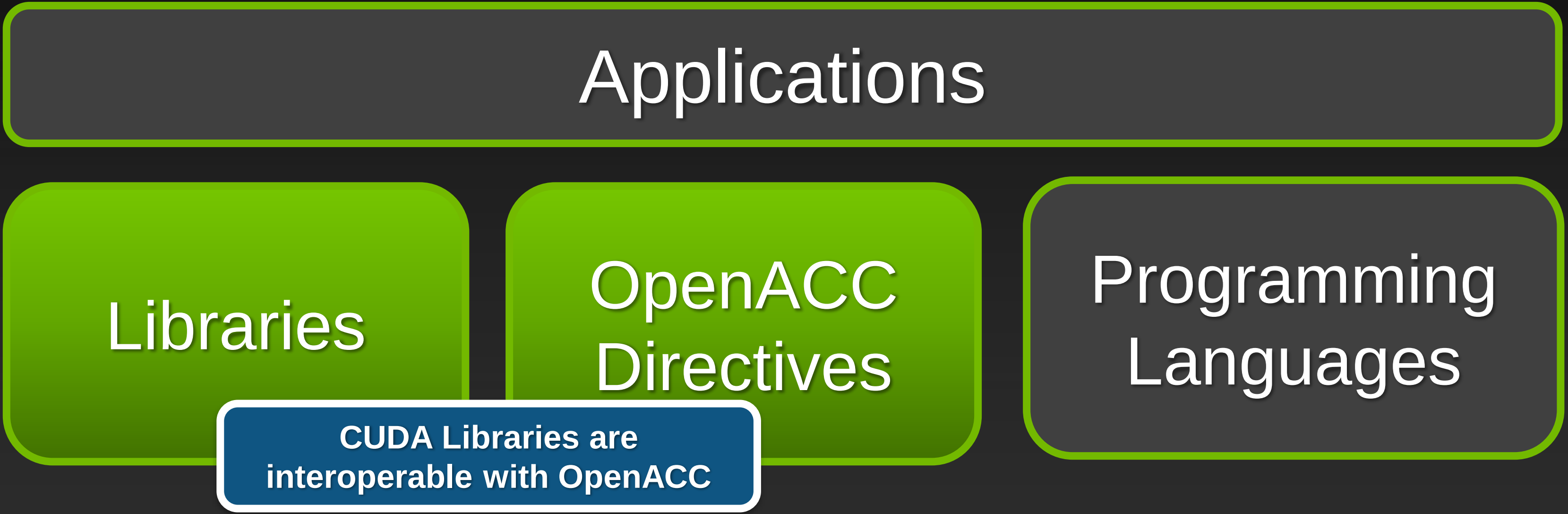
Using OpenACC With CUDA Libraries

John Urbanic
with NVIDIA
Pittsburgh Supercomputing Center

3 Ways to Accelerate Applications



Applications

Libraries

OpenACC Directives

Programming Languages

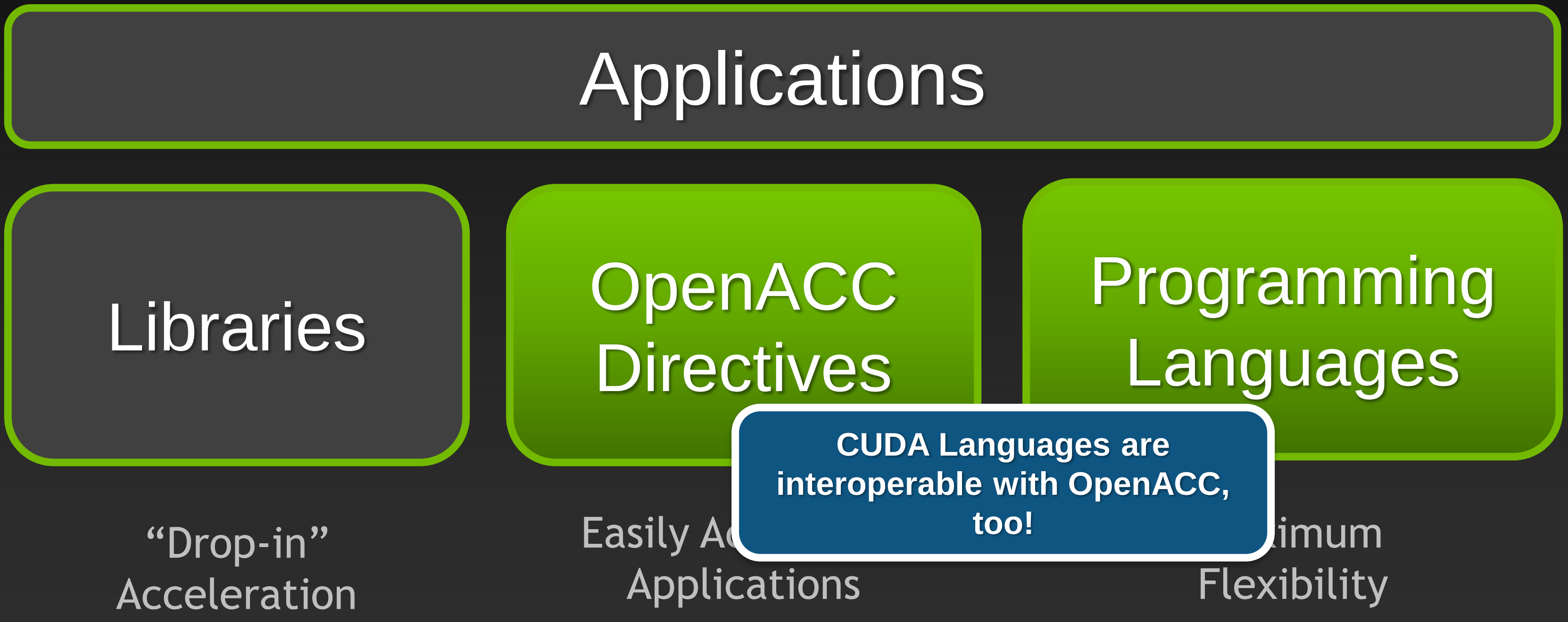
CUDA Libraries are interoperable with OpenACC

