Using OpenACC With CUDA Libraries

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3 Ways to Accelerate Applications

Applications

Libraries	OpenACC Directives	Programming Languages
"Drop-in" Acceleration	Easily Accelerate Applications	Maximum Flexibility

CUDA Libraries are interoperable with OpenACC

3 Ways to Accelerate Applications

Applications

Libraries

"Drop-in" Acceleration

OpenACC Directives

Easily Ac

Applications

Programming Languages

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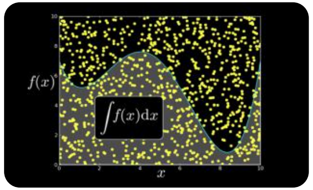
Flexibility

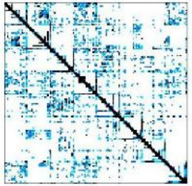
CUDA Languages are interoperable with OpenACC, too!

CUDA Libraries Overview

NVIDIA cuBLAS



NVIDIA cuRAND



NVIDIA cuSPARSE

NVIDIA NPP

GPU VSIPL

Vector Signal
Image Processing

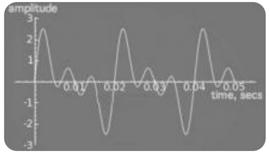
CULA | tools

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

Always more available at NVIDIA Developer site.

How To Use 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
- These same mechanisms are useful for interoperating with custom CUDA C, C++ and 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.

`use_device( 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 highlights follow. Code available with exercises in: `Exercises/Cufft-acc`

Source Excerpt

Allocating Data

```
// Allocate host memory for the signal and filter
Complex *h_signal = (Complex *)malloc(sizeof(Complex) * SIGNAL_SIZE);
Complex *h_filter_kernel = (Complex *)malloc(sizeof(Complex) * FILTER_KERNEL_SIZE);
      .
      .
      .

// Allocate device memory for signal
Complex *d_signal;
checkCudaErrors(cudaMalloc((void **)&d_signal, mem_size));
// Copy host memory to device
checkCudaErrors(cudaMemcpy(d_signal, h_padded_signal, mem_size, cudaMemcpyHostToDevice));

// Allocate device memory for filter kernel
Complex *d_filter_kernel;
checkCudaErrors(cudaMalloc((void **)&d_filter_kernel, mem_size));
```

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Source Excerpt

Sharing Device Data (d_signal, d_filter_kernel)

```
// 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);
```

OpenACC Routine

CUDA Routines

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 = /opt/pgi/13.10.0/linux86-64/2013/cuda/5.0
CCFLAGS = -I$(CUDA_PATH)/include -L$(CUDA_PATH)/lib64
          -lcudart -lcufft
```

Must use
PGI-provided
CUDA toolkit paths

Must link libcudart
and libcufft

Result

