



CUDA C BEST PRACTICES GUIDE

DG-05603-001_v4.0 | May 2011

Design Guide



DOCUMENT CHANGE HISTORY

DG-05603-001_v4.0

Version	Date	Authors	Description of Change
3.0	February 4, 2010	CW	See Section C.1
3.1	May 19, 2010	CW	See Section C.2
3.2	August 20, 2010	CW	See Section C.3
4.0	May 9, 2011	CW,NJ,VS	See Section C.4

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PREFACE

WHAT IS THIS DOCUMENT?

This Best Practices Guide is a manual to help developers obtain the best performance from the NVIDIA® CUDA™ architecture using version 4.0 of the CUDA Toolkit. It presents established optimization techniques and explains coding metaphors and idioms that can greatly simplify programming for the CUDA architecture.

While the contents can be used as a reference manual, you should be aware that some topics are revisited in different contexts as various programming and configuration topics are explored. As a result, it is recommended that first-time readers proceed through the guide sequentially. This approach will greatly improve your understanding of effective programming practices and enable you to better use the guide for reference later.

WHO SHOULD READ THIS GUIDE?

This guide is intended for programmers who have a basic familiarity with the CUDA programming environment. You have already downloaded and installed the CUDA Toolkit and have written successful programs using it. The discussions in this guide all use the C programming language, so you should be comfortable reading C.

This guide refers to and relies on several other documents that you should have at your disposal for reference, all of which are available at no cost from the CUDA website http://www.nvidia.com/object/cuda_develop.html. The following documents are especially important resources:

- ▶ CUDA Quickstart Guide
- ▶ CUDA C Programming Guide

- ▶ [CUDA Reference Manual](#)

Be sure to download the correct manual for the CUDA Toolkit version and operating system you are using.

RECOMMENDATIONS AND BEST PRACTICES

Throughout this guide, specific recommendations are made regarding the design and implementation of CUDA C code. These recommendations are categorized by priority, which is a blend of the effect of the recommendation and its scope. Actions that present substantial improvements for most CUDA applications have the highest priority, while small optimizations that affect only very specific situations are given a lower priority.

Before implementing lower priority recommendations, it is good practice to make sure all higher priority recommendations that are relevant have already been applied. This approach will tend to provide the best results for the time invested and will avoid the trap of premature optimization.

The criteria of benefit and scope for establishing priority will vary depending on the nature of the program. In this guide, they represent a typical case. Your code might reflect different priority factors. Regardless of this possibility, it is good practice to verify that no higher-priority recommendations have been overlooked before undertaking lower-priority items.

Appendix A of this document lists all the recommendations and best practices, grouping them by priority and adding some additional helpful observations.

Code samples throughout the guide omit error checking for conciseness. Production code should, however, systematically check the error code returned by each API call and check for failures in kernel launches (or groups of kernel launches in the case of concurrent kernels) by calling `cudaGetLastError()`.

CONTENTS

The remainder of this guide is divided into the following sections:

- ▶ [Parallel Computing with CUDA: Important aspects of the parallel programming architecture.](#)
- ▶ [Performance Metrics: How should performance be measured in CUDA applications and what are the factors that most influence performance?](#)
- ▶ [Memory Optimizations: Correct memory management is one of the most effective means of improving performance. This chapter explores the different kinds of memory available to CUDA applications.](#)

- ▶ Execution Configuration Optimizations: How to make sure your CUDA application is exploiting all the available resources on the GPU.
- ▶ Instruction Optimizations: Certain operations run faster than others. Using faster operations and avoiding slower ones often confers remarkable benefits.
- ▶ Control Flow: Carelessly designed control flow can force parallel code into serial execution; whereas thoughtfully designed control flow can help the hardware perform the maximum amount of work per clock cycle.
- ▶ Getting the Right Answer: How to debug code and how to handle differences in how the CPU and GPU represent floating-point values.

Chapter 1.

PARALLEL COMPUTING WITH CUDA

This chapter reviews heterogeneous computing with CUDA, explains the limits of performance improvement, and helps you choose the right version of CUDA and which application programming interface (API) to use when programming.

1.1 HETEROGENEOUS COMPUTING WITH CUDA

CUDA C programming involves running code on two different platforms concurrently: a *host* system with one or more CPUs and one or more *devices* (frequently graphics adapter cards) with CUDA-enabled NVIDIA GPUs.

While NVIDIA devices are frequently associated with rendering graphics, they are also powerful arithmetic engines capable of running thousands of lightweight threads in parallel. This capability makes them well suited to computations that can leverage parallel execution well.

However, the device is based on a distinctly different design from the host system, and it's important to understand those differences and how they determine the performance of CUDA applications to use CUDA effectively.

1.1.1 Differences Between Host and Device

The primary differences occur in threading and memory access:

- ▶ **Threading resources.** Execution pipelines on host systems can support a limited number of concurrent threads. Servers that have four quad-core processors today can run only 16 threads concurrently (32 if the CPUs support HyperThreading.) By comparison, the *smallest* executable unit of parallelism on a CUDA device comprises

32 threads (a *warp*). All NVIDIA GPUs can support at least 768 concurrently active threads per multiprocessor, and some GPUs support 1,024 or more active threads per multiprocessor (see Section F.1 of the *CUDA C Programming Guide*). On devices that have 30 multiprocessors (such as the NVIDIA® GeForce® GTX 280), this leads to more than 30,000 active threads.

- ▶ **Threads.** Threads on a CPU are generally heavyweight entities. The operating system must swap threads on and off of CPU execution channels to provide multithreading capability. Context switches (when two threads are swapped) are therefore slow and expensive. By comparison, threads on GPUs are extremely lightweight. In a typical system, thousands of threads are queued up for work (in warps of 32 threads each). If the GPU must wait on one warp of threads, it simply begins executing work on another. Because separate registers are allocated to all active threads, no swapping of registers or state need occur between GPU threads. Resources stay allocated to each thread until it completes its execution.
- ▶ **RAM.** Both the host system and the device have RAM. On the host system, RAM is generally equally accessible to all code (within the limitations enforced by the operating system). On the device, RAM is divided virtually and physically into different types, each of which has a special purpose and fulfills different needs. The types of device RAM are explained in the *CUDA C Programming Guide* and in Chapter 3 of this document.

These are the primary hardware differences between CPU hosts and GPU devices with respect to parallel programming. Other differences are discussed as they arise elsewhere in this document.

1.1.2 What Runs on a CUDA-Enabled Device?

Because of the considerable differences between the host and the device, it's important to partition applications so that each hardware system is doing the work it does best. The following issues should be considered when determining what parts of an application to run on the device:

- ▶ The device is ideally suited for computations that can be run on numerous data elements simultaneously in parallel. This typically involves arithmetic on large data sets (such as matrices) where the same operation can be performed across thousands, if not millions, of elements at the same time. This is a requirement for good performance on CUDA: the software must use a large number of threads. The support for running numerous threads in parallel derives from the CUDA architecture's use of a lightweight threading model.
- ▶ There should be some coherence in memory access by device code. Certain memory access patterns enable the hardware to coalesce groups of reads or writes of multiple data items into one operation. Data that cannot be laid out so as to enable coalescing, or that doesn't have enough locality to use textures or L1 efficiently, will not enjoy much of a performance benefit when used in computations on CUDA.

- ▶ To use CUDA, data values must be transferred from the host to the device along the PCI Express (PCIe) bus. These transfers are costly in terms of performance and should be minimized. (See Section 3.1.) This cost has several ramifications:

- The complexity of operations should justify the cost of moving data to and from the device. Code that transfers data for brief use by a small number of threads will see little or no performance benefit. The ideal scenario is one in which many threads perform a substantial amount of work.

For example, transferring two matrices to the device to perform a matrix addition and then transferring the results back to the host will not realize much performance benefit. The issue here is the number of operations performed per data element transferred. For the preceding procedure, assuming matrices of size $N \times N$, there are N^2 operations (additions) and $3N^2$ elements transferred, so the ratio of operations to elements transferred is 1:3 or $O(1)$. Performance benefits can be more readily achieved when this ratio is higher. For example, a matrix multiplication of the same matrices requires N^3 operations (multiply-add), so the ratio of operations to elements transferred is $O(N)$, in which case the larger the matrix the greater the performance benefit. The types of operations are an additional factor, as additions have different complexity profiles than, for example, trigonometric functions. It is important to include the overhead of transferring data to and from the device in determining whether operations should be performed on the host or on the device.

- Data should be kept on the device as long as possible. Because transfers should be minimized, programs that run multiple kernels on the same data should favor leaving the data on the device between kernel calls, rather than transferring intermediate results to the host and then sending them back to the device for subsequent calculations. So, in the previous example, had the two matrices to be added already been on the device as a result of some previous calculation, or if the results of the addition would be used in some subsequent calculation, the matrix addition should be performed locally on the device. This approach should be used even if one of the steps in a sequence of calculations could be performed faster on the host. Even a relatively slow kernel may be advantageous if it avoids one or more PCIe transfers. Section 3.1 provides further details, including the measurements of bandwidth between the host and the device versus within the device proper.

1.1.3 Maximum Performance Benefit



High Priority: To get the maximum benefit from CUDA, focus first on finding ways to parallelize sequential code.

The amount of performance benefit an application will realize by running on CUDA depends entirely on the extent to which it can be parallelized. As mentioned previously, code that cannot be sufficiently parallelized should run on the host, unless doing so would result in excessive transfers between the host and the device.

Amdahl's law specifies the maximum speed-up that can be expected by parallelizing portions of a serial program. Essentially, it states that the maximum speed-up (S) of a program is :

$$S = \frac{1}{(1 - P) + \frac{P}{N}}$$

where P is the fraction of the total serial execution time taken by the portion of code that can be parallelized and N is the number of processors over which the parallel portion of the code runs.