"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

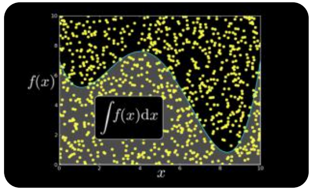
Easily Ac Applications

imum Flexibility

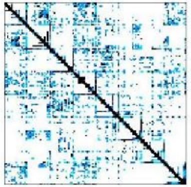
GPU Accelerated Libraries

“Drop-in” Acceleration for Your Applications

NVIDIA cuBLAS



NVIDIA cuRAND

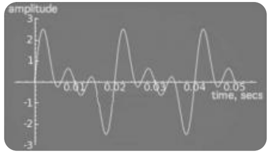

NVIDIA cuSPARSE

NVIDIA NPP

GPU VSIPL
Vector Signal Image Processing

CULA | tools
GPU Accelerated Linear Algebra

MAGMA
ICL UT
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

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

CUDA data in OpenACC

You have to allocate data memory on the host and device with alloc/cudaMalloc. deviceptr() lets OpenACC know that has happened.

```
float *a;
...
err = cudaMalloc(&a, sizeof(float)*n);
kernel<<<n/32,32>>>(a,...);
...
incr(a,n);

void incr(float* x, int n){
  #pragma acc parallel loop deviceptr(x)
  for (int i = 0; i < n; ++i)
    x[i] += 1.0f;
}
```

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

If the data is on the device - say it has been *create()*ed - then host_data use_device() allows us to grab that device pointer on the host so that we can pass it along to some CUDA routine elsewhere.

```
a = (float*)malloc(sizeof(float)*n);
#pragma acc data create(a[0:n])
{
   #pragma acc host_data use_device(a)
   {
      incr(a,n);
   }
}

----- separate file with CUDA code -----
__global__ inckernel(float* x, int n){ ... }

void incr(float* x, int n){
  inckernel<<<n/32,n>>>(x,n);
}
```

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/OpenACC/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));
```

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;
        }
    }
}
```

Implementation note: 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

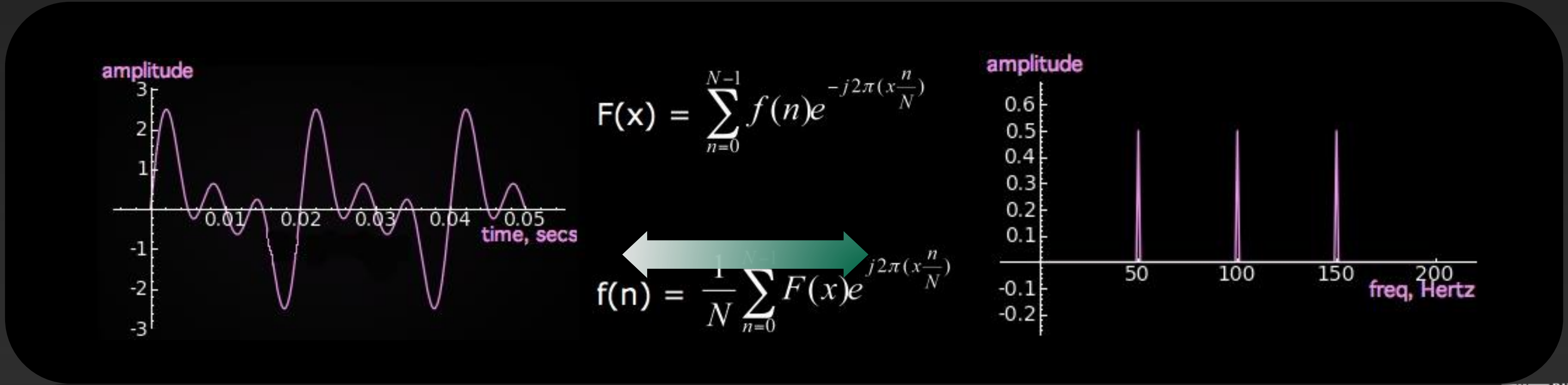
- Use deviceptr data clause to pass pre-allocated device data to OpenACC regions and loops
- Use host_data to get device address for pointers inside acc data regions
- The same techniques shown here can be used to share device data between OpenACC loops and
  - Your custom CUDA C/C++/Fortran/etc. device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