```
instr009@nid27635:~/Cufft> aprun -n 1 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: 6.576960 ms (0.186368 for point-wise convolution)
Test PASSED
```

CUFFT + cudaMemcpy

OpenACC

Summary

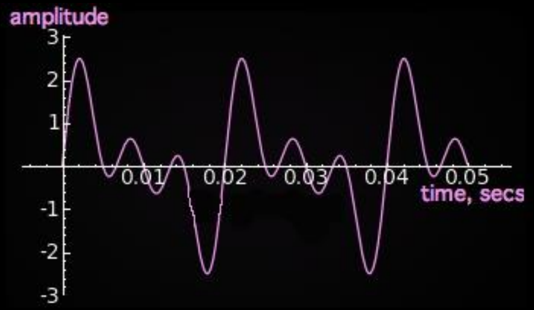
- Use deviceptr data clause to pass pre-allocated device data to OpenACC regions and loops
- Use host_data to get device address for pointers inside acc data regions
- The same techniques shown here can be used to share device data between OpenACC loops and
  - Your custom CUDA C/C++/Fortran/etc. device code
  - Any CUDA Library that uses CUDA device pointers

Appendix

Compelling Cases For Various Libraries Of Possible Interest To You

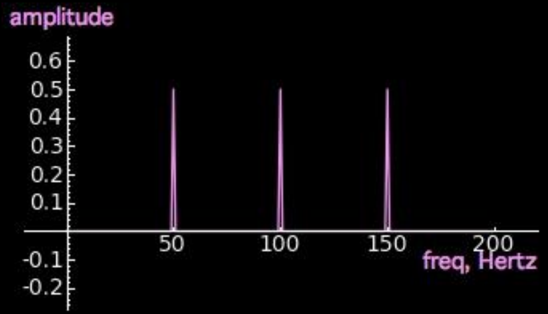
cuFFT: Multi-dimensional FFTs

- 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



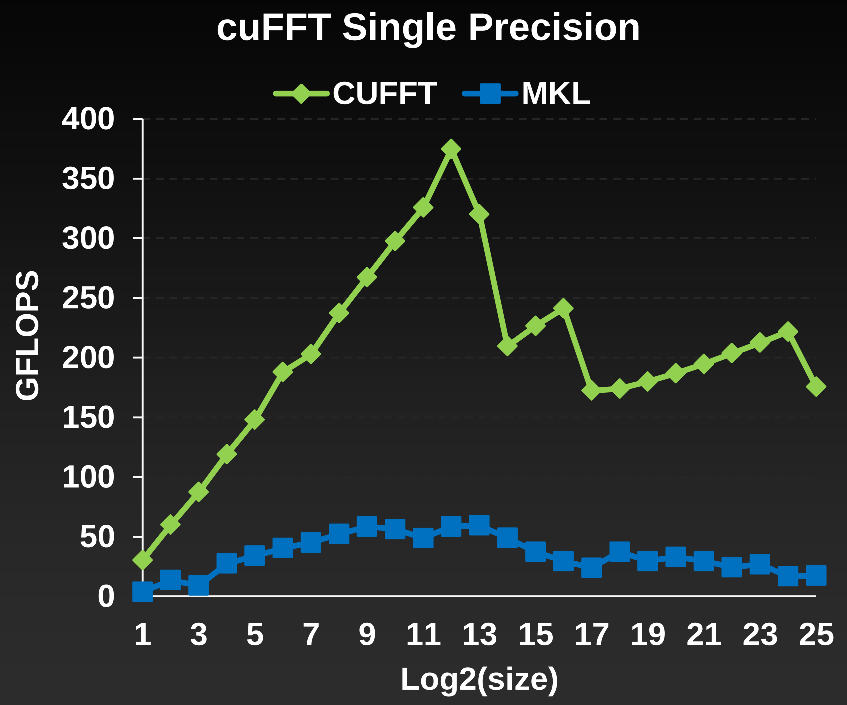
$$F(x) = \sum_{n=0}^{N-1} f(n) e^{-j2\pi(x\frac{n}{N})}$$

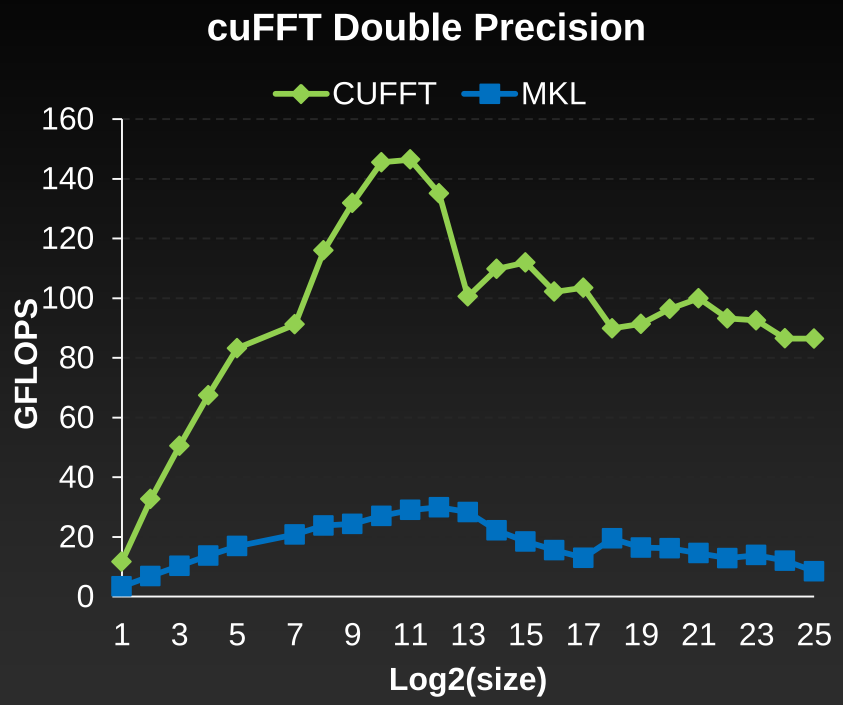
$$f(n) = \frac{1}{N} \sum_{n=0} F(x) e^{j2\pi(x\frac{n}{N})}$$