The larger N is (that is, the greater the number of processors), the smaller the P/N fraction. It can be simpler to view N as a very large number, which essentially transforms the equation into $S = 1 / 1 - P$. Now, if $\frac{3}{4}$ of a program is parallelized, the maximum speed-up over serial code is $1 / (1 - \frac{3}{4}) = 4$.

For most purposes, the key point is that the greater P is, the greater the speed-up. An additional caveat is implicit in this equation, which is that if P is a small number (so not substantially parallel), increasing N does little to improve performance. To get the largest lift, best practices suggest spending most effort on increasing P ; that is, by maximizing the amount of code that can be parallelized.

1.2 UNDERSTANDING THE PROGRAMMING ENVIRONMENT

With each generation of NVIDIA processors, new features are added to the GPU that CUDA can leverage. Consequently, it's important to understand the characteristics of the architecture.

Programmers should be aware of two version numbers. The first is the compute capability, and the second is the version number of the CUDA Runtime and CUDA Driver APIs.

1.2.1 CUDA Compute Capability

The *compute capability* describes the features of the hardware and reflects the set of instructions supported by the device as well as other specifications, such as the maximum number of threads per block and the number of registers per multiprocessor. Higher compute capability versions are supersets of lower (that is, earlier) versions, and so they are backward compatible.

The compute capability of the GPU in the device can be queried programmatically as illustrated in the CUDA SDK in the `deviceQuery` sample. The output for that program is shown in Figure 1.1. This information is obtained by calling `cudaGetDeviceProperties()` and accessing the information in the structure it returns.

```

C:\WINDOWS\system32\cmd.exe
There is 1 device supporting CUDA

Device 0: "Quadro FX 570"
Major revision number:          1
Minor revision number:          1
Total amount of global memory:  268107776 bytes
Number of multiprocessors:       16
Number of cores:                 128
Total amount of constant memory: 65536 bytes
Total amount of shared memory per block: 16384 bytes
Total number of registers available per block: 8192
Warp size:                       32
Maximum number of threads per block: 512
Maximum sizes of each dimension of a block: 512 x 512 x 64
Maximum sizes of each dimension of a grid: 65535 x 65535 x 1
Maximum memory pitch:           262144 bytes
Texture alignment:               256 bytes
Clock rate:                       0.41 GHz
Concurrent copy and execution:    Yes

Test PASSED

Press ENTER to exit...

```

Figure 1.1 Sample CUDA Configuration Data Reported by `deviceQuery`

The major and minor revision numbers of the compute capability are shown on the third and fourth lines of Figure 1.1. Device 0 of this system has compute capability 1.1.

More details about the compute capabilities of various GPUs are in Appendices A and F of the *CUDA C Programming Guide*. In particular, developers should note the number of multiprocessors on the device, the number of registers and the amount of memory available, and any special capabilities of the device.

1.2.2 Additional Hardware Data

Certain hardware features are not described by the compute capability. For example, the ability to overlap kernel execution with asynchronous data transfers between the host and the device is available on most but not all GPUs with compute capability 1.1. In such cases, call `cudaGetDeviceProperties()` to determine whether the device is capable of a certain feature. For example, the `deviceOverlap` field of the device property structure

indicates whether overlapping kernel execution and data transfers is possible (displayed in the “Concurrent copy and execution” line of Figure 1.1); likewise, the `canMapHostMemory` field indicates whether zero-copy data transfers can be performed.

1.2.3 CUDA Runtime and CUDA Driver API Version

The CUDA Driver API and the CUDA Runtime are two of the programming interfaces to CUDA. Their version number enables developers to check the features associated with these APIs and decide whether an application requires a newer (later) version than the one currently installed. This is important because the CUDA Driver API is *backward compatible but not forward compatible*, meaning that applications, plug-ins, and libraries (including the CUDA Runtime) compiled against a particular version of the Driver API will continue to work on subsequent (later) driver releases. However, applications, plug-ins, and libraries (including the CUDA Runtime) compiled against a particular version of the Driver API may not work on earlier versions of the driver, as illustrated in Figure 1.2.

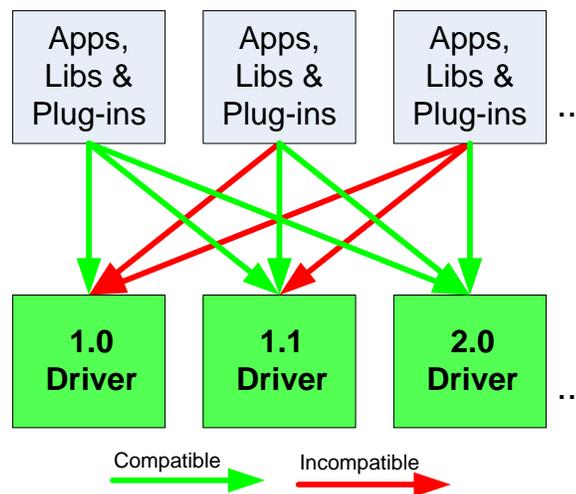


Figure 1.2 Compatibility of CUDA versions

1.2.4 Which Version to Target

When in doubt about the compute capability of the hardware that will be present at runtime, it is best to assume a compute capability of 1.0 as defined in the *CUDA C Programming Guide*, Section F.1.

To target specific versions of NVIDIA hardware and CUDA software, use the `-arch`, `-code`, and `-gencode` options of `nvcc`. Code that contains double-precision arithmetic, for example, must be compiled with “`-arch=sm_13`” (or higher compute capability), otherwise double-precision arithmetic will get demoted to single-precision

arithmetic (see Section 7.2.1). This and other compiler switches are discussed further in Appendix B.

1.3 CUDA APIS

The host runtime component of the CUDA software environment can be used only by host functions. It provides functions to handle the following:

- ▶ Device management
- ▶ Context management
- ▶ Memory management
- ▶ Code module management
- ▶ Execution control
- ▶ Texture reference management
- ▶ Interoperability with OpenGL and Direct3D

It comprises two APIs:

- ▶ A low-level API called the CUDA Driver API
- ▶ A higher-level API called the CUDA Runtime API that is implemented on top of the CUDA Driver API

Since version 3.1 of the CUDA software, these APIs are interoperable; applications can do most operations in the more streamlined CUDA Runtime API while seamlessly interoperating with the lower-level interfaces provided by the CUDA Driver API on an as-needed basis.

Most commonly, applications will use the CUDA Runtime API, which greatly eases device management by providing implicit initialization, context management, and device code module management.

In contrast, while the CUDA Driver API offers more explicit control in certain limited circumstances, it requires more code and is somewhat harder to program. For example, it is more difficult to configure and launch kernels using the CUDA Driver API, since the execution configuration and kernel parameters must be specified with explicit function calls instead of the execution configuration syntax (<<<...>>>).

The C/C++ host code generated by `nvcc` utilizes the CUDA Runtime, so applications that link to this code will depend on the CUDA Runtime; similarly, any code that uses the CUBLAS, CUFFT, and other CUDA Toolkit libraries will also depend on the CUDA Runtime, which is used internally by these libraries.

The two APIs can be easily distinguished: the CUDA Driver API is delivered through the `nvcuda/libcuda` dynamic library and all its entry points are prefixed with `cu`; while

the CUDA Runtime is delivered through the `cuda` dynamic library and all its entry points are prefixed with `cuda`. Note that the APIs relate only to host code; the kernels that are executed on the device are the same, regardless of which API is used.

The functions that make up these two APIs are explained in the *CUDA Reference Manual*.

1.3.1 CUDA Runtime API

The CUDA Runtime handles kernel loading and setting up kernel parameters and launch configuration before the kernel is launched. The implicit code initialization, CUDA context management, CUDA module management (cubin to function mapping), kernel configuration, and parameter passing are all performed by the CUDA Runtime.

It comprises two principal parts:

- ▶ A C-style function interface (`cuda_runtime_api.h`).
- ▶ C++-style convenience wrappers (`cuda_runtime.h`) built on top of the C-style functions.

For more information on the Runtime API, refer to Section 3.2 of the *CUDA C Programming Guide*.

1.3.2 CUDA Driver API

The Driver API is a lower-level API than the Runtime API. The Driver API has these advantages:

- ▶ More control over device contexts
- ▶ No C extensions in the host code, so the host code can be compiled with compilers other than `nvcc` and the host compiler it calls by default

Its primary disadvantages are as follows:

- ▶ Much more verbose code
- ▶ Linking against the CUDA Driver library requires additional application complexity, since the driver may or may not be installed on a given target machine
- ▶ Requires explicit management of device contexts and device code modules

For more information on the Driver API, refer to Section 3.3 of the *CUDA C Programming Guide*.

1.3.3 When to Use Which API

The previous section lists some of the salient differences between the two APIs. A key point is that for every Runtime API function, there is an equivalent Driver API function. The Driver API does include a few functions omitted from the Runtime API, such as

functions for the explicit management of CUDA contexts, but most applications will not need these additional functions (and, when they do, driver/runtime interoperability allows the selective use of these functions on an as-needed basis), so use of the Runtime API for most purposes is generally preferred.

