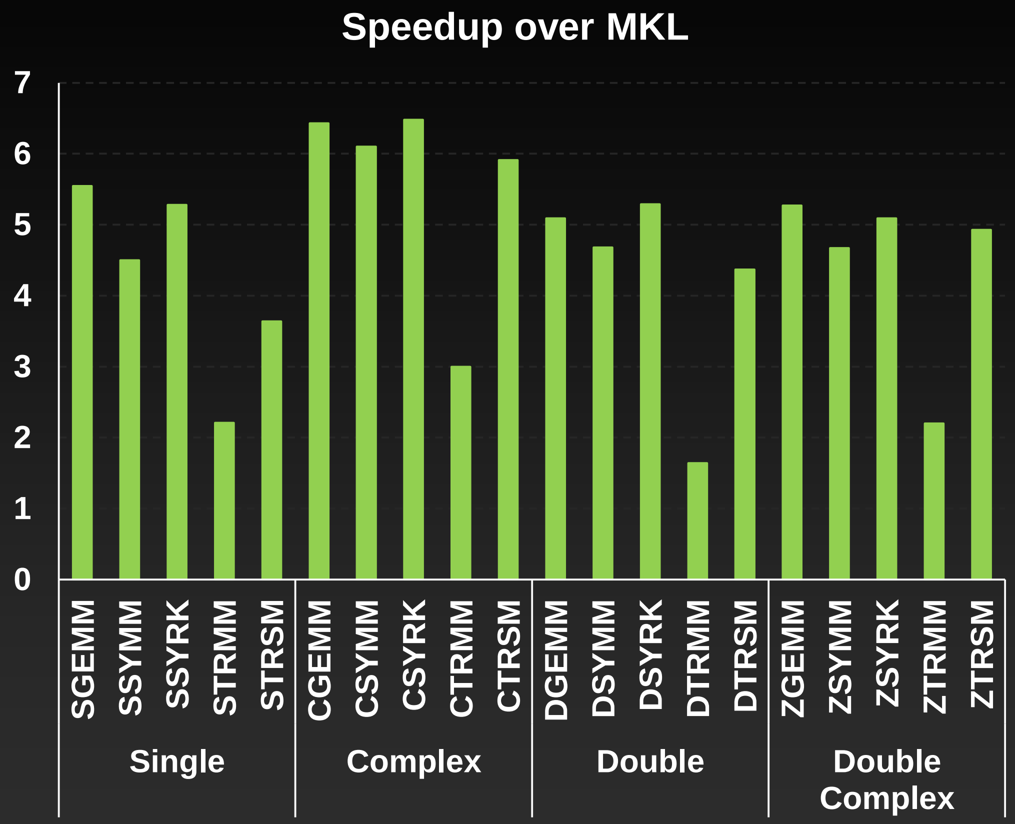
cuBLAS: Dense Linear Algebra on GPUs

- Complete BLAS implementation plus useful extensions
  - Supports all 152 standard routines for single, double, complex, and double complex
- New in CUDA 4.1
  - New batched GEMM API provides >4x speedup over MKL
    - Useful for batches of 100+ small matrices from 4x4 to 128x128
  - 5%-10% performance improvement to large GEMMs