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

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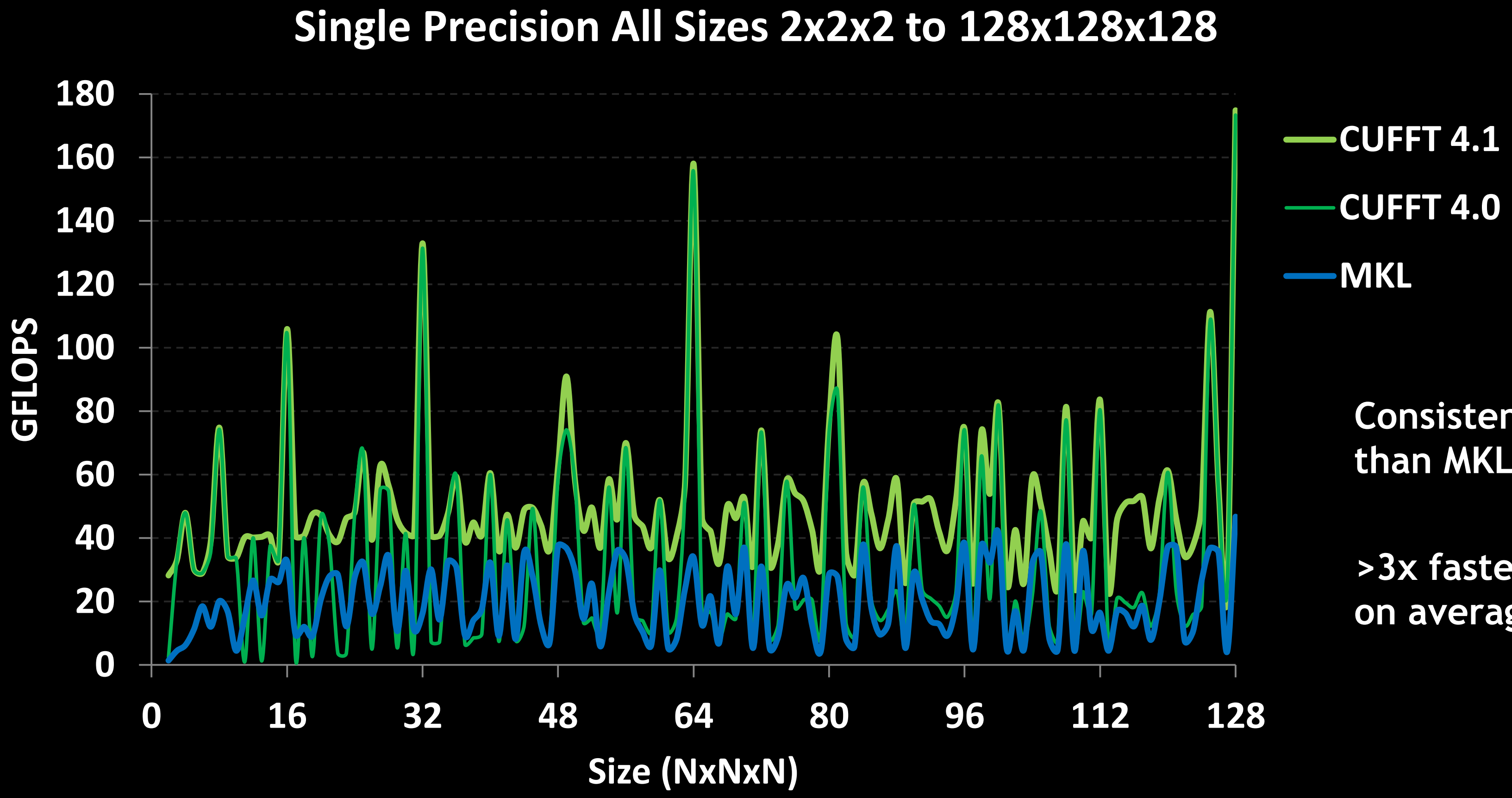
CUDA 4.1 optimizes 3D transforms



Consistently faster than MKL

>3x faster than 4.0 on average

Performance may vary based on OS version and motherboard configuration

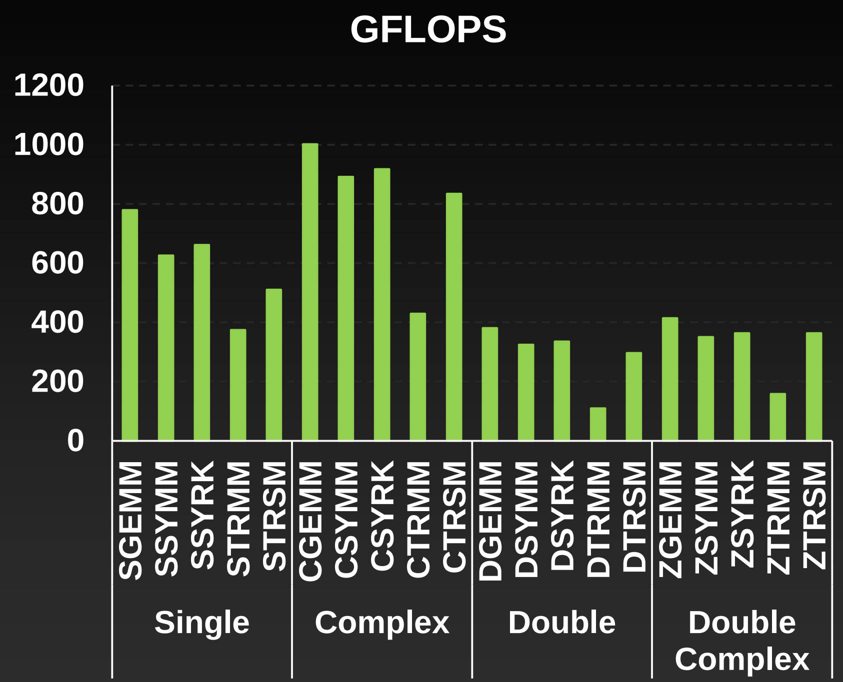
- cuFFT 4.1 on Tesla M2090, ECC on
- MKL 10.2.3, TYAN FT72-B7015 Xeon x5680 Six-Core @ 3.33 GHz

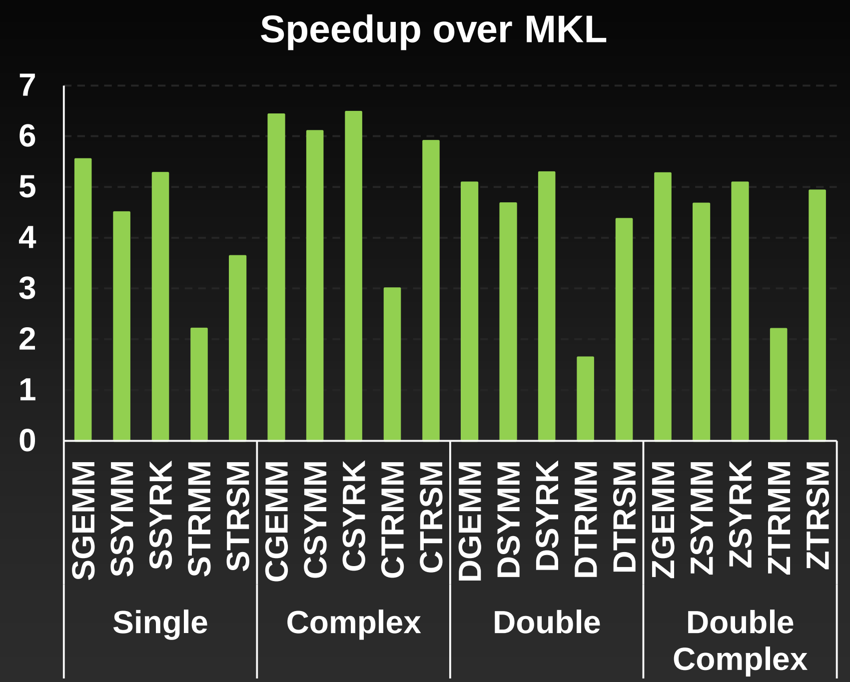
cuBLAS: Dense Linear Algebra on GPUs