1.3.4 Comparing Code for Different APIs

To illustrate the difference in code between the Runtime and Driver APIs, compare Listings 1.1 and 1.2, which are examples of a vector addition in which two arrays are added.

```
const unsigned int cnBlockSize = 512;
const unsigned int cnBlocks    = 3;
const unsigned int cnDimension = cnBlocks * cnBlockSize;

// create CUDA device & context
cudaSetDevice( 0 );    // pick first device

// allocate host vectors
float * pA = new float[cnDimension];
float * pB = new float[cnDimension];
float * pC = new float[cnDimension];

// initialize host memory
randomInit(pA, cnDimension);
randomInit(pB, cnDimension);

// allocate device memory
float *pDeviceMemA, *pDeviceMemB, *pDeviceMemC;
cudaMalloc(&pDeviceMemA, cnDimension * sizeof(float));
cudaMalloc(&pDeviceMemB, cnDimension * sizeof(float));
cudaMalloc(&pDeviceMemC, cnDimension * sizeof(float));

// copy host vectors to device
cudaMemcpy(pDeviceMemA, pA, cnDimension * sizeof(float),
           cudaMemcpyHostToDevice);
cudaMemcpy(pDeviceMemB, pB, cnDimension * sizeof(float),
           cudaMemcpyHostToDevice);

vectorAdd<<<cnBlocks, cnBlockSize>>> (pDeviceMemA, pDeviceMemB,
                                     pDeviceMemC);

// copy result from device to host
cudaMemcpy ((void *) pC, pDeviceMemC, cnDimension * sizeof(float),
           cudaMemcpyDeviceToHost);

delete[] pA;
delete[] pB;
```

```
delete[] pC;

cudaFree(pDeviceMemA);
cudaFree(pDeviceMemB);
cudaFree(pDeviceMemC);
```

Listing 1.1 Host code for adding two vectors using the CUDA Runtime

Listing 1.1 consists of 27 lines of code. Listing 1.2 shows the same functionality implemented using the CUDA Driver API.

```
const unsigned int cnBlockSize = 512;
const unsigned int cnBlocks    = 3;
const unsigned int cnDimension = cnBlocks * cnBlockSize;

CUdevice    hDevice;
CUcontext   hContext;
CUmodule    hModule;
CUfunction  hFunction;

// create CUDA device & context
cuInit(0);
cuDeviceGet(&hContext, 0); // pick first device
cuCtxCreate(&hContext, 0, hDevice);

cuModuleLoad(&hModule, "vectorAdd.cubin");
cuModuleGetFunction(&hFunction, hModule, "vectorAdd");

// allocate host vectors
float * pA = new float[cnDimension];
float * pB = new float[cnDimension];
float * pC = new float[cnDimension];

// initialize host memory
randomInit(pA, cnDimension);
randomInit(pB, cnDimension);

// allocate memory on the device
CUdeviceptr pDeviceMemA, pDeviceMemB, pDeviceMemC;
cuMemAlloc(&pDeviceMemA, cnDimension * sizeof(float));
cuMemAlloc(&pDeviceMemB, cnDimension * sizeof(float));
cuMemAlloc(&pDeviceMemC, cnDimension * sizeof(float));

// copy host vectors to device
cuMemcpyHtoD(pDeviceMemA, pA, cnDimension * sizeof(float));
cuMemcpyHtoD(pDeviceMemB, pB, cnDimension * sizeof(float));

// set up parameter values
cuFuncSetBlockShape(cuFunction, cnBlockSize, 1, 1);
#define ALIGN_UP(offset, alignment) \
```

```

        (offset) = ((offset) + (alignment) - 1) & ~((alignment) - 1)
int offset = 0;
ALIGN_UP(offset, __alignof(pDeviceMemA));
cuParamSetv(cuFunction, offset, &ptr, sizeof(pDeviceMemA));
offset += sizeof(pDeviceMemA);
ALIGN_UP(offset, __alignof(pDeviceMemB));
cuParamSetv(cuFunction, offset, &ptr, sizeof(pDeviceMemB));
offset += sizeof(pDeviceMemB);
ALIGN_UP(offset, __alignof(pDeviceMemC));
cuParamSetv(cuFunction, offset, &ptr, sizeof(pDeviceMemC));
offset += sizeof(pDeviceMemC);
cuParamSetSize(cuFunction, offset);

// execute kernel
cuLaunchGrid(cuFunction, cnBlocks, 1);

// copy the result from device back to host
cuMemcpyDtoH((void *) pC, pDeviceMemC,
             cnDimension * sizeof(float));

delete[] pA;
delete[] pB;
delete[] pC;

cuMemFree(pDeviceMemA);
cuMemFree(pDeviceMemB);
cuMemFree(pDeviceMemC);

```

Listing 1.2 Host code for adding two vectors using the CUDA Driver API

Listing 1.2 contains 50 lines of code and performs several lower-level operations than the Runtime API. These additional calls are evident in several places, especially the setup necessary in the Driver API prior to the kernel launch.

Chapter 2.

PERFORMANCE METRICS

When attempting to optimize CUDA code, it pays to know how to measure performance accurately and to understand the role that bandwidth plays in performance measurement. This chapter discusses how to correctly measure performance using CPU timers and CUDA events. It then explores how bandwidth affects performance metrics and how to mitigate some of the challenges it poses.

2.1 TIMING

CUDA calls and kernel executions can be timed using either CPU or GPU timers. This section examines the functionality, advantages, and pitfalls of both approaches.

2.1.1 Using CPU Timers

Any CPU timer can be used to measure the elapsed time of a CUDA call or kernel execution. The details of various CPU timing approaches are outside the scope of this document, but developers should always be aware of the resolution their timing calls provide.

When using CPU timers, it is critical to remember that many CUDA API functions are asynchronous; that is, they return control back to the calling CPU thread prior to completing their work. All kernel launches are asynchronous, as are memory-copy functions with the `ASYNC` suffix on their names. Therefore, to accurately measure the elapsed time for a particular call or sequence of CUDA calls, it is necessary to synchronize the CPU thread with the GPU by calling `cudaThreadSynchronize()` immediately before starting and stopping the CPU timer.

`cudaThreadSynchronize()` blocks the calling CPU thread until all CUDA calls previously issued by the thread are completed.

Although it is also possible to synchronize the CPU thread with a particular stream or event on the GPU, these synchronization functions are not suitable for timing code in streams other than the default stream. `cudaStreamSynchronize()` blocks the CPU thread until all CUDA calls previously issued into the given stream have completed.

`cudaEventSynchronize()` blocks until a given event in a particular stream has been recorded by the GPU. Because the driver may interleave execution of CUDA calls from other non-default streams, calls in other streams may be included in the timing.

Because the default stream, stream 0, exhibits synchronous behavior (an operation in the default stream can begin only after all preceding calls in any stream have completed; and no subsequent operation in any stream can begin until it finishes), these functions can be used reliably for timing in the default stream.

Be aware that CPU-to-GPU synchronization points such as those mentioned in this section imply a stall in the GPU's processing pipeline and should thus be used sparingly to minimize their performance impact.

2.1.2 Using CUDA GPU Timers

The CUDA event API provides calls that create and destroy events, record events (via timestamp), and convert timestamp differences into a floating-point value in milliseconds. Listing 2.1 illustrates their use.

```
cudaEvent_t start, stop;
float time;

cudaEventCreate(&start);
cudaEventCreate(&stop);

cudaEventRecord( start, 0 );
kernel<<<grid,threads>>> ( d_odata, d_idata, size_x, size_y,
                          NUM_REPS );
cudaEventRecord( stop, 0 );
cudaEventSynchronize( stop );

cudaEventElapsedTime( &time, start, stop );
cudaEventDestroy( start );
cudaEventDestroy( stop );
```

Listing 2.1 How to time code using CUDA events

Here `cudaEventRecord()` is used to place the `start` and `stop` events into the default stream, stream 0. The device will record a timestamp for the event when it reaches that event in the stream. The `cudaEventElapsedTime()` function returns the time elapsed between the recording of the `start` and `stop` events. This value is expressed in

milliseconds and has a resolution of approximately half a microsecond. Like the other calls in this listing, their specific operation, parameters, and return values are described in the *CUDA Reference Manual*. Note that the timings are measured on the GPU clock, so the timing resolution is operating-system-independent.

2.2 BANDWIDTH

Bandwidth—the rate at which data can be transferred—is one of the most important gating factors for performance. Almost all changes to code should be made in the context of how they affect bandwidth. As described in Chapter 3 of this guide, bandwidth can be dramatically affected by the choice of memory in which data is stored, how the data is laid out and the order in which it is accessed, as well as other factors.

To measure performance accurately, it is useful to calculate theoretical and effective bandwidth. When the latter is much lower than the former, design or implementation details are likely to reduce bandwidth, and it should be the primary goal of subsequent optimization efforts to increase it.



High Priority: Use the effective bandwidth of your computation as a metric when measuring performance and optimization benefits.

2.2.1 Theoretical Bandwidth Calculation

Theoretical bandwidth can be calculated using hardware specifications available in the product literature. For example, the NVIDIA GeForce GTX 280 uses DDR (double data rate) RAM with a memory clock rate of 1,107 MHz and a 512-bit wide memory interface.

Using these data items, the peak theoretical memory bandwidth of the NVIDIA GeForce GTX 280 is 141.6 GB/sec:

$$(1107 \times 10^6 \times (512/8) \times 2) / 10^9 = 141.6 \text{ GB/sec}$$

In this calculation, the memory clock rate is converted in to Hz, multiplied by the interface width (divided by 8, to convert bits to bytes) and multiplied by 2 due to the double data rate. Finally, this product is divided by 10^9 to convert the result to GB/sec (GBps).

Note that some calculations use $1,024^3$ instead of 10^9 for the final calculation. In such a case, the bandwidth would be 131.9 GBps. It is important to use the same divisor when calculating theoretical and effective bandwidth so that the comparison is valid.

2.2.2 Effective Bandwidth Calculation

Effective bandwidth is calculated by timing specific program activities and by knowing how data is accessed by the program. To do so, use this equation:

$$\text{Effective bandwidth} = ((B_r + B_w) / 10^9) / \text{time}$$

Here, the effective bandwidth is in units of GBps, B_r is the number of bytes read per kernel, B_w is the number of bytes written per kernel, and time is given in seconds.