cuBLAS Level 3 Performance

Up to 1 TFLOPS sustained performance and >6x speedup over Intel MKL

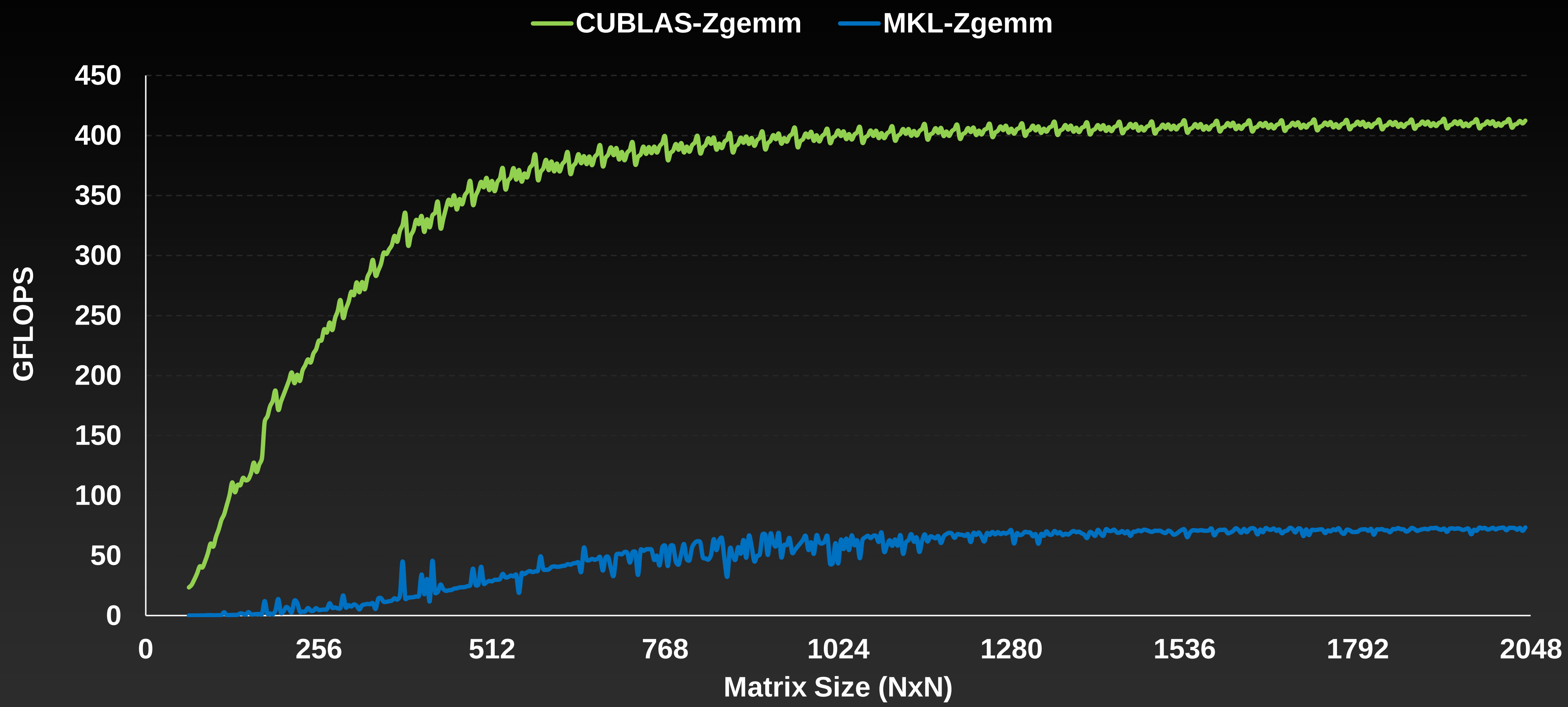




- 4Kx4K matrix size
- cuBLAS 4.1, Tesla M2090 (Fermi), ECC on
- MKL 10.2.3, TYAN FT72-B7015 Xeon x5680 Six-Core @ 3.33 GHz