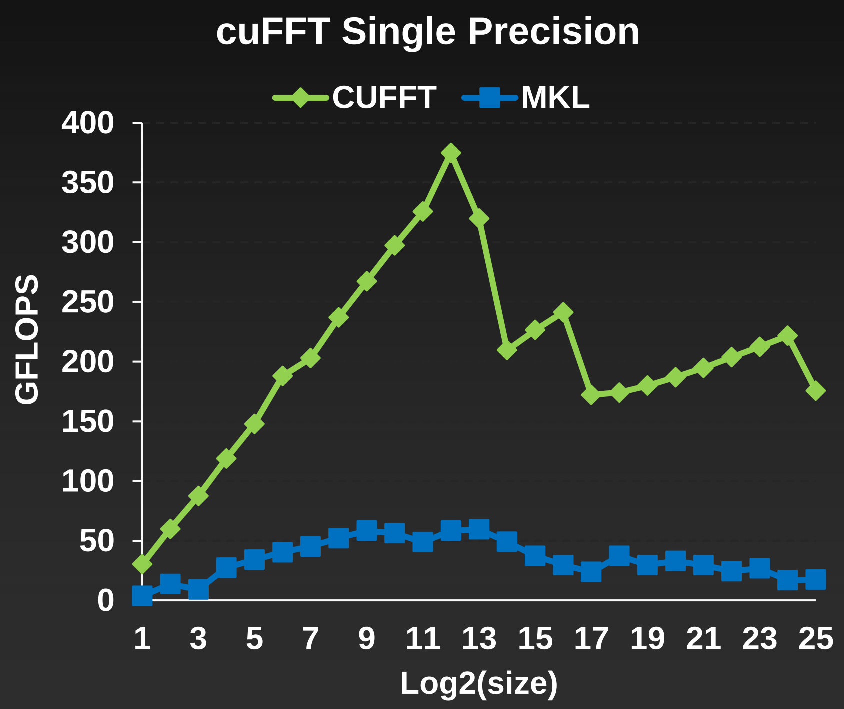


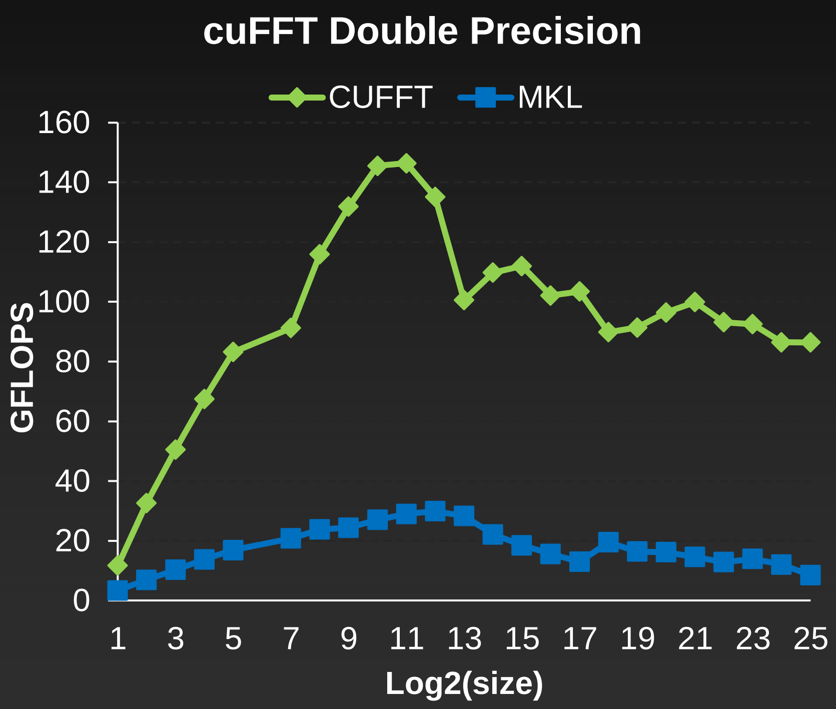
$$F(x) = \sum_{n=0}^{N-1} f(n) e^{-j2\pi(x\frac{n}{N})}$$