For example, to compute the effective bandwidth of a 2048 x 2048 matrix copy, the following formula could be used:

$$\text{Effective bandwidth} = ((2048^2 \times 4 \times 2) / 10^9) / \text{time}$$

The number of elements is multiplied by the size of each element (4 bytes for a float), multiplied by 2 (because of the read *and* write), divided by 10^9 (or $1,024^3$) to obtain GB of memory transferred. This number is divided by the time in seconds to obtain GBps.

2.2.3 Throughput Reported by cudaprof

The memory throughput reported in the summary table of cudaprof, the CUDA Visual Profiler, differs from the effective bandwidth obtained by the calculation in Section 2.2.2 in several respects.

The first difference is that cudaprof measures throughput using a subset of the GPU's multiprocessors and then extrapolates that number to the entire GPU, thus reporting an estimate of the data throughput.

The second and more important difference is that because the minimum memory transaction size is larger than most word sizes, the memory throughput reported by the profiler includes the transfer of data not used by the kernel.

The effective bandwidth calculation in Section 2.2.2, however, includes only data transfers that are relevant to the algorithm. As such, the effective bandwidth will be smaller than the memory throughput reported by cudaprof and is the number to use when optimizing memory performance.

However, it's important to note that both numbers are useful. The profiler memory throughput shows how close the code is to the hardware limit, and the comparison of the effective bandwidth with the profiler number presents a good estimate of how much bandwidth is wasted by suboptimal coalescing of memory accesses.

Chapter 3.

MEMORY OPTIMIZATIONS

Memory optimizations are the most important area for performance. The goal is to maximize the use of the hardware by maximizing bandwidth. Bandwidth is best served by using as much fast memory and as little slow-access memory as possible. This chapter discusses the various kinds of memory on the host and device and how best to set up data items to use the memory effectively.

3.1 DATA TRANSFER BETWEEN HOST AND DEVICE

The peak bandwidth between the device memory and the GPU is much higher (141 GBps on the NVIDIA GeForce GTX 280, for example) than the peak bandwidth between host memory and device memory (8 GBps on the PCIe ×16 Gen2). Hence, for best overall application performance, it is important to minimize data transfer between the host and the device, even if that means running kernels on the GPU that do not demonstrate any speed-up compared with running them on the host CPU.



High Priority: Minimize data transfer between the host and the device, even if it means running some kernels on the device that do not show performance gains when compared with running them on the host CPU.

Intermediate data structures should be created in device memory, operated on by the device, and destroyed without ever being mapped by the host or copied to host memory.

Also, because of the overhead associated with each transfer, batching many small transfers into one larger transfer performs significantly better than making each transfer separately.

Finally, higher bandwidth between the host and the device is achieved when using *page-locked* (or *pinned*) memory, as discussed in the *CUDA C Programming Guide* and Section 3.1.1 of this document.

3.1.1 Pinned Memory

Page-locked or pinned memory transfers attain the highest bandwidth between the host and the device. On PCIe ×16 Gen2 cards, for example, pinned memory can attain greater than 5 GBps transfer rates.

Pinned memory is allocated using the `cudaMallocHost()` or `cudaHostAlloc()` functions in the Runtime API. The `bandwidthTest.cu` program in the CUDA SDK shows how to use these functions as well as how to measure memory transfer performance.

Pinned memory should not be overused. Excessive use can reduce overall system performance because pinned memory is a scarce resource. How much is too much is difficult to tell in advance, so as with all optimizations, test the applications and the systems they run on for optimal performance parameters.

3.1.2 Asynchronous Transfers and Overlapping Transfers with Computation

Data transfers between the host and the device using `cudaMemcpy()` are blocking transfers; that is, control is returned to the host thread only after the data transfer is complete. The `cudaMemcpyAsync()` function is a non-blocking variant of `cudaMemcpy()` in which control is returned immediately to the host thread. In contrast with `cudaMemcpy()`, the asynchronous transfer version *requires* pinned host memory (see Section 3.1.1), and it contains an additional argument, a stream ID. A *stream* is simply a sequence of operations that are performed in order on the device. Operations in different streams can be interleaved and in some cases overlapped—a property that can be used to hide data transfers between the host and the device.

Asynchronous transfers enable overlap of data transfers with computation in two different ways. On all CUDA-enabled devices, it is possible to overlap host computation with asynchronous data transfers and with device computations. For example, Listing 3.1 demonstrates how host computation in the routine `cpuFunction()` is performed while data is transferred to the device and a kernel using the device is executed.

```
cudaMemcpyAsync(a_d, a_h, size, cudaMemcpyHostToDevice, 0);
kernel<<<grid, block>>>(a_d);
cpuFunction();
```

Listing 3.1 Overlapping computation and data transfers

The last argument to the `cudaMemcpyAsync()` function is the stream ID, which in this case uses the default stream, stream 0. The kernel also uses the default stream, and it will not

begin execution until the memory copy completes; therefore, no explicit synchronization is needed. Because the memory copy and the kernel both return control to the host immediately, the host function `cpuFunction()` overlaps their execution.

In Listing 3.1, the memory copy and kernel execution occur sequentially. On devices that are capable of “concurrent copy and execute,” it is possible to overlap kernel execution on the device with data transfers between the host and the device. Whether a device has this capability is indicated by the `deviceOverlap` field of a `cudaDeviceProp` variable (or listed in the output of the `deviceQuery` SDK sample). On devices that have this capability, the overlap once again requires pinned host memory, and, in addition, the data transfer and kernel must use different, non-default streams (streams with non-zero stream IDs). Non-default streams are required for this overlap because memory copy, memory set functions, and kernel calls that use the default stream begin only after all preceding calls on the device (in any stream) have completed, and no operation on the device (in any stream) commences until they are finished.

Listing 3.2 illustrates the basic technique.

```
cudaStreamCreate(&stream1);
cudaStreamCreate(&stream2);
cudaMemcpyAsync(a_d, a_h, size, cudaMemcpyHostToDevice, stream1);
kernel<<<grid, block, 0, stream2>>>(otherData_d);
```

Listing 3.2 Concurrent copy and execute

In this code, two streams are created and used in the data transfer and kernel executions as specified in the last arguments of the `cudaMemcpyAsync` call and the kernel’s execution configuration.

Listing 3.2 demonstrates how to overlap kernel execution with asynchronous data transfer. This technique could be used when the data dependency is such that the data can be broken into chunks and transferred in multiple stages, launching multiple kernels to operate on each chunk as it arrives. Listings 3.3a and 3.3b demonstrate this. They produce equivalent results. The first segment shows the reference sequential implementation, which transfers and operates on an array of N floats (where N is assumed to be evenly divisible by `nThreads`).

```
cudaMemcpy(a_d, a_h, N*sizeof(float), dir);
kernel<<<N/nThreads, nThreads>>>(a_d);
```

Listing 3.3a Sequential copy and execute

Listing 3.3b shows how the transfer and kernel execution can be broken up into `nStreams` stages. This approach permits some overlapping of the data transfer and execution.

```
size=N*sizeof(float)/nStreams;
for (i=0; i<nStreams; i++) {
```

```

offset = i*N/nStreams;
cudaMemcpyAsync(a_d+offset, a_h+offset, size, dir, stream[i]);
}
for (i=0; i<nStreams; i++) {
    offset = i*N/nStreams;
    kernel<<<N/(nThreads*nStreams), nThreads,
        0, stream[i]>>>(a_d+offset);
}

```

Listing 3.3b Staged concurrent copy and execute

(In Listing 3.3b, it is assumed that N is evenly divisible by $nThreads * nStreams$.) Because execution within a stream occurs sequentially, none of the kernels will launch until the data transfers in their respective streams complete. Current hardware can simultaneously process an asynchronous data transfer and execute kernels. (It should be mentioned that it is not possible to overlap a blocking transfer with an asynchronous transfer, because the blocking transfer occurs in the default stream, and so it will not begin until all previous CUDA calls complete. It will not allow any other CUDA call to begin until it has completed.) A diagram depicting the timeline of execution for the two code segments is shown in Figure 3.1, and $nStreams=4$ for Listing 3.3b is shown in the bottom half.

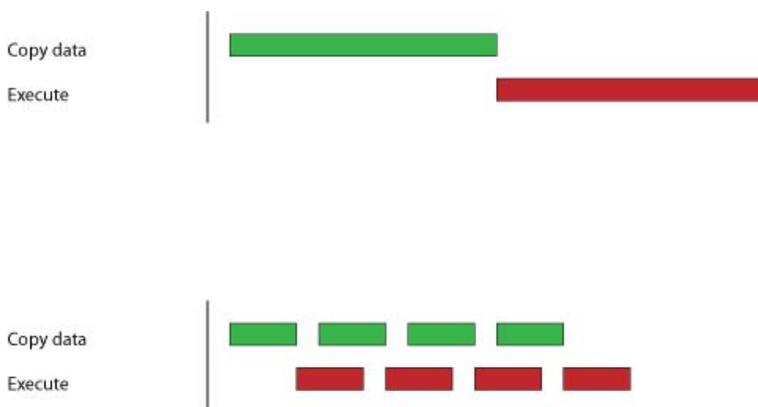


Figure 3.1 Timeline Comparison for Sequential (top) and Concurrent (bottom) Copy and Kernel Execution

For this example, it is assumed that the data transfer and kernel execution times are comparable. In such cases, and when the execution time (t_E) exceeds the transfer time (t_T), a rough estimate for the overall time is $t_E + t_T/nStreams$ for the staged version versus $t_E + t_T$ for the sequential version. If the transfer time exceeds the execution time, a rough estimate for the overall time is $t_T + t_E/nStreams$.