Performance may vary based on OS version and motherboard configuration

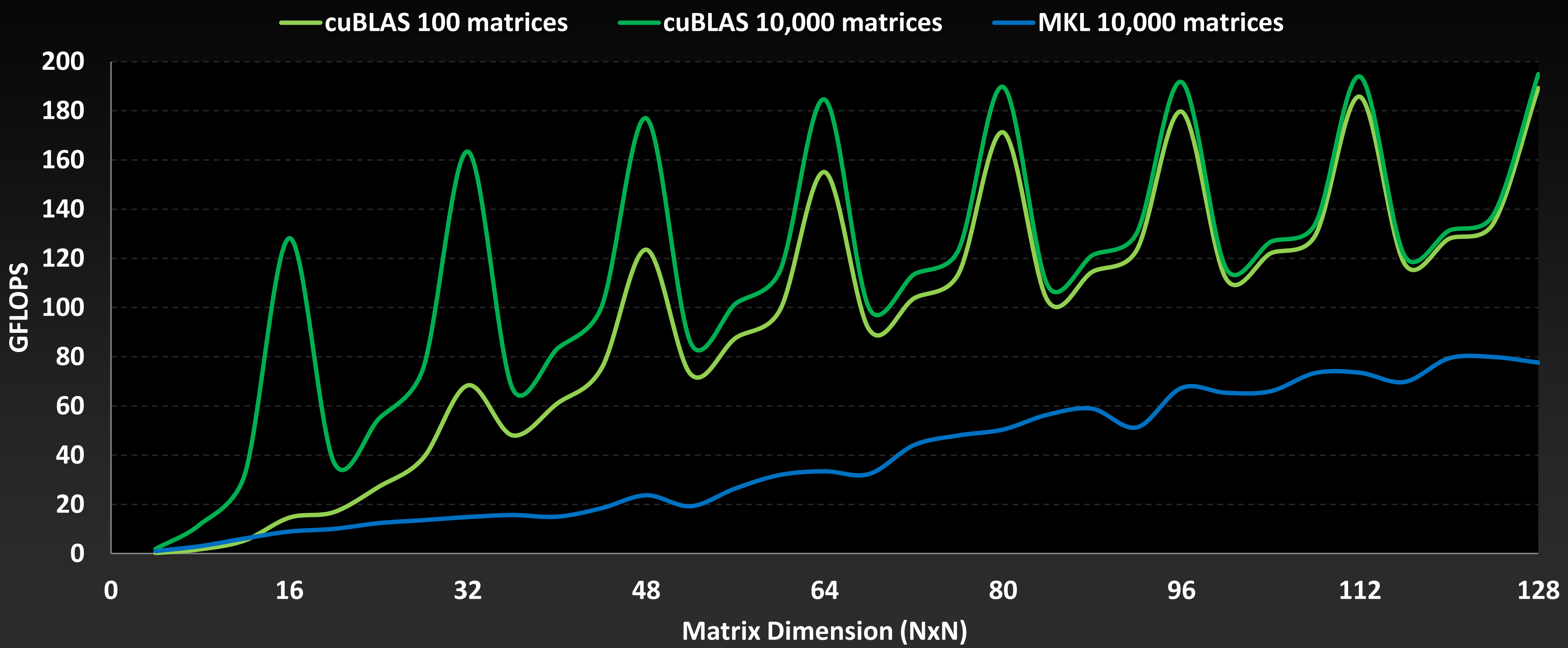
ZGEMM Performance vs Intel MKL



- cuBLAS 4.1 on Tesla M2090, ECC on
- MKL 10.2.3, TYAN FT72-B7015 Xeon x5680 Six-Core @ 3.33 GHz

Performance may vary based on OS version and motherboard configuration

cuBLAS Batched GEMM API improves performance on batches of small matrices



- cuBLAS 4.1 on Tesla M2090, ECC on
- MKL 10.2.3, TYAN FT72-B7015 Xeon x5680 Six-Core @ 3.33 GHz

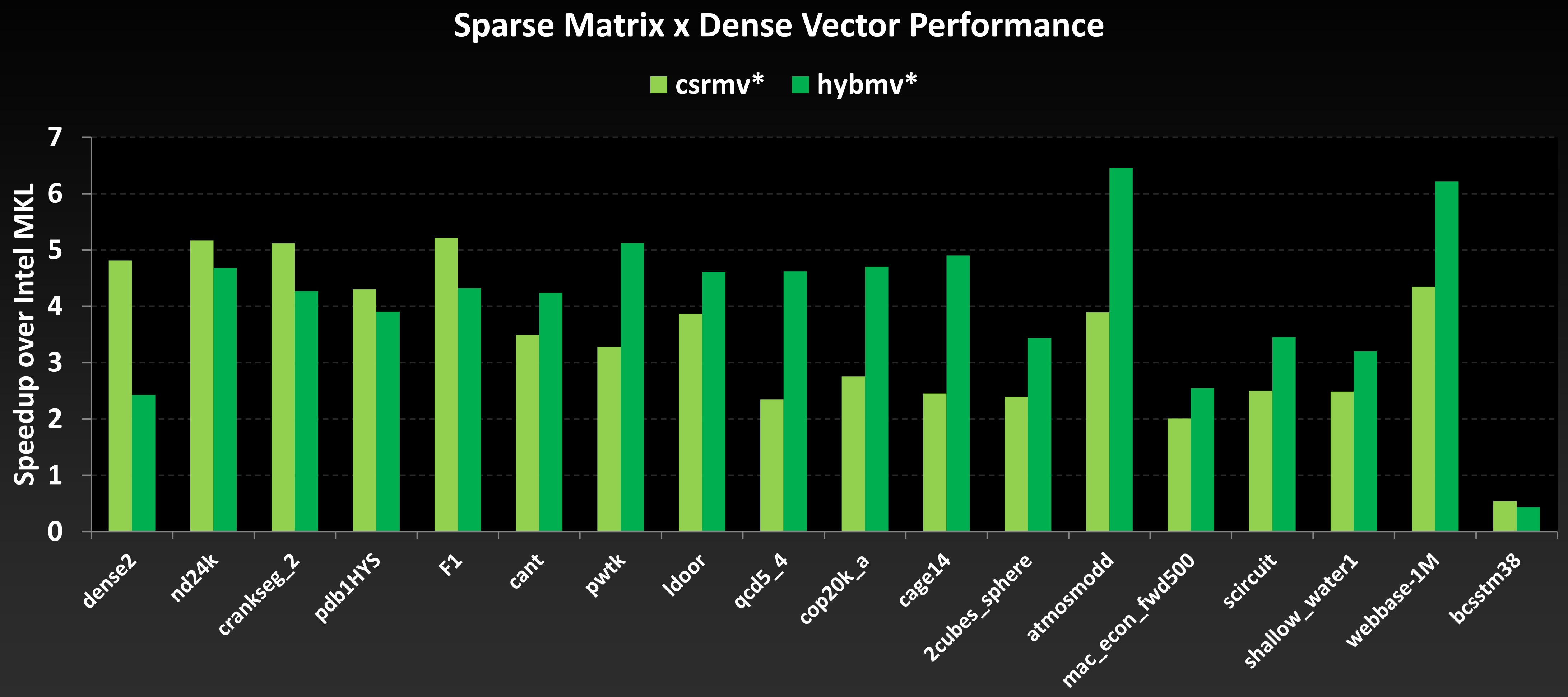
Performance may vary based on OS version and motherboard configuration

cuSPARSE: Sparse linear algebra routines

- Sparse matrix-vector multiplication & triangular solve
  - APIs optimized for iterative methods
- New in 4.1
  - Tri-diagonal solver with speedups up to 10x over Intel MKL
  - ELL-HYB format offers 2x faster matrix-vector multiplication