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

FFTs up to 10x Faster than MKL

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

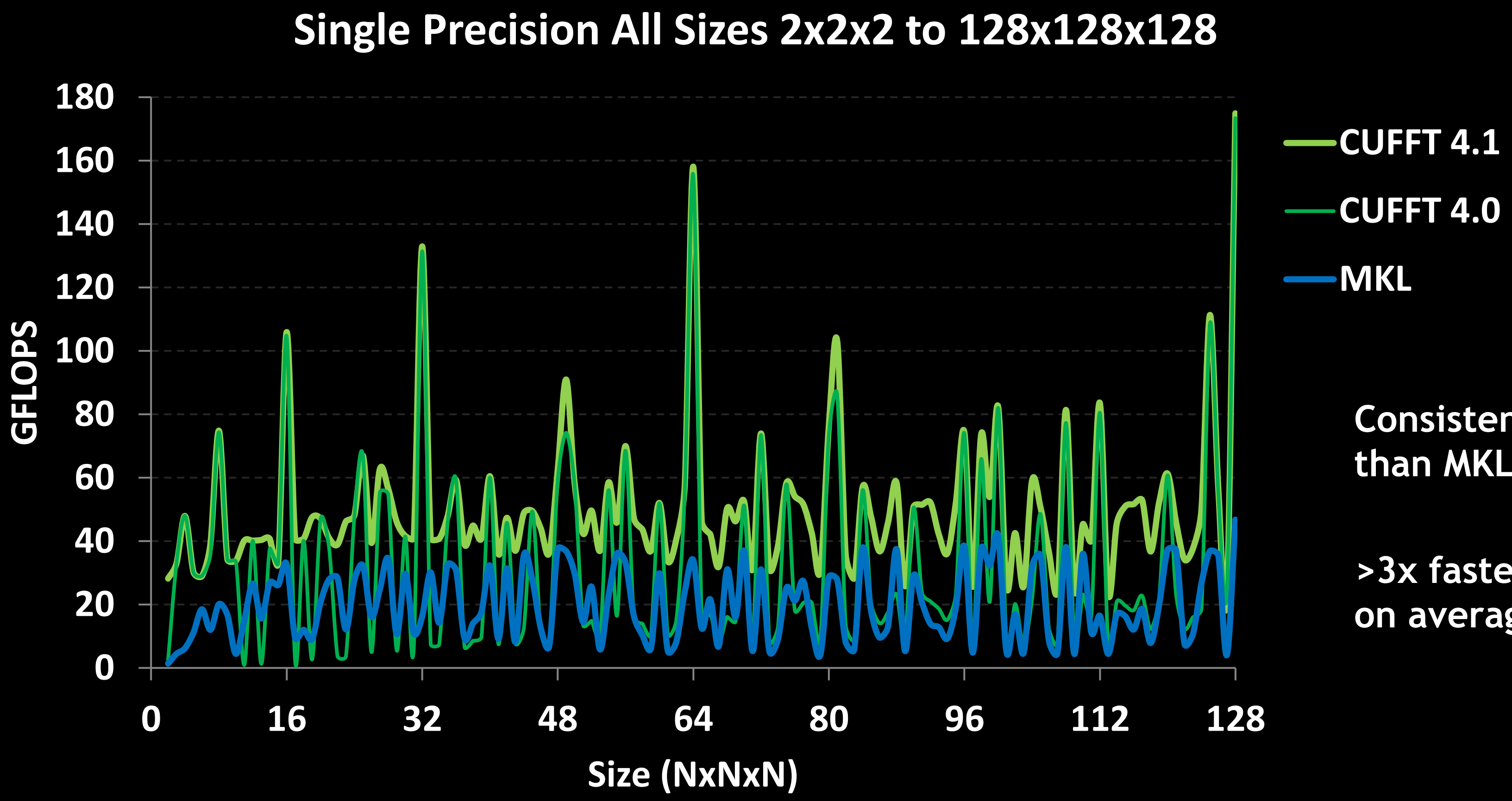




- Measured on sizes that are exactly powers-of-2
- cuFFT 4.1 on Tesla M2090, ECC on
- MKL 10.2.3, TYAN FT72-B7015 Xeon x5680 Six-Core @ 3.33 GHz

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

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

PITTSBURGH SUPERCOMPUTING CENTER

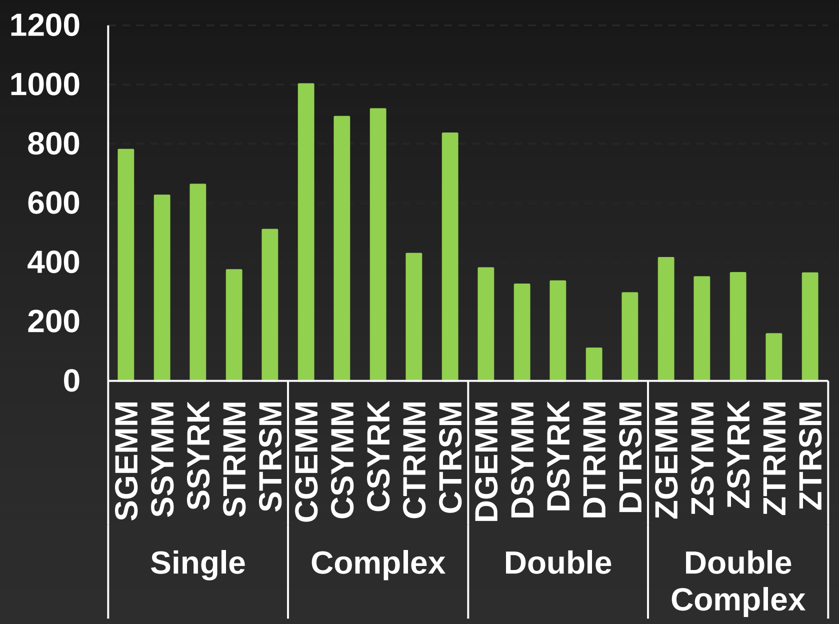
cuBLAS: Dense Linear Algebra on GPUs

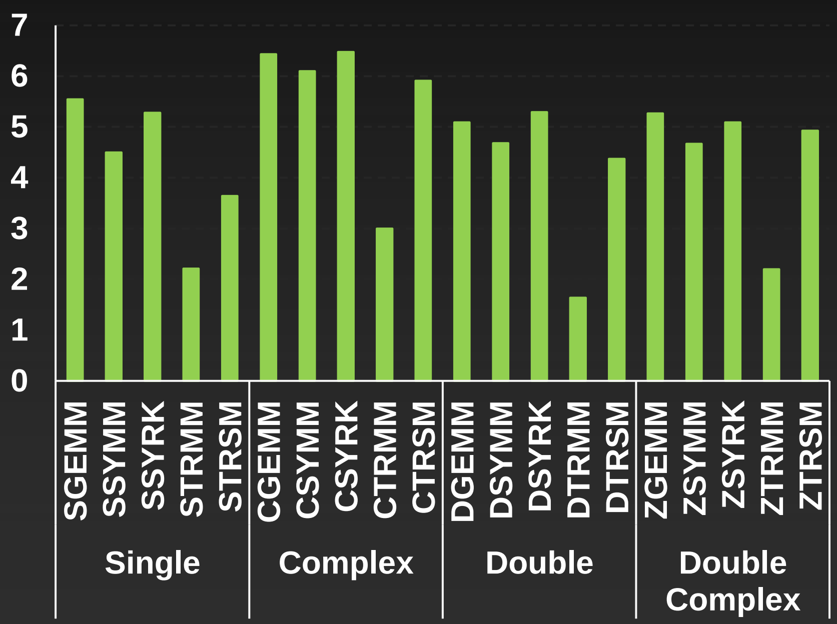
- Complete BLAS implementation plus useful extensions
  - Supports all 152 standard routines for single, double, complex, and double complex