3.1.3 Zero Copy

Zero copy is a feature that was added in version 2.2 of the CUDA Toolkit. It enables GPU threads to directly access host memory. For this purpose, it requires mapped pinned (non-pageable) memory. On integrated GPUs (e.g., mobile GPUs for notebooks), mapped pinned memory is always a performance gain because it avoids superfluous copies as integrated GPU and CPU memory are physically the same. On discrete GPUs, mapped pinned memory is advantageous only in certain cases. Because the data is not cached on the GPU on devices of compute capability 1.x, mapped pinned memory should be read or written only once, and the global loads and stores that read and write the memory should be coalesced. Zero copy can be used in place of streams because kernel-originated data transfers automatically overlap kernel execution without the overhead of setting up and determining the optimal number of streams.



Low Priority: Use zero-copy operations on integrated GPUs for CUDA Toolkit version 2.2 and later.

The host code in Listing 3.4 shows how zero copy is typically set up.

```
float *a_h, *a_map;
...
cudaGetDeviceProperties(&prop, 0);
if (!prop.canMapHostMemory)
    exit(0);
cudaSetDeviceFlags(cudaDeviceMapHost);
cudaHostAlloc(&a_h, nBytes, cudaHostAllocMapped);
cudaHostGetDevicePointer(&a_map, a_h, 0);
kernel<<<gridSize, blockSize>>>(a_map);
```

Listing 3.4 Zero-copy host code

In this code, the `canMapHostMemory` field of the structure returned by `cudaGetDeviceProperties()` is used to check that the device supports mapping host memory to the device's address space. Page-locked memory mapping is enabled by calling `cudaSetDeviceFlags()` with `cudaDeviceMapHost`. Note that `cudaSetDeviceFlags()` must be called prior to setting a device or making a CUDA call that requires state (that is, essentially, before a context is created). Page-locked mapped host memory is allocated using `cudaHostAlloc()`, and the pointer to the mapped device address space is obtained via the function `cudaHostGetDevicePointer()`. In the code in Listing 3.4, `kernel()` can reference the mapped pinned host memory using the pointer `a_map` in exactly the same way as it would if `a_map` referred to a location in device memory.

3.2 DEVICE MEMORY SPACES

CUDA devices use several memory spaces, which have different characteristics that reflect their distinct usages in CUDA applications. These memory spaces include global, local, shared, texture, and registers, as shown in Figure 3.2.

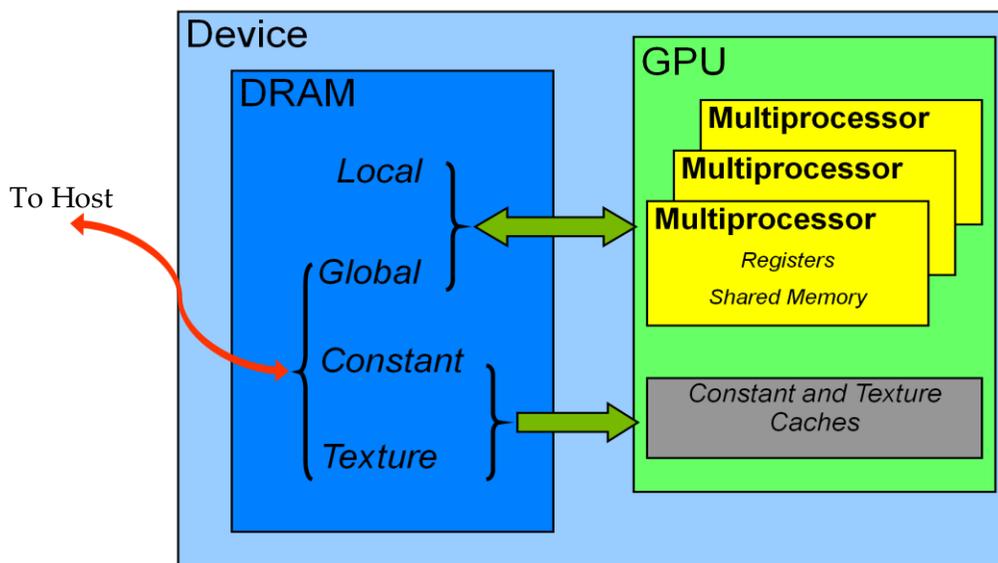


Figure 3.2 Memory Spaces on a CUDA Device

Of these different memory spaces, global and texture memory are the most plentiful; see Section F.1 of the *CUDA C Programming Guide* for the amounts of memory available in each memory space at each compute capability level. Global, local, and texture memory have the greatest access latency, followed by constant memory, registers, and shared memory.

The various principal traits of the memory types are shown in Table 3.1.

Table 3.1 Salient Features of Device Memory

Memory	Location on/off chip	Cached	Access	Scope	Lifetime
Register	On	n/a	R/W	1 thread	Thread
Local	Off	†	R/W	1 thread	Thread
Shared	On	n/a	R/W	All threads in block	Block
Global	Off	†	R/W	All threads + host	Host allocation
Constant	Off	Yes	R	All threads + host	Host allocation
Texture	Off	Yes	R	All threads + host	Host allocation

† Cached only on devices of compute capability 2.x.

In the case of texture access, if a texture reference is bound to a linear (and, as of version 2.2 of the CUDA Toolkit, pitch-linear) array in global memory, then the device code can write to the underlying array. Reading from a texture while writing to its underlying global memory array in the same kernel launch should be avoided because the texture caches are read-only and are not invalidated when the associated global memory is modified.

3.2.1 Coalesced Access to Global Memory

High Priority: Ensure global memory accesses are coalesced whenever possible.

Perhaps the single most important performance consideration in programming for the CUDA architecture is coalescing global memory accesses. Global memory loads and stores by threads of a half warp (for devices of compute capability 1.x) or of a warp (for devices of compute capability 2.x) are coalesced by the device into as few as one transaction when certain access requirements are met.

To understand these access requirements, global memory should be viewed in terms of aligned segments of 16 and 32 words. Figure 3.3 helps explain the coalescing of 32-bit words (such as floats) by a half warp. It shows global memory as rows of 64-byte aligned segments (16 floats). Two rows of the same color represent a 128-byte aligned segment. A half warp of threads that accesses the global memory is indicated at the bottom of the figure. Note that this figure assumes a device of compute capability 1.x.

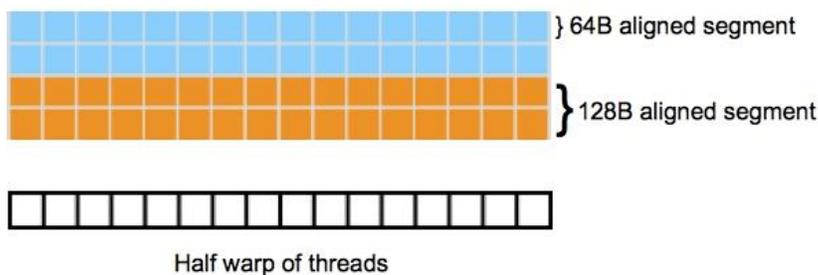


Figure 3.3 Linear Memory Segments and Threads in a Half Warp

The access requirements for coalescing depend on the compute capability of the device:

- ▶ On devices of compute capability 1.0 or 1.1, the k -th thread in a half warp must access the k -th word in a segment aligned to 16 times the size of the elements being accessed; however, not all threads need to participate.
- ▶ On devices of compute capability 1.2 or 1.3, coalescing is achieved for any pattern of accesses that fits into a segment size of 32 bytes for 8-bit words, 64 bytes for 16-bit words, or 128 bytes for 32- and 64-bit words. Smaller transactions may be issued to

avoid wasting bandwidth. More precisely, the following protocol is used to issue a memory transaction for a half warp:

- Find the memory segment that contains the address requested by the lowest numbered active thread. Segment size is 32 bytes for 8-bit data, 64 bytes for 16-bit data, and 128 bytes for 32-, 64-, and 128-bit data.
- Find all other active threads whose requested address lies in the same segment, and reduce the transaction size if possible:
 - If the transaction is 128 bytes and only the lower or upper half is used, reduce the transaction size to 64 bytes.
 - If the transaction is 64 bytes and only the lower or upper half is used, reduce the transaction size to 32 bytes.
- Carry out the transaction and mark the serviced threads as inactive.
- Repeat until all threads in the half warp are serviced.
- On devices of compute capability 2.x, memory accesses by the threads of a warp are coalesced into the minimum number of L1-cache-line-sized aligned transactions necessary to satisfy all threads; see Section F.4.2 of the *CUDA C Programming Guide*.

These concepts are illustrated in the following simple examples.

3.2.1.1 A Simple Access Pattern

The first and simplest case of coalescing can be achieved by any CUDA-enabled device: the k -th thread accesses the k -th word in a segment. Note that not all threads need to participate. (See Figure 3.4. Note that this figure assumes a device of compute capability 1.x, but that the figure would be much the same except twice as wide for devices of compute capability 2.x.)

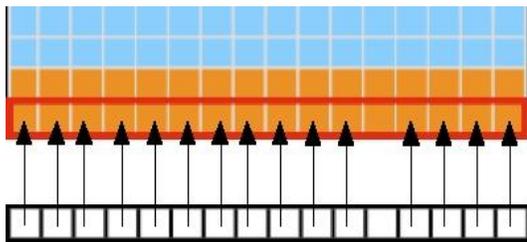


Figure 3.4 Coalesced Access—All Threads but One Access the Corresponding Word in a Segment

This access pattern results in a single 64-byte transaction, indicated by the red rectangle. Note that even though one word is not requested, all data in the segment are fetched. If accesses by threads were permuted within this segment, still one 64-byte transaction

would be performed by a device with compute capability 1.2 or higher, but 16 serialized transactions would be performed by a device with compute capability 1.1 or lower.