- 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

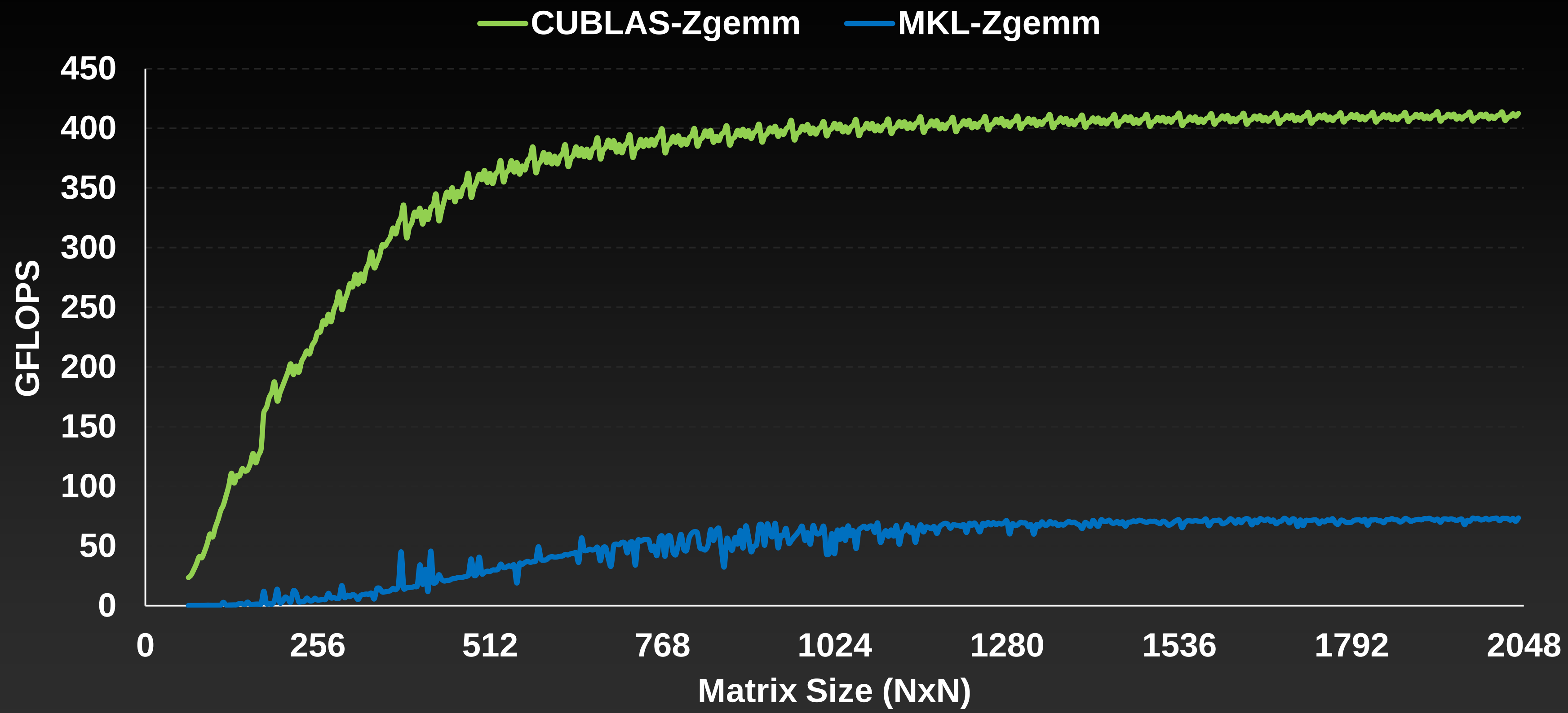




- 4Kx4K matrix size
- cuBLAS 4.1, Tesla M2090 (Fermi), ECC on
- MKL 10.2.3, TYAN FT72-B7015 Xeon x5680 Six-Core @

Performance may vary based on OS version and motherboard configuration

ZGEMM Performance vs Intel MKL



Performance may vary based on OS version and motherboard configuration

- cuBLAS 4.1 on Tesla M2090, ECC on
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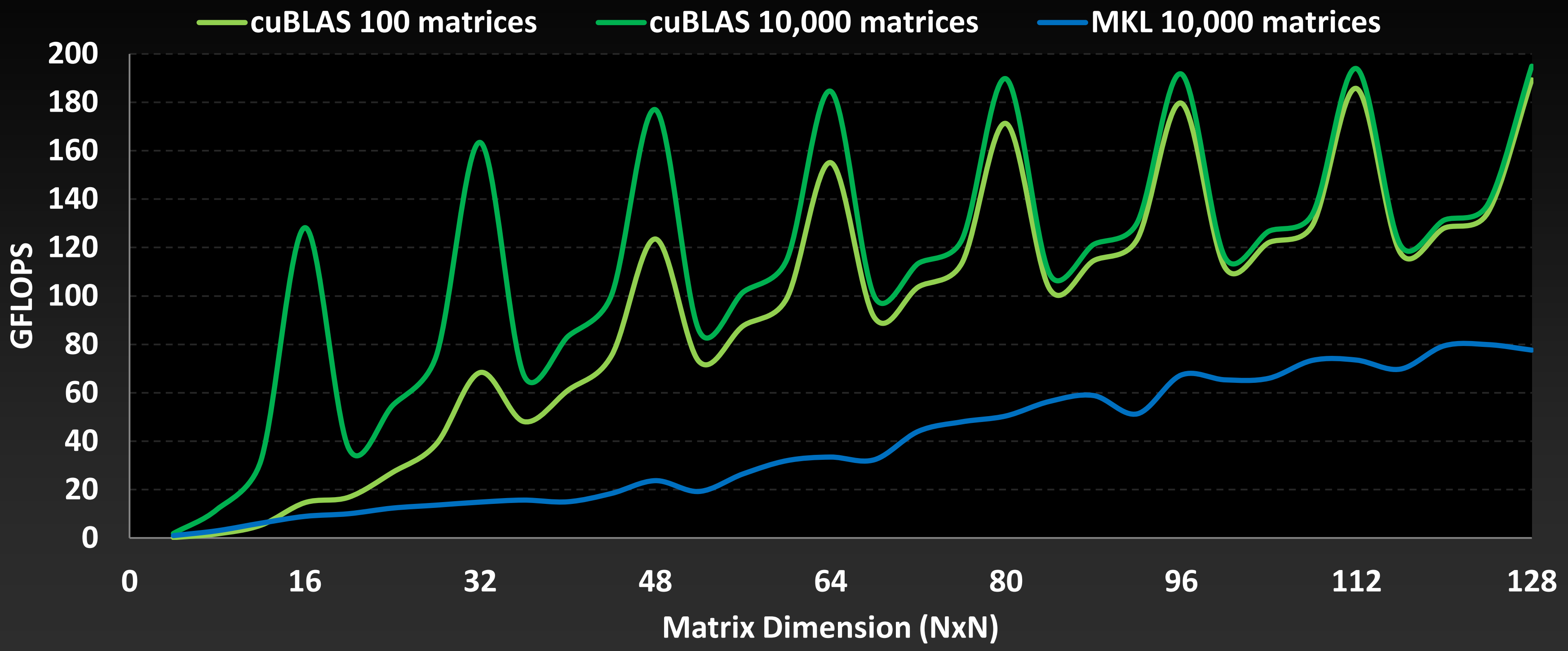