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix} = \alpha \begin{bmatrix} 1.0 & \cdots & \cdots & \cdots \\ 2.0 & 3.0 & \cdots & \cdots \\ \cdots & \cdots & 4.0 & \cdots \\ 5.0 & \cdots & 6.0 & 7.0 \end{bmatrix} \begin{bmatrix} 1.0 \\ 2.0 \\ 3.0 \\ 4.0 \end{bmatrix} + \beta \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix}$$

cuSPARSE is >6x Faster than Intel MKL

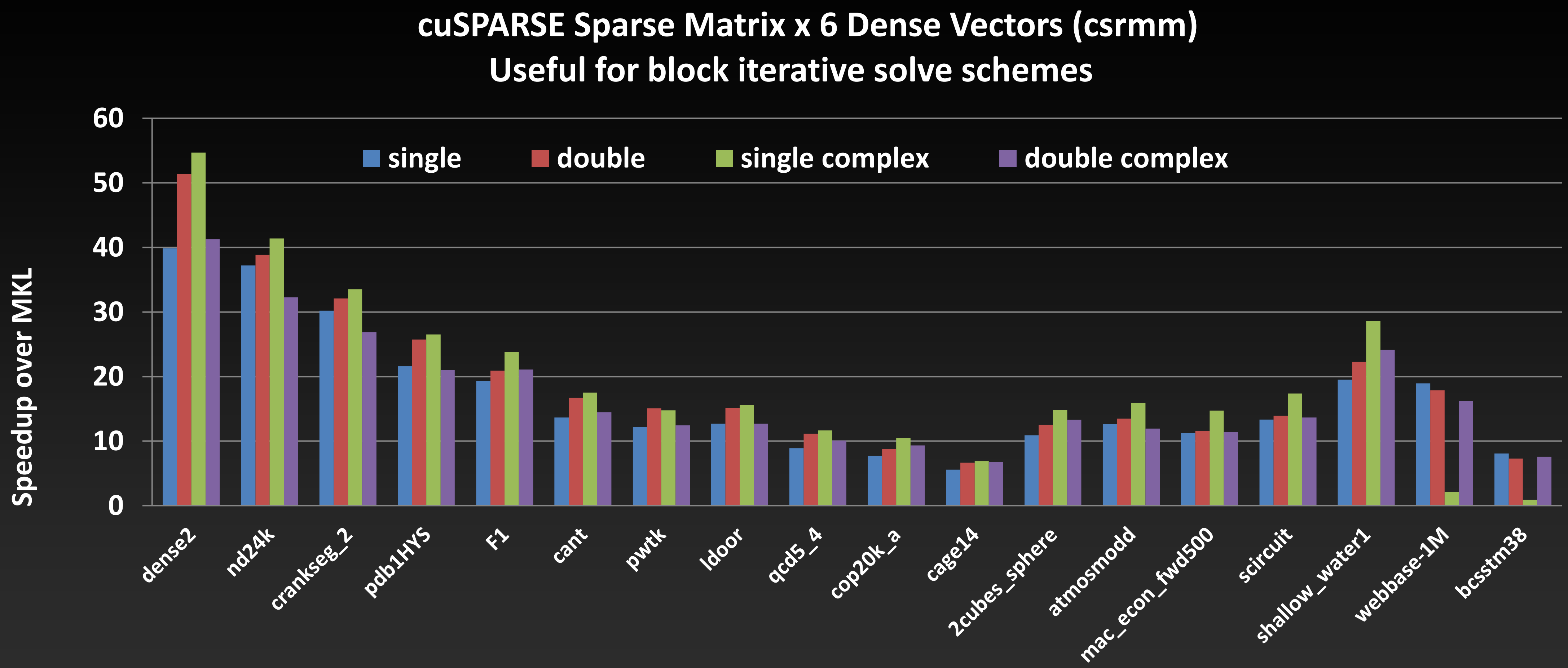


**Average speedup over single, double, single complex & double-complex*

Performance may vary based on OS version and motherboard configuration

- cuSPARSE 4.1, Tesla M2090 (Fermi), ECC on
- MKL 10.2.3, TYAN FT72-B7015 Xeon x5680 Six-Core @ 3.33 GHz