3.2.1.2 A Sequential but Misaligned Access Pattern

If sequential threads in a half warp access memory that is sequential but not aligned with the segments, then a separate transaction results for each element requested on a device with compute capability 1.1 or lower. On a device with compute capability 1.2 or higher, several different scenarios can arise depending on whether all addresses for a half warp fall within a single 128-byte segment. If the addresses fall within a 128-byte segment, then a single 128-byte transaction is performed, as shown in Figure 3.5. Again, this figure assumes a device of compute capability 1.x.

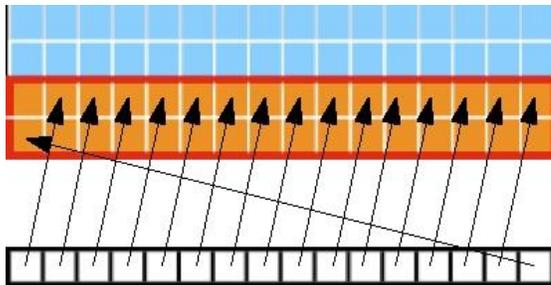


Figure 3.5 Unaligned Sequential Addresses that Fit within a Single 128-Byte Segment

If a half warp accesses memory that is sequential but split across two 128-byte segments, then two transactions are performed. In the following case, illustrated in Figure 3.6, one 64-byte transaction and one 32-byte transaction result. Again, this figure assumes a device of compute capability 1.x.

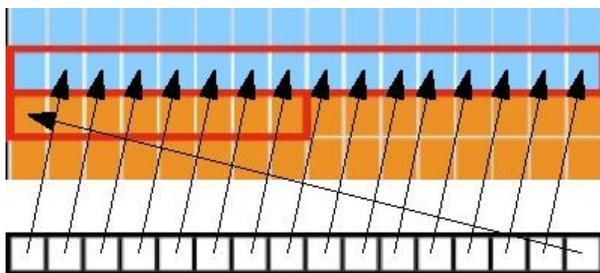


Figure 3.6 Misaligned Sequential Addresses that Fall within Two 128-Byte Segments

Memory allocated through the Runtime API, such as via `cudaMalloc()`, is guaranteed to be aligned to at least 256 bytes. Therefore, choosing sensible thread block sizes, such as multiples of 16, facilitates memory accesses by half warps that are aligned to segments.

In addition, the qualifiers `__align__(8)` and `__align__(16)` can be used when defining structures to ensure alignment to segments.

3.2.1.3 Effects of Misaligned Accesses

It is easy and informative to explore the ramifications of misaligned accesses using a simple copy kernel, such as the one in Listing 3.5.

```
__global__ void offsetCopy(float *odata, float* idata, int offset)
{
    int xid = blockIdx.x * blockDim.x + threadIdx.x + offset;
    odata[xid] = idata[xid];
}
```

Listing 3.5 A copy kernel that illustrates misaligned accesses

In Listing 3.5, data is copied from the input array `idata` to the output array, both of which exist in global memory. The kernel is executed within a loop in host code that varies the parameter `offset` from 1 to 32. (Figure 3.5 and Figure 3.6 correspond to offsets of 1 and 17, respectively.) The effective bandwidth for the copy with various offsets on an NVIDIA GeForce GTX 280 (with compute capability 1.3) and an NVIDIA GeForce GTX 8800 (compute capability 1.0) are shown in Figure 3.7.

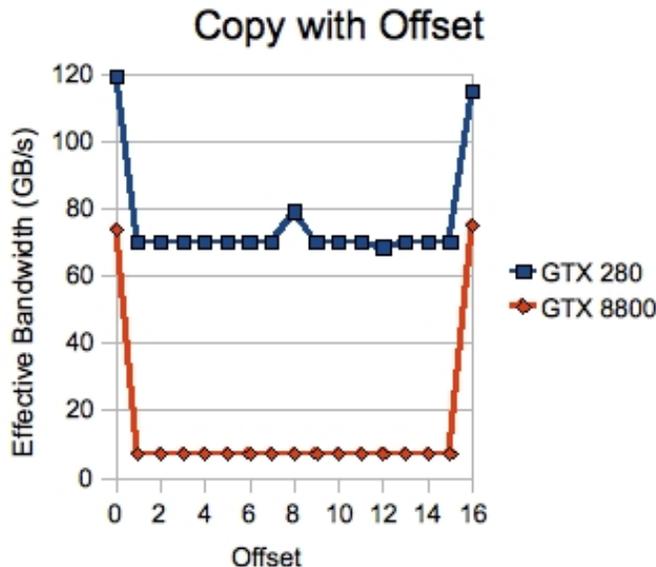


Figure 3.7 Performance of `offsetCopy` kernel

For the NVIDIA GeForce GTX 8800 device, global memory accesses with no offset or with offsets that are multiples of 16 result in a single transaction per half warp and an effective bandwidth of approximately 74 GBps. Otherwise, 16 transactions are issued per half warp resulting in an effective bandwidth of approximately 7 GBps. This roughly 8x

performance degradation is due to the fact that 32 bytes, the minimum transaction size, are fetched for each thread. However, only 4 bytes of data are used for each 32 bytes fetched—resulting in the $4/32=1/8$ performance relative to the fully coalesced case. The two numbers also reflect the different data represented by effective bandwidth (4 bytes) versus actual bandwidth (32 bytes).

Because of this possible performance degradation, memory coalescing is the most critical aspect of performance optimization of device memory. For devices of compute capability 1.2 and 1.3, the situation is less dire for misaligned accesses because, in all cases, access by a half warp of threads in this kernel results in either one or two transactions.

On the NVIDIA GeForce GTX 280 device, this results in an effective bandwidth of between 120 GBps for a single transaction and 70 GBps for two transactions per half warp. The number of transactions issued for a half warp of threads depends on the offset and whether the warp is even- or odd-numbered. For offsets of 0 or 16, each half warp results in a single 64-byte transaction (Figure 3.4). For offsets of 1 through 7 or 9 through 15, even-numbered warps result in a single 128-byte transaction (Figure 3.5) and odd-numbered warps result in two transactions: one 64-byte and one 32-byte (Figure 3.6). For offsets of 8, even-numbered warps result in one 128-byte transaction and odd-numbered warps result in two 32-byte transactions. The two 32-byte transactions, rather than a 64- and a 32-byte transaction, are responsible for the blip at the offset of 8 in Figure 3.7.

3.2.1.4 Strided Accesses

Although the relaxed coalescing restrictions for devices with compute capability 1.2 or higher achieve one-half full bandwidth for the offset copy case just described, performance on such devices can degrade when successive threads access memory locations that have non-unit strides. This pattern occurs frequently when dealing with multidimensional data or matrices; for example, when a half warp of threads accesses matrix elements column-wise and the matrix is stored in row-major order.

To illustrate the effect of strided access on effective bandwidth, see the following kernel `strideCopy()`, which copies data with a stride of `stride` elements between threads from `idata` to `odata`.

```
__global__ void strideCopy(float *odata, float* idata, int stride)
{
    int xid = (blockIdx.x*blockDim.x + threadIdx.x)*stride;
    odata[xid] = idata[xid];
}
```

Listing 3.6 A kernel to illustrate non-unit stride data copy

Figure 3.8 illustrates a situation that can be created using the code in Listing 3.6; namely, threads within a half warp access memory with a stride of 2. This action is coalesced into a single 128-byte transaction on an NVIDIA GeForce GTX 280 (compute capability 1.3).

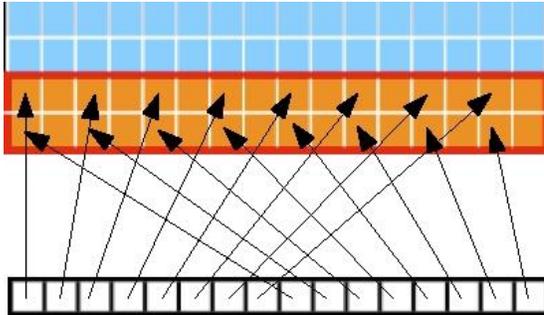


Figure 3.8 A half warp accessing memory with a stride of 2

Although a stride of 2 results in a single transaction, note that half the elements in the transaction are not used and represent wasted bandwidth. As the stride increases, the effective bandwidth decreases until the point where 16 transactions are issued for the 16 threads in a half warp, as indicated in Figure 3.9.

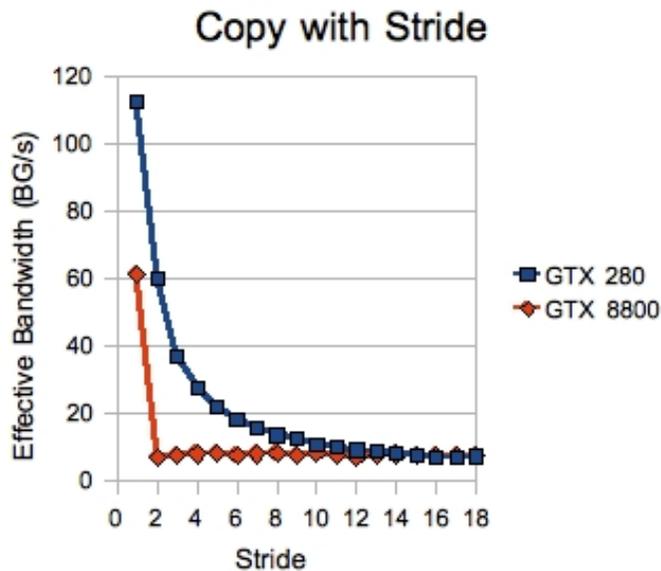


Figure 3.9 Performance of strideCopy Kernel

Note, however, that on the NVIDIA GTX 8800 device (compute capability 1.0), any non-unit stride results in 16 separate transactions per half warp.

As illustrated in Figure 3.9, non-unit stride global memory accesses should be avoided whenever possible. One method for doing so utilizes shared memory, which is discussed in the next section.