cuBLAS Batched GEMM API improves performance on batches of small matrices



- cuBLAS 4.1 on Tesla M2090, ECC on
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Performance may vary based on OS version and motherboard configuration

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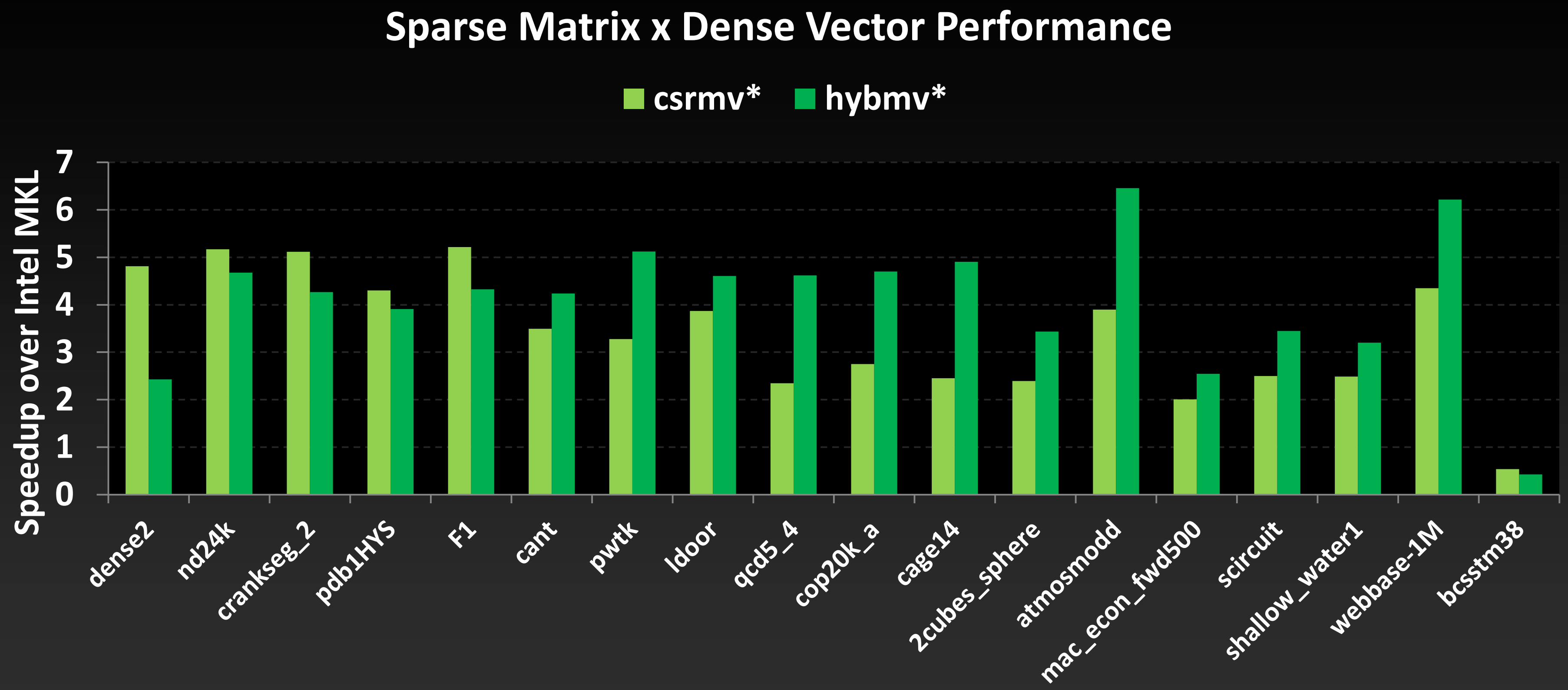
cuSPARSE: Sparse linear algebra routines

- 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

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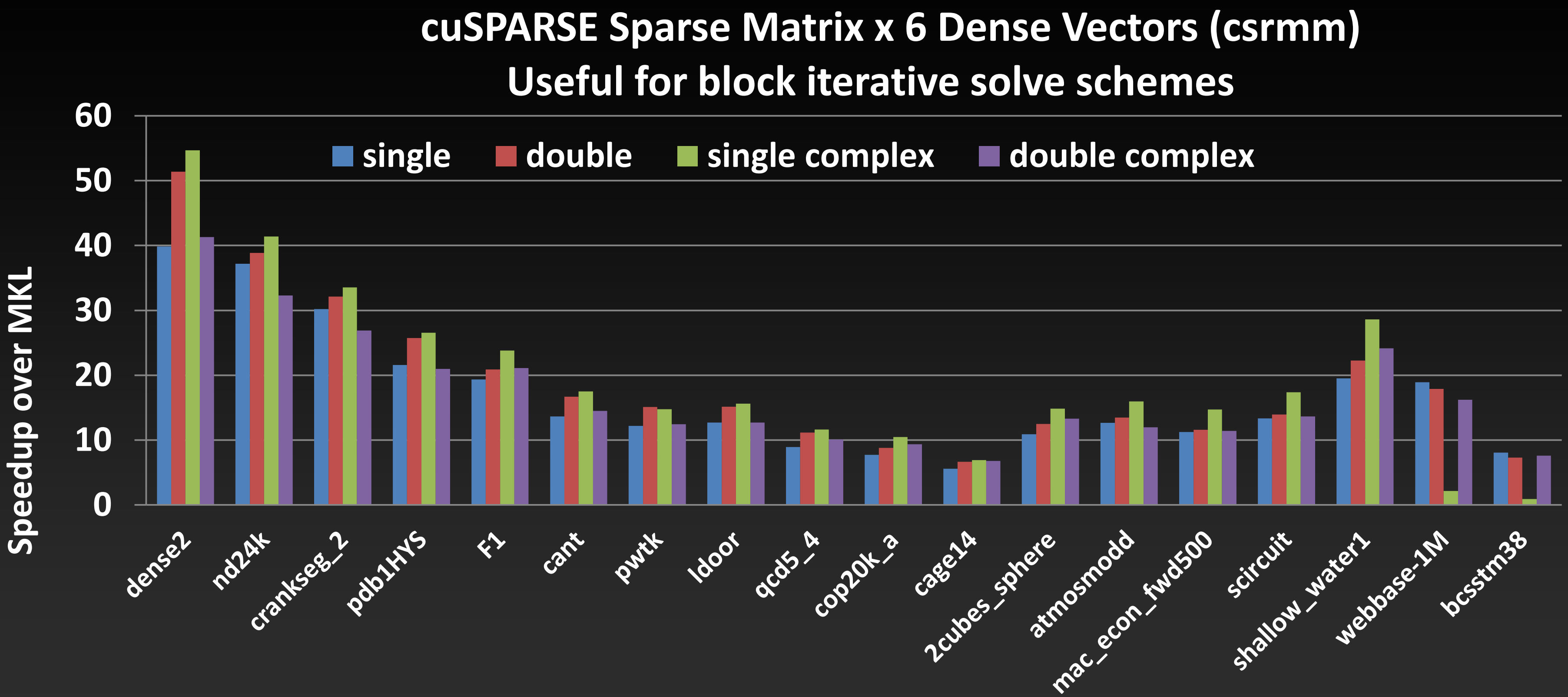