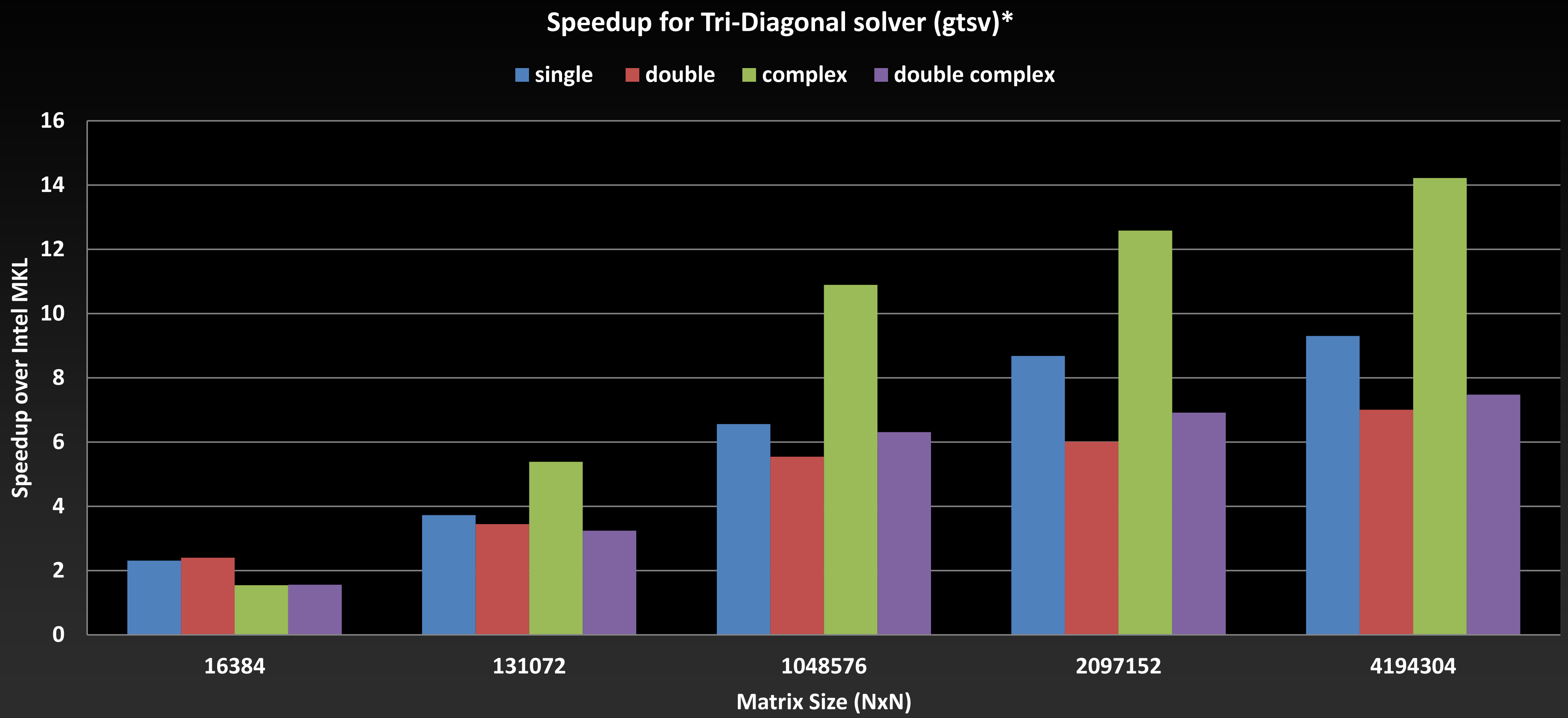
Up to 40x faster with 6 CSR Vectors



Performance may vary based on OS version and motherboard configuration

- cuSPARSE 4.1, Tesla M2090 (Fermi), ECC on
- MKL 10.2.3, TYAN FT72-B7015 Xeon x5680 Six-Core @ 3.33 GHz

Tri-diagonal solver performance vs. MKL



**Parallel GPU implementation does not include pivoting*

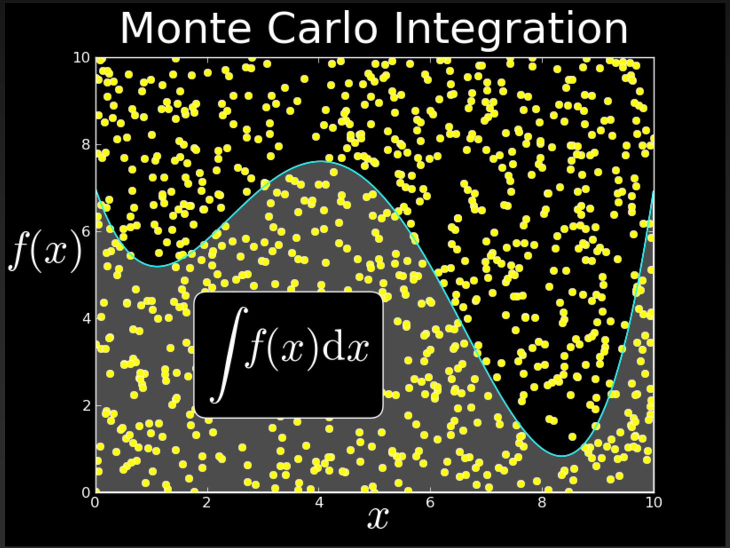
Performance may vary based on OS version and motherboard configuration