- 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


GFLOPS

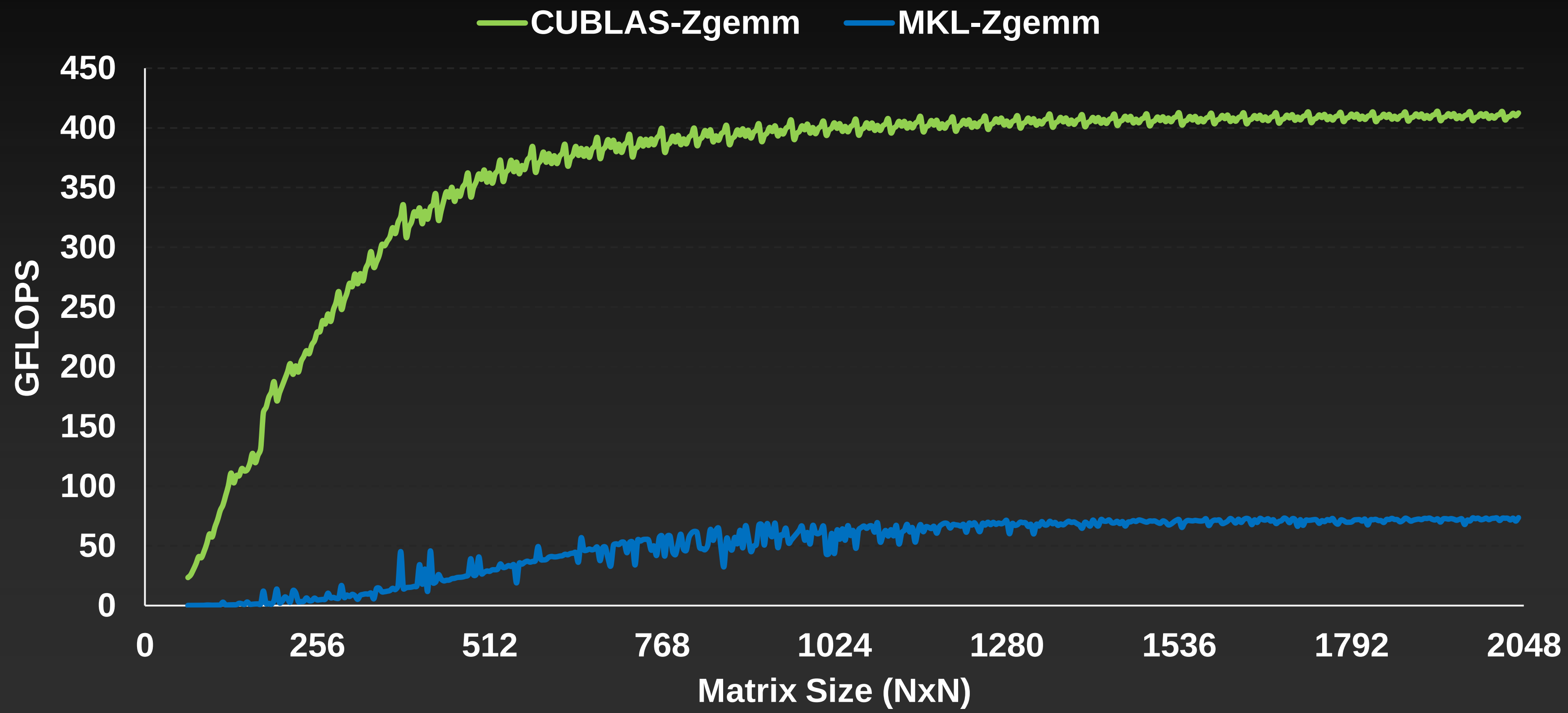

Speedup over MKL

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

PITTSBURGH SUPERCOMPUTING CENTER

Performance may vary based on OS version and motherboard configuration

ZGEMM Performance vs Intel MKL

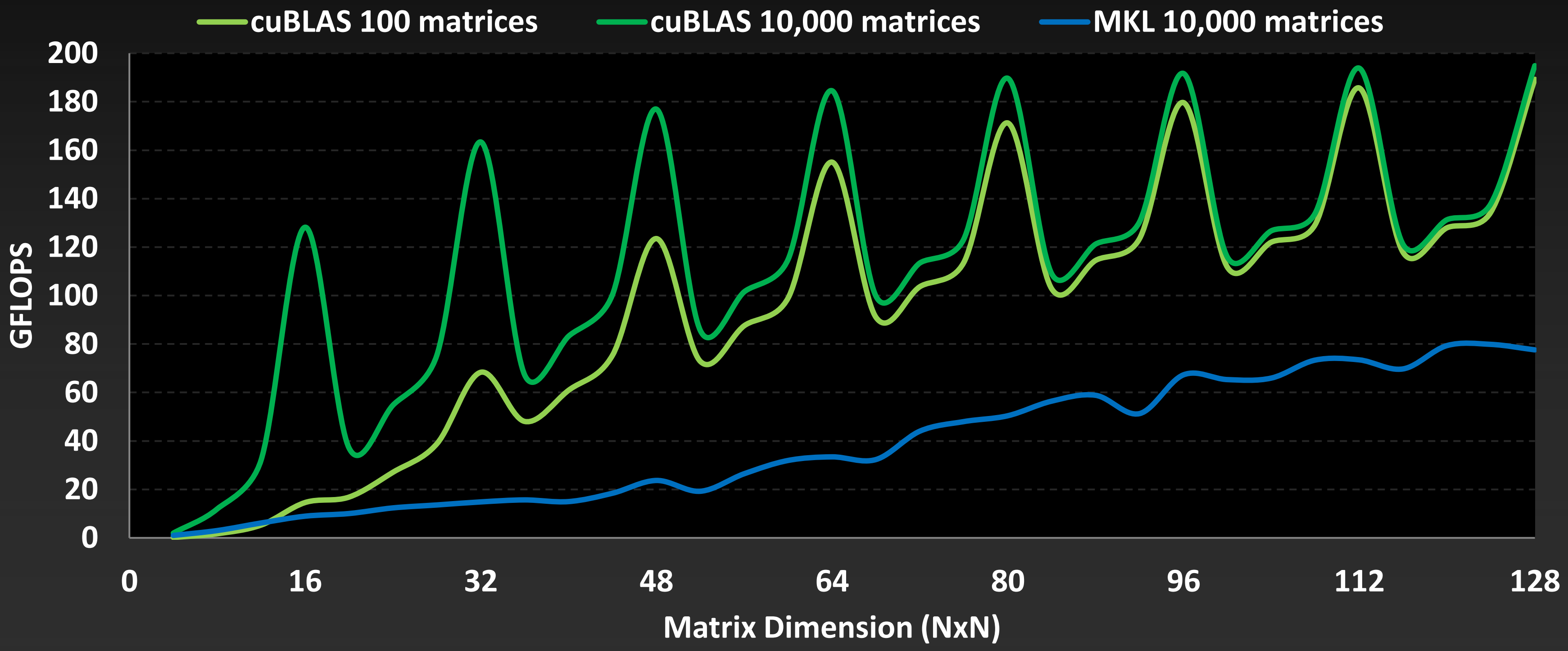


- cuBLAS 4.1 on Tesla M2090, ECC on
- MKL 10.2.3, TYAN FT72-B7015 Xeon x5680 Six-Core @ 3.33 GHz