3.2.2 Shared Memory

Because it is on-chip, shared memory is much faster than local and global memory. In fact, uncached shared memory latency is roughly 100x lower than global memory latency—provided there are no bank conflicts between the threads, as detailed in the following section.

3.2.2.1 Shared Memory and Memory Banks

To achieve high memory bandwidth for concurrent accesses, shared memory is divided into equally sized memory modules (*banks*) that can be accessed simultaneously. Therefore, any memory load or store of n addresses that spans n distinct memory banks can be serviced simultaneously, yielding an effective bandwidth that is n times as high as the bandwidth of a single bank.

However, if multiple addresses of a memory request map to the same memory bank, the accesses are serialized. The hardware splits a memory request that has bank conflicts into as many separate conflict-free requests as necessary, decreasing the effective bandwidth by a factor equal to the number of separate memory requests. The one exception here is when all threads in a half warp address the same shared memory location, resulting in a broadcast. Devices of compute capability 2.x have the additional ability to multicast shared memory accesses (i.e., to send copies of the same value to several but not all threads of the warp).

To minimize bank conflicts, it is important to understand how memory addresses map to memory banks and how to optimally schedule memory requests.



Medium Priority: Accesses to shared memory should be designed to avoid serializing requests due to bank conflicts.

Shared memory banks are organized such that successive 32-bit words are assigned to successive banks and each bank has a bandwidth of 32 bits per clock cycle. The bandwidth of shared memory is 32 bits per bank per clock cycle.

For devices of compute capability 1.x, the warp size is 32 threads and the number of banks is 16. A shared memory request for a warp is split into one request for the first half of the warp and one request for the second half of the warp. Note that no bank conflict occurs if only one memory location per bank is accessed by a half warp of threads.

For devices of compute capability 2.x, the warp size is 32 threads and the number of banks is also 32. A shared memory request for a warp is not split as with devices of

compute capability 1.x, meaning that bank conflicts *can* occur between threads in the first half of a warp and threads in the second half of the same warp (see Section F.4.3 of the *CUDA C Programming Guide*).

Refer to the *CUDA C Programming Guide* for more information on how accesses and banks can be matched to avoid conflicts.

3.2.2.2 Shared Memory in Matrix Multiplication ($C = AB$)

Shared memory enables cooperation between threads in a block. When multiple threads in a block use the same data from global memory, shared memory can be used to access the data from global memory only once. Shared memory can also be used to avoid uncoalesced memory accesses by loading and storing data in a coalesced pattern from global memory and then reordering it in shared memory. Aside from memory bank conflicts, there is no penalty for non-sequential or unaligned accesses by a half warp in shared memory.

The use of shared memory is illustrated via the simple example of a matrix multiplication $C = AB$ for the case with A of dimension $M \times 16$, B of dimension $16 \times N$, and C of dimension $M \times N$. To keep the kernels simple, M and N are multiples of 16. A natural decomposition of the problem is to use a block and tile size of 16×16 threads. Therefore, in terms of 16×16 tiles, A is a column matrix, B is a row matrix, and C is their outer product. (See Figure 3.10) A grid of $N/16$ by $M/16$ blocks is launched, where each thread block calculates the elements of a different tile in C from a single tile of A and a single tile of B .

Note that the example discussed throughout this section assumes compute capability 1.x; the example would be much the same for compute capability 2.x, except that it would have a width of 32 instead of 16.

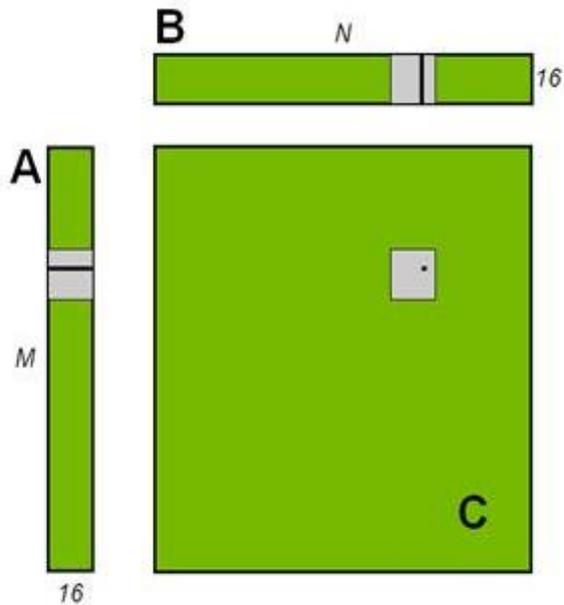


Figure 3.10 Block-Column Matrix (A) Multiplied by Block-Row Matrix (B) with Resulting Product Matrix (C)

To do this, the `simpleMultiply` kernel (Listing 3.7) calculates the output elements of a tile of matrix C.

```
__global__ void simpleMultiply(float *a, float* b, float *c,
                              int N)
{
    int row = blockIdx.y * blockDim.y + threadIdx.y;
    int col = blockIdx.x * blockDim.x + threadIdx.x;
    float sum = 0.0f;
    for (int i = 0; i < TILE_DIM; i++) {
        sum += a[row*TILE_DIM+i] * b[i*N+col];
    }
    c[row*N+col] = sum;
}
```

Listing 3.7 Unoptimized matrix multiplication

In Listing 3.7, `a`, `b`, and `c` are pointers to global memory for the matrices A, B, and C, respectively; `blockDim.x`, `blockDim.y`, and `TILE_DIM` are all 16. Each thread in the 16×16 block calculates one element in a tile of C. `row` and `col` are the row and column of the element in C being calculated by a particular thread. The `for` loop over `i` multiplies a row of A by a column of B, which is then written to C.

The effective bandwidth of this kernel is only 8.7 GBps on an NVIDIA GeForce GTX 280 and 0.7 GBps on an NVIDIA GeForce GTX 8800. To analyze performance, it is necessary to consider how half warps of threads access global memory in the `for` loop. Each half

warp of threads calculates one row of a tile of C, which depends on a single row of A and an entire tile of B as illustrated in Figure 3.11.

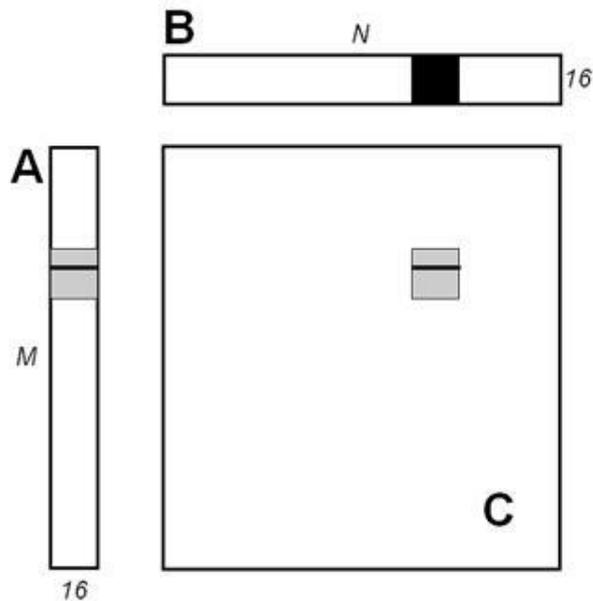


Figure 3.11 Computing a Row (Half Warp) of a Tile In C Using One Row of A and an Entire Tile of B

For each iteration i of the `for` loop, all threads in a half warp read the same value from global memory (the index `row*TILE_DIM+i` is constant within a half warp), resulting in 16 transactions for compute capability 1.1 or lower, and 1 transaction for compute capability 1.2 or higher. Even though the operation requires only 1 transaction for compute capability 1.2 or higher, there is wasted bandwidth in the transaction because only 4 bytes out of a 32-byte transaction are used. For each iteration, the 16 threads in a half warp read a row of the B tile, which is a sequential and coalesced access for all compute capabilities.

The performance on a device of any compute capability can be improved by reading a tile of A into shared memory as shown in Listing 3.8.

```
__global__ void coalescedMultiply(float *a, float* b, float *c,
                                int N)
{
    __shared__ float aTile[TILE_DIM][TILE_DIM];

    int row = blockIdx.y * blockDim.y + threadIdx.y;
    int col = blockIdx.x * blockDim.x + threadIdx.x;
    float sum = 0.0f;
    aTile[threadIdx.y][threadIdx.x] = a[row*TILE_DIM+threadIdx.x];
```

```

for (int i = 0; i < TILE_DIM; i++) {
    sum += aTile[threadIdx.y][i] * b[i*N+col];
}
c[row*N+col] = sum;
}

```

Listing 3.8 Using shared memory to improve the global memory load efficiency in matrix multiplication

In Listing 3.8, each element in a tile of A is read from global memory only once, in a fully coalesced fashion (with no wasted bandwidth), to shared memory. Within each iteration of the `for` loop, a value in shared memory is broadcast to all threads in a half warp.

In Listing 3.8, a `__syncthreads()` synchronization barrier call is not needed after reading the tile of A into shared memory because only threads within the half warp that write the data into shared memory read the data. This kernel has an effective bandwidth of 14.3 GBps on an NVIDIA GeForce GTX 280, and 8.2 GBps on an NVIDIA GeForce GTX 8800.