- cuSPARSE 4.1, Tesla M2090 (Fermi), ECC on
- MKL 10.2.3, TYAN FT72-B7015 Xeon x5680 Six-Core @ 3.33 GHz

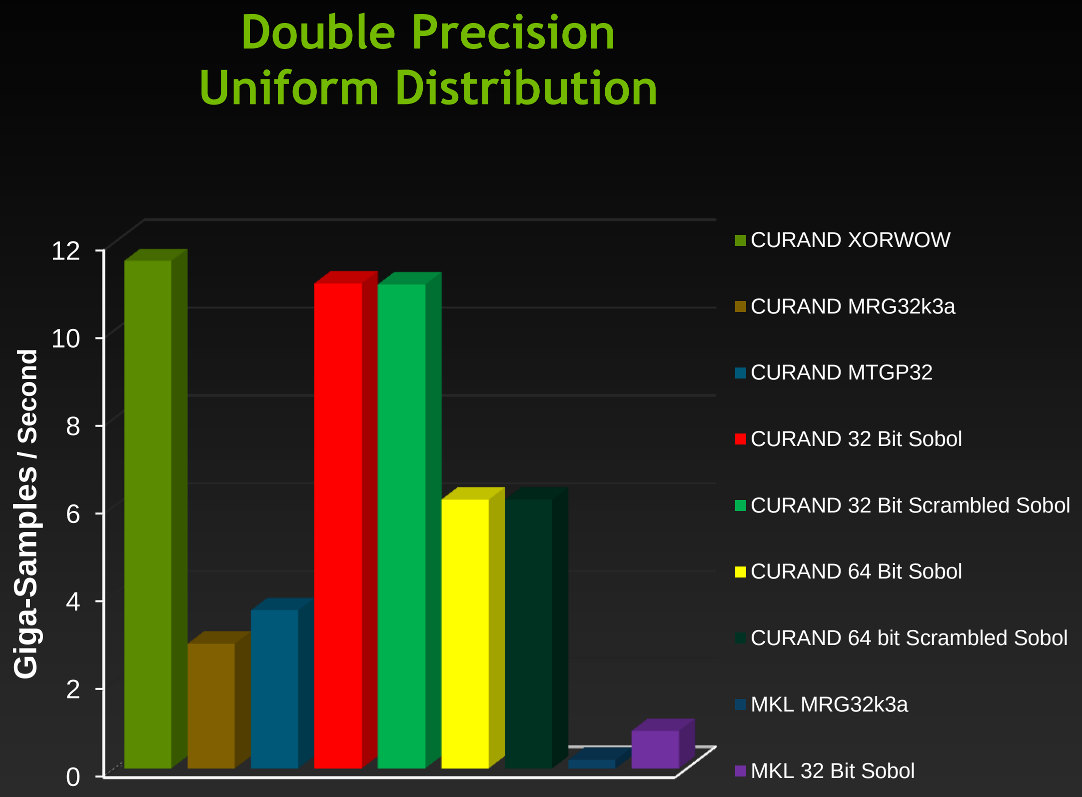
cuRAND: Random Number Generation

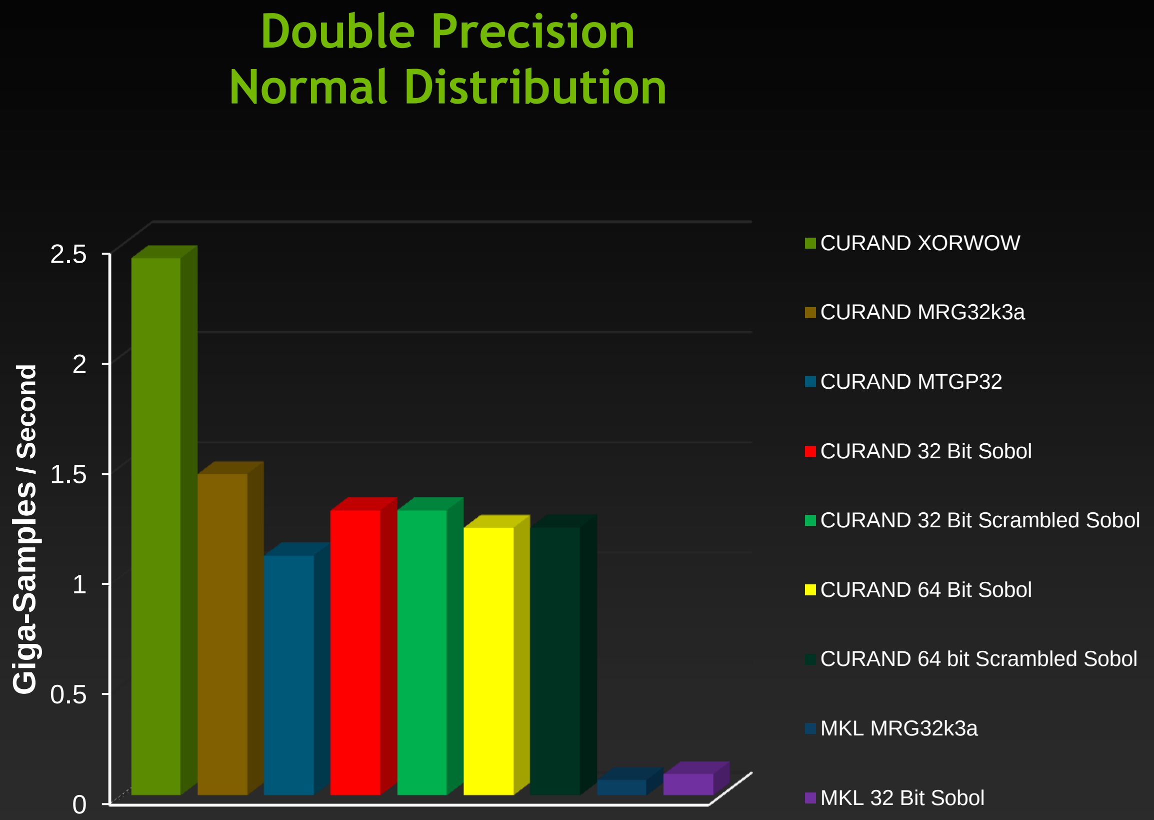
- Pseudo- and Quasi-RNGs
- Supports several output distributions
- Statistical test results reported in documentation

- New commonly used RNGs in CUDA 4.1
  - MRG32k3a RNG
  - MTGP11213 Mersenne Twister RNG



cuRAND Performance compared to Intel MKL