Performance may vary based on OS version and motherboard configuration

PITTSBURGH SUPERCOMPUTING CENTER

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

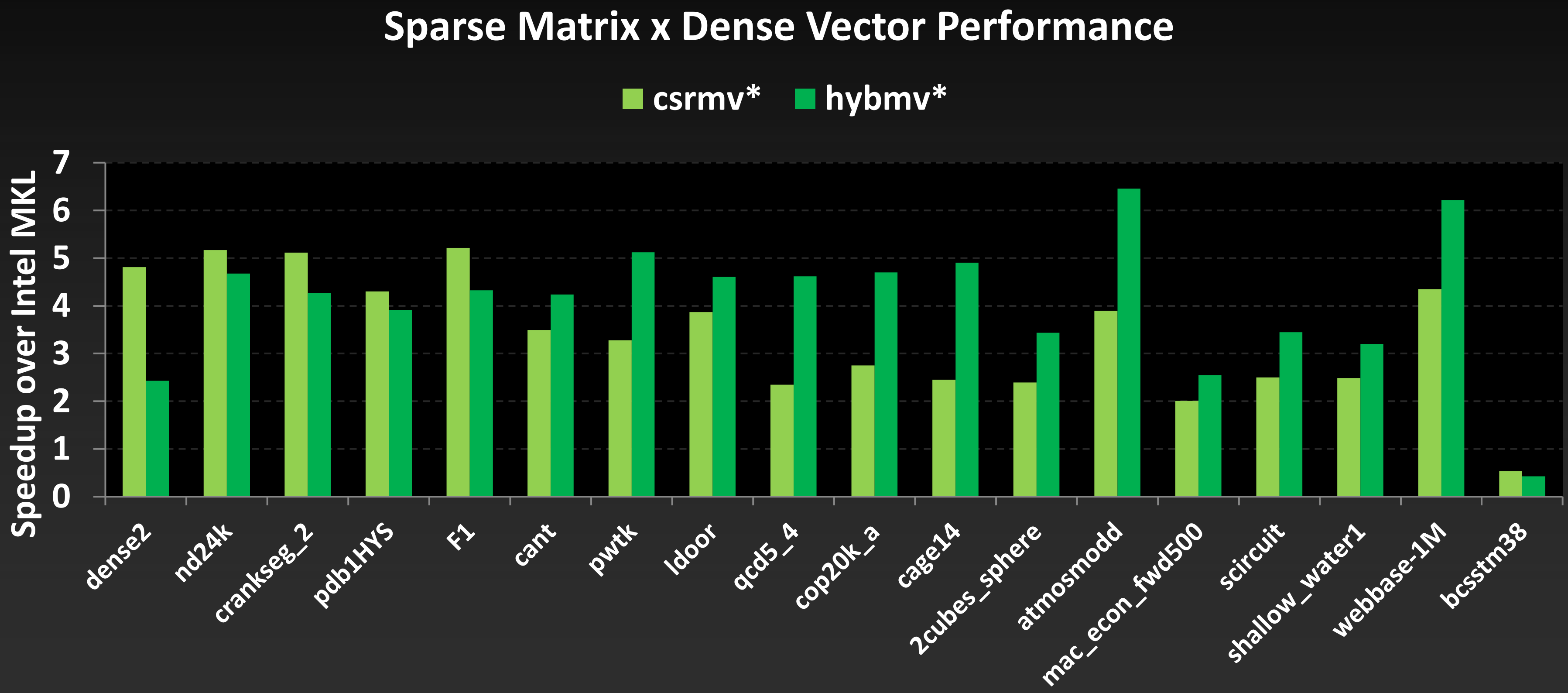
PITTSBURGH SUPERCOMPUTING CENTER

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


Sparse Matrix x Dense Vector Performance