Up to 40x faster with 6 CSR Vectors



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 @

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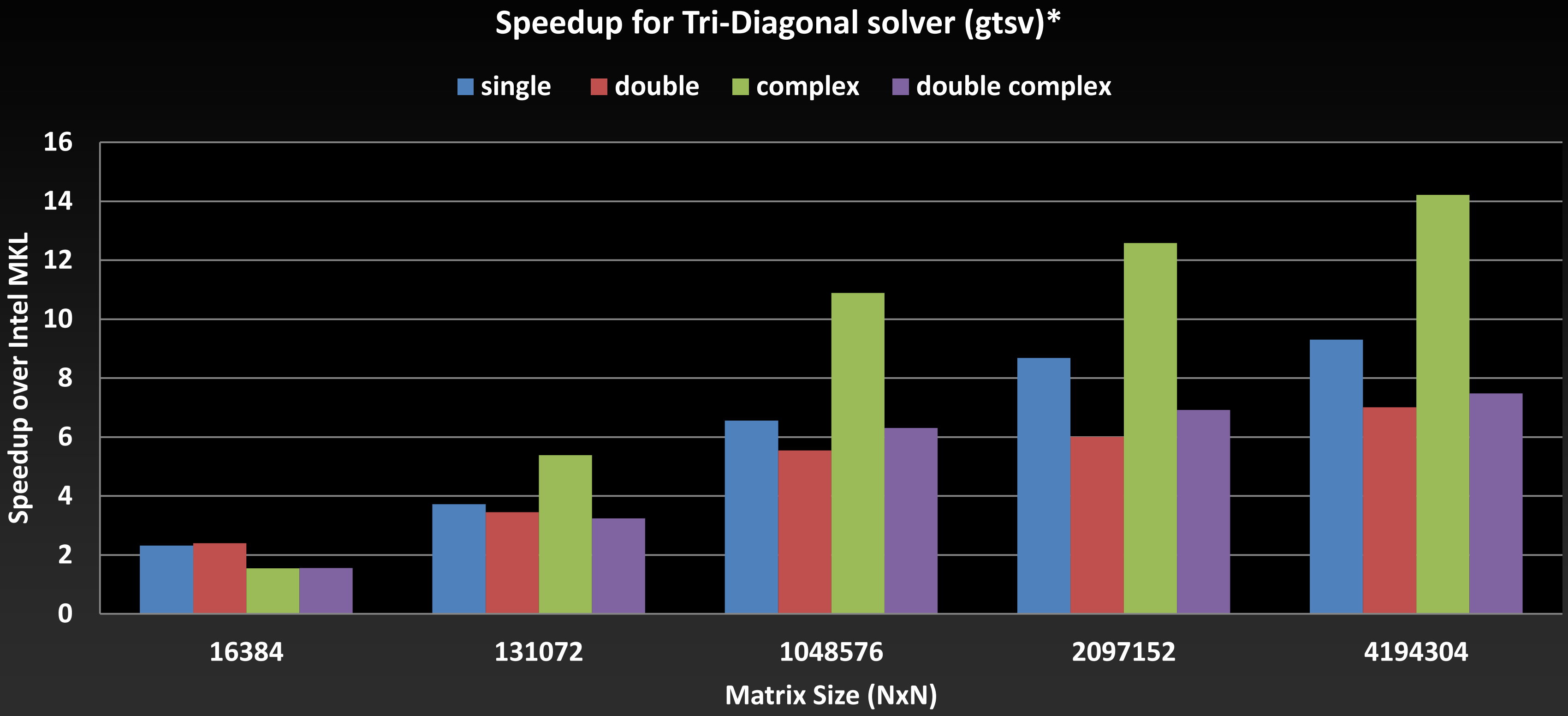
Tri-diagonal solver performance vs. MKL



**Parallel GPU implementation does not include pivoting*

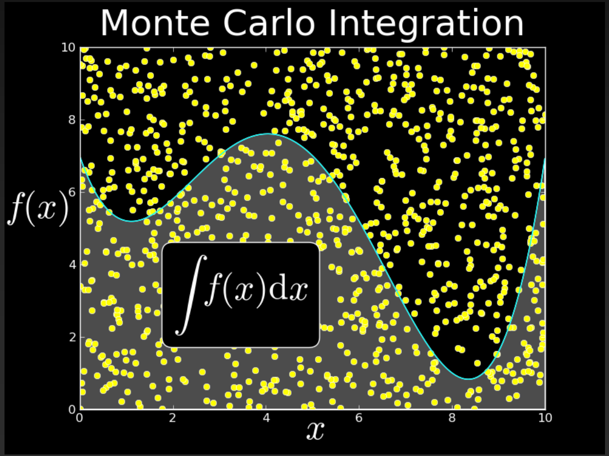
Performance may vary based on OS version and motherboard configuration

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

cuRAND: Random Number Generation

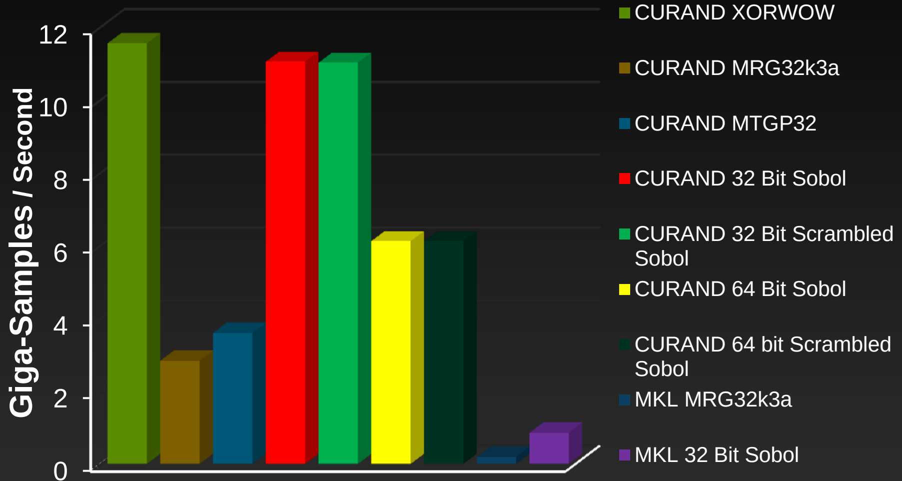