Performance may vary based on OS version and motherboard configuration

- cuRAND 4.1, Tesla M2090 (Fermi), ECC on
- MKL 10.2.3, TYAN FT72-B7015 Xeon x5680 @ 3.33 GHz

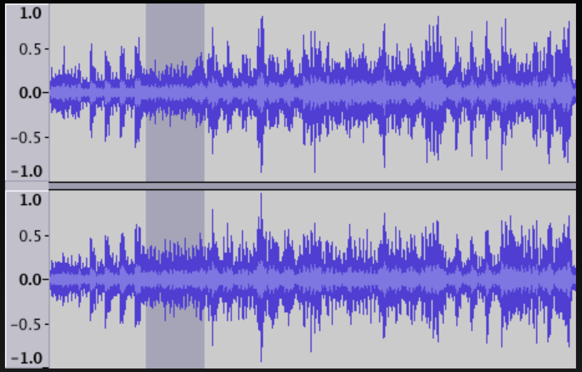
1000+ New Imaging Functions in NPP 4.1

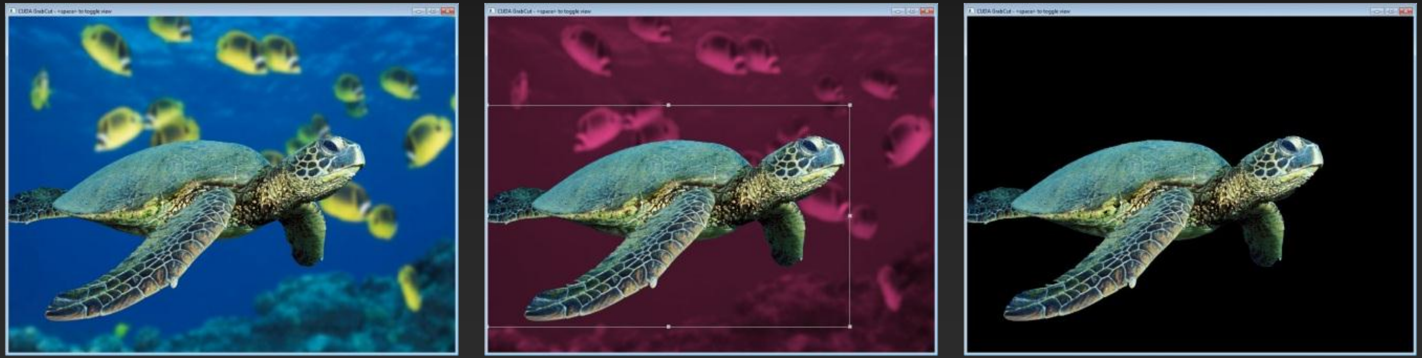
Up to 40x speedups

- NVIDIA Performance Primitives (NPP) library includes over 2200 GPU-accelerated functions for image & signal processing

  Arithmetic, Logic, Conversions, Filters, Statistics, etc.