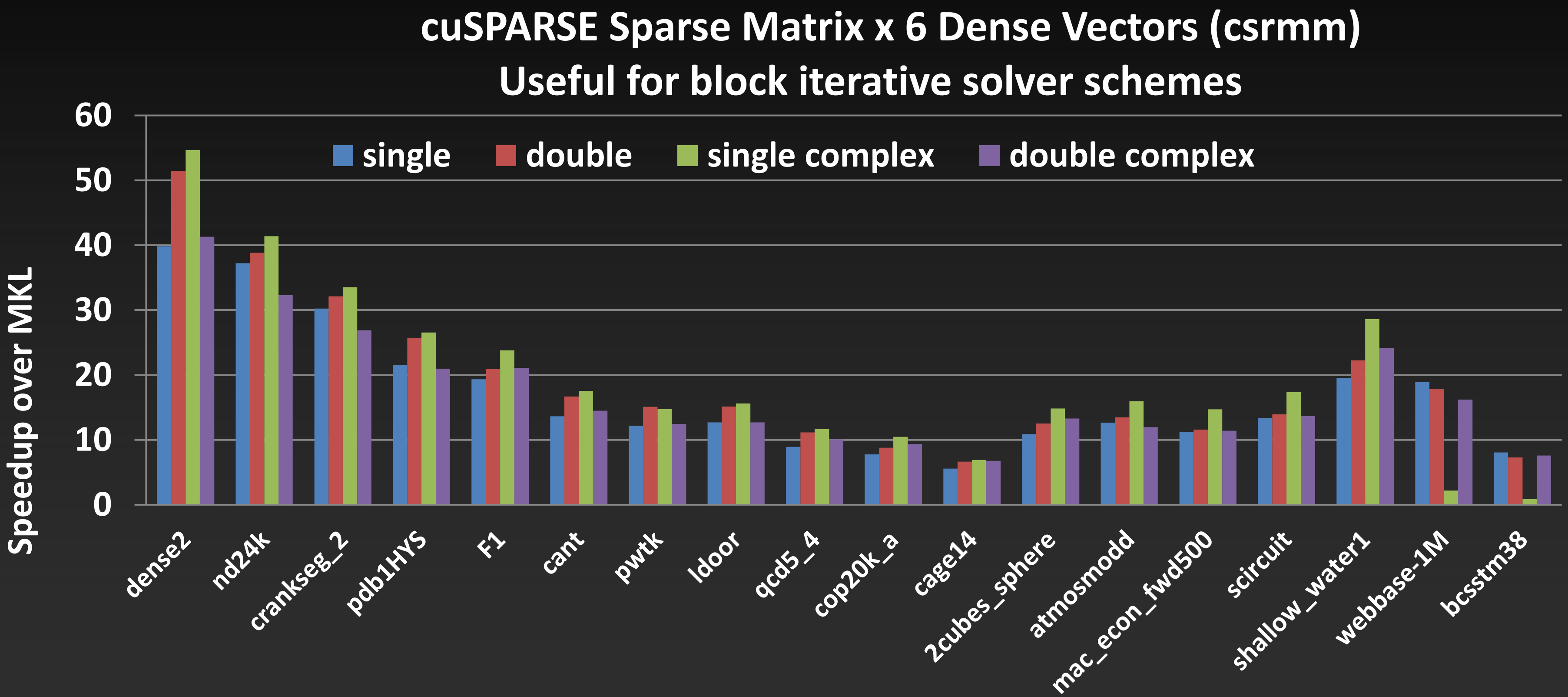
*Average speedup over single, double, single complex & double-complex

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

PITTSBURGH SUPERCOMPUTING CENTER

Up to 40x faster with 6 CSR Vectors



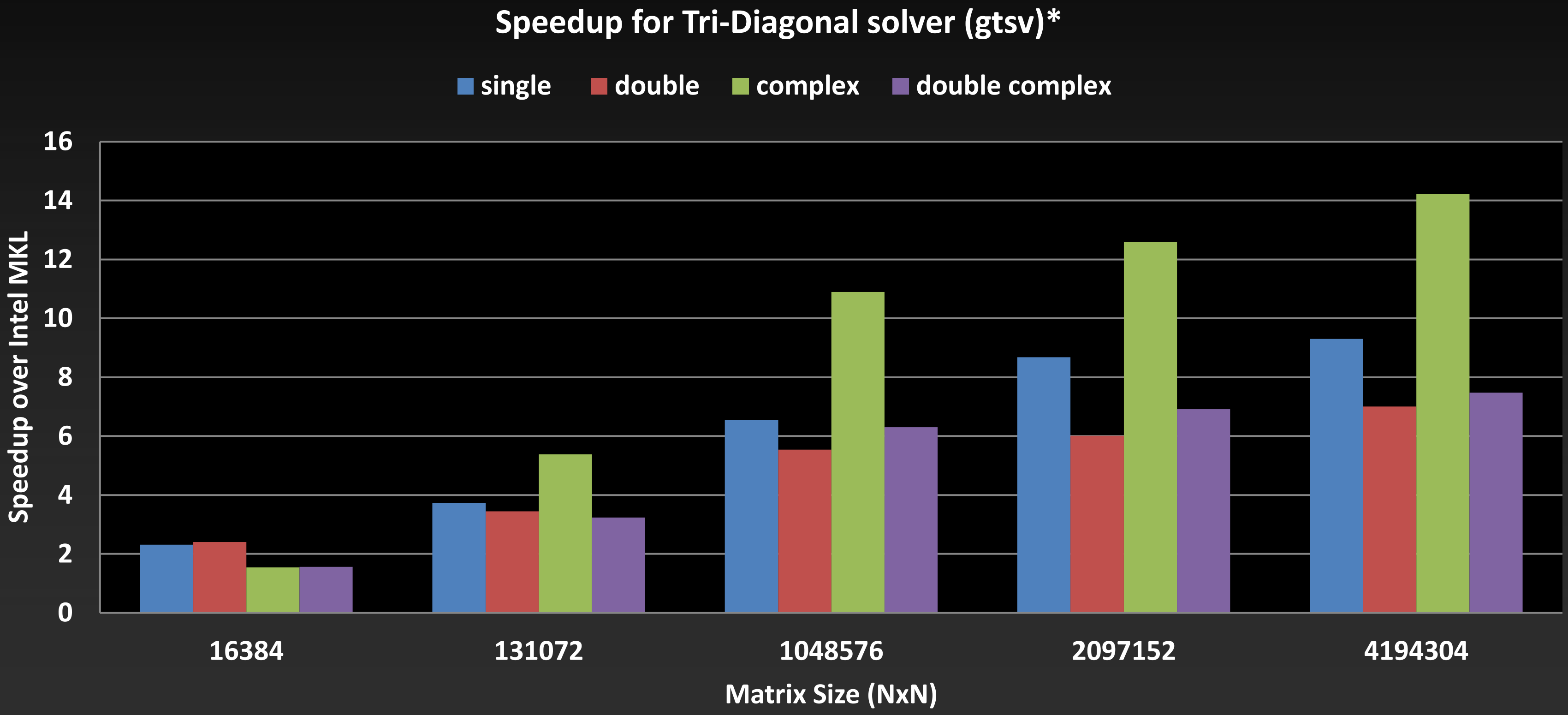
cuSPARSE Sparse Matrix x 6 Dense Vectors (csrmm)
Useful for block iterative solver schemes