- Pseudo- and Quasi-RNGs
- Supports several output distributions
- Statistical test results reported in documentation

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

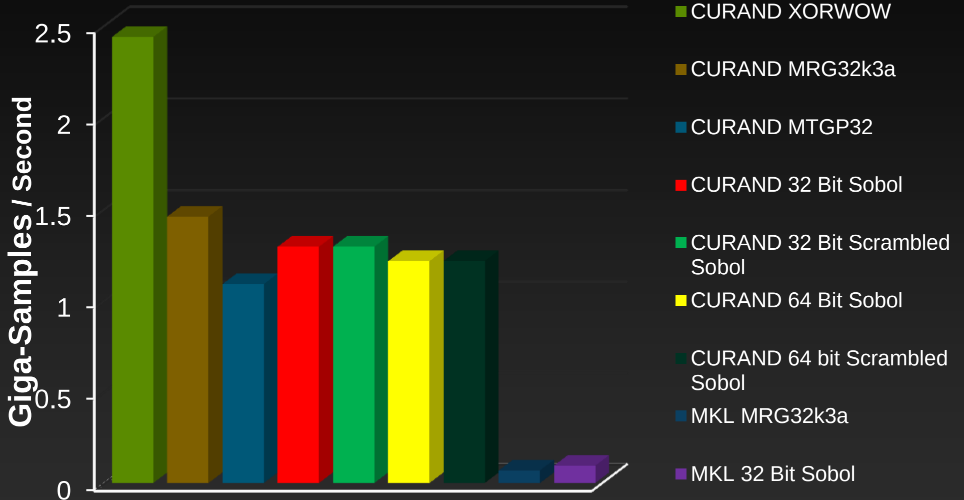


cuRAND Performance compared to Intel MKL

Double Precision Uniform Distribution



Double Precision Normal Distribution



Performance may vary based on OS version and motherboard configuration

- cuRAND 4.1, Tesla M2090 (Fermi), ECC on
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