- Most are 5x-10x faster than analogous routines in Intel IPP





http://developer.nvidia.com/content/graphcuts-using-npp

* NPP 4.1, NVIDIA C2050 (Fermi)
* IPP 6.1, Dual Socket Core™ i7 920 @ 2.67GHz

Using CUDA Libraries with OpenACC

Sharing data with libraries

- CUDA libraries and OpenACC both operate on device arrays
- OpenACC provides mechanisms for interop with library calls
  - deviceptr data clause
  - host_data construct
- Note: same mechanisms useful for interop with custom CUDA C/C++/Fortran code

deviceptr Data Clause

`deviceptr( list )` Declares that the pointers in *list* refer to device pointers that need not be allocated or moved between the host and device for this pointer.

Example:

C

```
#pragma acc data deviceptr(d_input)
```

Fortran

```
$!acc data deviceptr(d_input)
```

host_data Construct

Makes the address of device data available on the host.

`deviceptr( list )` Tells the compiler to use the device address for any variable in *list*. Variables in the list must be present in device memory due to data regions that contain this construct

Example

C

```
#pragma acc host_data use_device(d_input)
```

Fortran

```
$!acc host_data use_device(d_input)
```

Example: 1D convolution using CUFFT

- Perform convolution in frequency space
  1. Use CUFFT to transform input signal and filter kernel into the frequency domain
  2. Perform point-wise complex multiply and scale on transformed signal
  3. Use CUFFT to transform result back into the time domain
- We will perform step 2 using OpenACC
- Code walk-through follows. Code available with exercises.
  - In `exercises/cufft-acc`

Source Excerpt

```
// Transform signal and kernel
error = cufftExecC2C(plan, (cufftComplex *)d_signal,
                     (cufftComplex *)d_signal, CUFFT_FORWARD);
error = cufftExecC2C(plan, (cufftComplex *)d_filter_kernel,
                     (cufftComplex *)d_filter_kernel, CUFFT_FORWARD);

// Multiply the coefficients together and normalize the result
printf("Performing point-wise complex multiply and scale.\n");
complexPointwiseMulAndScale(new_size,
                            (float *restrict)d_signal,
                            (float *restrict)d_filter_kernel);

// Transform signal back
error = cufftExecC2C(plan, (cufftComplex *)d_signal,
                     (cufftComplex *)d_signal, CUFFT_INVERSE);
```

This function must execute on device data

OpenACC convolution code

```
void complexPointwiseMulAndScale(int n, float *restrict signal,
                                 float *restrict filter_kernel)
{
// Multiply the coefficients together and normalize the result
#pragma acc data deviceptr(signal, filter_kernel)
    {
#pragma acc kernels loop independent
        for (int i = 0; i < n; i++) {
            float ax = signal[2*i];
            float ay = signal[2*i+1];
            float bx = filter_kernel[2*i];
            float by = filter_kernel[2*i+1];
            float s = 1.0f / n;
            float cx = s * (ax * bx - ay * by);
            float cy = s * (ax * by + ay * bx);
            signal[2*i] = cx;
            signal[2*i+1] = cy;
        }
    }
}
```

Note: The PGI C compiler does not currently support structs in OpenACC loops, so we cast the Complex* pointers to float* pointers and use interleaved indexing

Linking CUFFT

- `#include "cufft.h"`
- Compiler command line options:

```
CUDA_PATH = /usr/local/pgi/linux86-64/2012/cuda/4.0
CCFLAGS = -I$(CUDA_PATH)/include -L$(CUDA_PATH)/lib64
          -lcudart -lcufft
```

Must use PGI-provided CUDA toolkit paths

Must link libcudart and libcufft

Results

```
[harrism@kollman0 cufft-acc]$ ./cufft_acc
Transforming signal cufftExecC2C
Performing point-wise complex multiply and scale.
Transforming signal back cufftExecC2C
Performing Convolution on the host and checking correctness

Signal size: 500000, filter size: 33
Total Device Convolution Time: 11.461152 ms (0.242624 for point-wise convolution)
Test PASSED
```

CUFFT + cudaMemcpy

OpenACC

Summary

- Use deviceptr data clause to pass pre-allocated device data to OpenACC regions and loops
- Use host_data to get device address for pointers inside acc data regions

- The same techniques shown here can be used to share device data between OpenACC loops and
  - Your custom CUDA C/C++/Fortran/etc. device code
  - Any CUDA Library that uses CUDA device pointers

Thank you