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

PITTSBURGH
SUPERCOMPUTING
CENTER

Performance may vary based on OS version and motherboard configuration

Tri-diagonal solver performance vs. MKL



Speedup for Tri-Diagonal solver (gtsv)*

**Parallel GPU implementation does not include pivoting*

Performance may vary based on OS version and motherboard configuration

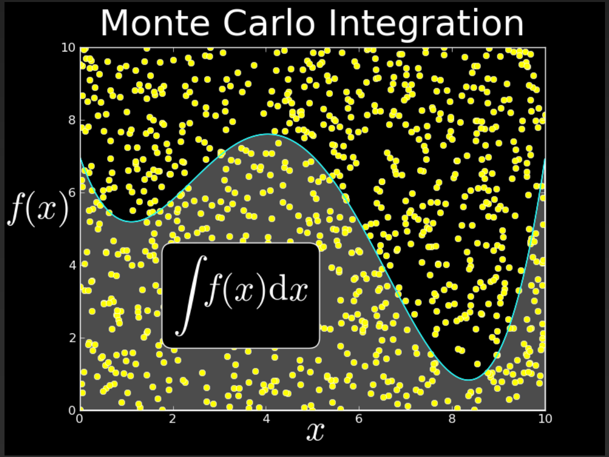
- cuSPARSE 4.1, Tesla M2090 (Fermi), ECC on
- MKL 10.2.3, TYAN FT72-B7015 Xeon x5680 Six-Core @

PITTSBURGH SUPERCOMPUTING CENTER

cuRAND: Random Number Generation

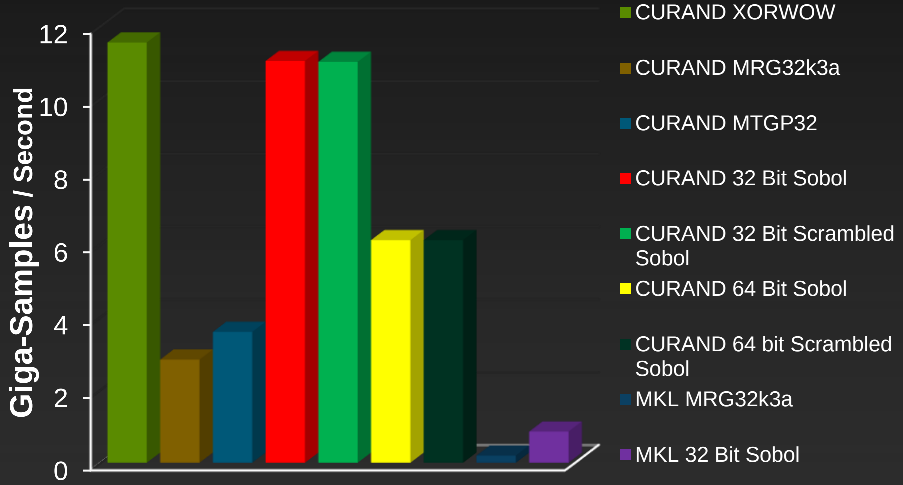
- Pseudo- and Quasi-RNGs
- Supports several output distributions
- Statistical test results reported in documentation

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

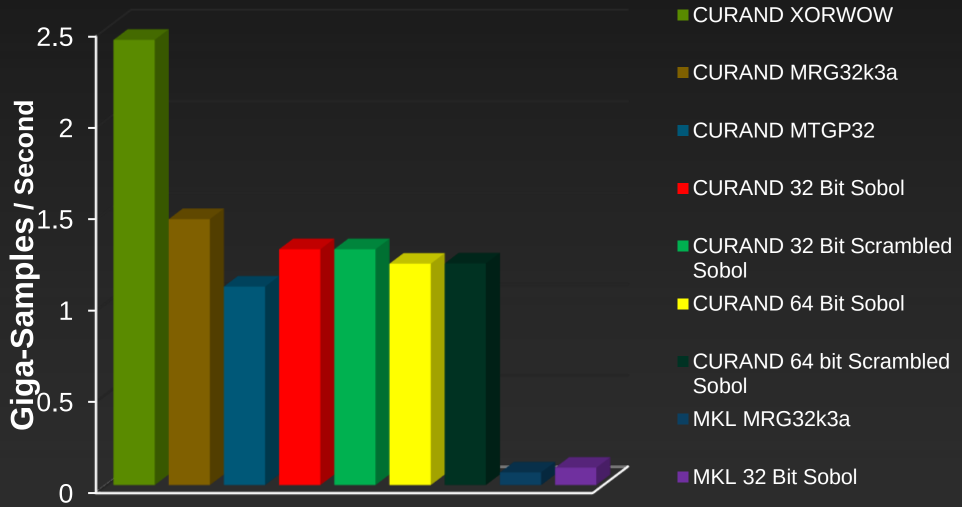


cuRAND Performance compared to Intel MKL

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
- MKL 10.2.3, TYAN FT72-B7015 Xeon x5680 @

PITTSBURGH SUPERCOMPUTING CENTER