A further improvement can be made to how Listing 3.8 deals with matrix B. In calculating a tile's row of matrix C, the entire tile of B is read. The repeated reading of the B tile can be eliminated by reading it into shared memory once (Listing 3.9).

```

__global__ void sharedABMultiply(float *a, float* b, float *c,
                                int N)
{
    __shared__ float aTile[TILE_DIM][TILE_DIM],
                  bTile[TILE_DIM][TILE_DIM];
    int row = blockIdx.y * blockDim.y + threadIdx.y;
    int col = blockIdx.x * blockDim.x + threadIdx.x;
    float sum = 0.0f;
    aTile[threadIdx.y][threadIdx.x] = a[row*TILE_DIM+threadIdx.x];
    bTile[threadIdx.y][threadIdx.x] = b[threadIdx.y*N+col];
    __syncthreads();
    for (int i = 0; i < TILE_DIM; i++) {
        sum += aTile[threadIdx.y][i] * bTile[i][threadIdx.x];
    }
    c[row*N+col] = sum;
}

```

Listing 3.9 Improvement by reading additional data into shared memory

Note that in Listing 3.9, a `__syncthreads()` call is required after reading the B tile because a warp reads data from shared memory that were written to shared memory by different warps. The effective bandwidth of this routine is 29.7 GBps on an NVIDIA GeForce GTX 280 and 15.7 GBps on an NVIDIA GeForce GTX 8800. Note that the performance improvement is not due to improved coalescing in either case, but to avoiding redundant transfers from global memory.

The results of the various optimizations are summarized in Table 3.2.

Table 3.2 Performance Improvements Optimizing $C = AB$ Matrix Multiply

Optimization	NVIDIA GeForce GTX 280	NVIDIA GeForce GTX 8800
No optimization	8.7 GBps	0.7 GBps
Coalesced using shared memory to store a tile of A	14.3 GBps	8.2 GBps
Using shared memory to eliminate redundant reads of a tile of B	29.7 GBps	15.7 GBps



Medium Priority: Use shared memory to avoid redundant transfers from global memory.

3.2.2.3 Shared Memory in Matrix Multiplication ($C = AA^T$)

A variant of the previous matrix multiplication can be used to illustrate how strided accesses to global memory, as well as shared memory bank conflicts, are handled. This variant simply uses the transpose of A rather than B, or $C = AA^T$.

As in the previous section, this example assumes compute capability 1.x; it would have a width of 32 rather than 16 for compute capability 2.x.

A simple implementation for $C = AA^T$ is shown in Listing 3.10.

```
__global__ void simpleMultiply(float *a, float *c, int M)
{
    int row = blockIdx.y * blockDim.y + threadIdx.y;
    int col = blockIdx.x * blockDim.x + threadIdx.x;
    float sum = 0.0f;
    for (int i = 0; i < TILE_DIM; i++) {
        sum += a[row*TILE_DIM+i] * a[col*TILE_DIM+i];
    }
    c[row*M+col] = sum;
}
```

Listing 3.10 Unoptimized handling of strided accesses to global memory

In Listing 3.10, the *row*-th, *col*-th element of C is obtained by taking the dot product of the *row*-th and *col*-th rows of A. The effective bandwidth for this kernel is 1.1 GBps on an NVIDIA GeForce GTX 280 and 0.5 GBps on an NVIDIA GeForce GTX 8800. These results are substantially lower than the corresponding measurements for the $C = AB$ kernel. The difference is in how threads in a half warp access elements of A in the

second term, `a[col*TILE_DIM+i]`, for each iteration `i`. For a half warp of threads, `col` represents sequential columns of the transpose of `A`, and therefore `col*TILE_DIM` represents a strided access of global memory with a stride of 16. This results in uncoalesced memory accesses on devices with compute capability 1.1 or lower and plenty of wasted bandwidth on devices with compute capability 1.2 or higher. The way to avoid strided access is to use shared memory as before, except in this case a half warp reads a row of `A` into a column of a shared memory tile, as shown in Listing 3.11.

```

__global__ void coalescedMultiply(float *a, float *c, int M)
{
    __shared__ float aTile[TILE_DIM][TILE_DIM],
                  transposedTile[TILE_DIM][TILE_DIM];
    int row = blockIdx.y * blockDim.y + threadIdx.y;
    int col = blockIdx.x * blockDim.x + threadIdx.x;
    float sum = 0.0f;
    aTile[threadIdx.y][threadIdx.x] = a[row*TILE_DIM+threadIdx.x];
    transposedTile[threadIdx.x][threadIdx.y] =
        a[(blockIdx.x*blockDim.x + threadIdx.y)*TILE_DIM +
          threadIdx.x];
    __syncthreads();
    for (int i = 0; i < TILE_DIM; i++) {
        sum += aTile[threadIdx.y][i] * transposedTile[i][threadIdx.x];
    }
    c[row*M+col] = sum;
}

```

Listing 3.11 An optimized version of Listing 3.10 using coalesced reads from global memory

Listing 3.11 uses the shared `transposedTile` to avoid uncoalesced accesses in the second term in the dot product, and the shared `aTile` technique from the previous example to avoid uncoalesced accesses in the first term. The effective bandwidth of this kernel is 24.9 GBps on an NVIDIA GeForce GTX 280 and 13.2 GBps on an NVIDIA GeForce GTX 8800. These results are slightly lower than those obtained by the final kernel for `C = AB`. The cause of the difference is shared memory bank conflicts.

The reads of elements in `transposedTile` within the `for` loop are free of conflicts, because threads of each half warp read across rows of the tile, resulting in unit stride across the banks. However, bank conflicts occur when copying the tile from global memory into shared memory. To enable the loads from global memory to be coalesced, data are read from global memory sequentially. However, this requires writing to shared memory in columns, and because of the use of 16×16 tiles in shared memory, this results in a stride between threads of 16 banks. These 16-way bank conflicts are very expensive. The simple remedy is to pad the shared memory array so that it has an extra column, as in the following line of code.

```

__shared__ float transposedTile[TILE_DIM][TILE_DIM+1];

```

This padding eliminates the conflicts entirely, because now the stride between threads is 17 banks (33 banks for compute capability 2.x), which, due to modular arithmetic used to compute bank indices, is equivalent to a unit stride. After this change, the effective bandwidth is 30.4 GBps on an NVIDIA GeForce GTX 280 and 15.6 GBps on an NVIDIA GeForce GTX 8800, which is comparable to the results from the last $C = AB$ kernel.

The results of these optimizations are summarized in Table 3.3.

Table 3.3 Performance Improvements Optimizing $C = AA^T$ Matrix Multiplication

Optimization	NVIDIA GeForce GTX 280	NVIDIA GeForce GTX 8800
No optimization	1.1 GBps	0.5 GBps
Using shared memory to coalesce global reads	24.9 GBps	13.2 GBps
Removing bank conflicts	30.4 GBps	15.6 GBps

These results should be compared with those in Table 3.2. As can be seen from these tables, judicious use of shared memory can dramatically improve performance.

The examples in this section have illustrated three reasons to use shared memory:

- ▶ To enable coalesced accesses to global memory, especially to avoid large strides (for general matrices, strides are much larger than 16)
- ▶ To eliminate (or reduce) redundant loads from global memory
- ▶ To avoid wasted bandwidth

3.2.2.4 Shared Memory Use by Kernel Arguments

Shared memory holds the parameters or arguments that are passed to kernels at launch. In kernels with long argument lists, it can be valuable to put some arguments into constant memory (and reference them there) rather than consume shared memory.



Low Priority: For kernels with long argument lists, place some arguments into constant memory to save shared memory.

3.2.3 Local Memory

Local memory is so named because its scope is local to the thread, not because of its physical location. In fact, local memory is off-chip. Hence, access to local memory is as expensive as access to global memory. Like global memory, local memory is not cached on devices of compute capability 1.x. In other words, the term “local” in the name does not imply faster access.

Local memory is used only to hold automatic variables. This is done by the `nvcc` compiler when it determines that there is insufficient register space to hold the variable. Automatic variables that are likely to be placed in local memory are large structures or arrays that would consume too much register space and arrays that the compiler determines may be indexed dynamically.

Inspection of the PTX assembly code (obtained by compiling with `-ptx` or `-keep` command-line options to `nvcc`) reveals whether a variable has been placed in local memory during the first compilation phases. If it has, it will be declared using the `.local` mnemonic and accessed using the `ld.local` and `st.local` mnemonics. If it has not, subsequent compilation phases might still decide otherwise, if they find the variable consumes too much register space for the targeted architecture. There is no way to check this for a specific variable, but the compiler reports total local memory usage per kernel (`lmem`) when run with the `--ptxas-options=-v` option.

3.2.4 Texture Memory

The read-only texture memory space is cached. Therefore, a texture fetch costs one device memory read only on a cache miss; otherwise, it just costs one read from the texture cache. The texture cache is optimized for 2D spatial locality, so threads of the same warp that read texture addresses that are close together will achieve best performance. Texture memory is also designed for streaming fetches with a constant latency; that is, a cache hit reduces DRAM bandwidth demand, but not fetch latency.

In certain addressing situations, reading device memory through texture fetching can be an advantageous alternative to reading device memory from global or constant memory.

3.2.4.1 Textured Fetch vs. Global Memory Read

Device memory reads through texture fetching present several potential benefits over reads from global memory:

- ▶ They are cached, unlike global memory reads in devices of compute capability 1.x. This results in potentially higher achieved bandwidth if there is 2D locality in the texture fetches and can be used to avoid uncoalesced loads from global memory. (Note that the L1 cache in devices of compute capability 2.x has a higher bandwidth than the texture cache, potentially obviating this benefit in these devices, depending on access pattern.)
- ▶ Packed data can be unpacked into separate variables in a single operation.
- ▶ 8-bit and 16-bit integer input data may be optionally converted to 32-bit floating-point values in the range `[0.0, 1.0]` or `[-1.0, 1.0]`.

Listings 3.12 and 3.13 illustrate how textures can be used to avoid uncoalesced global memory accesses in the following variation of the `offsetCopy` kernel. This copy performs a shift in data, as demonstrated in the following kernel.

```
__global__ void shiftCopy(float *odata, float *idata, int shift)
{
    int xid = blockIdx.x * blockDim.x + threadIdx.x;
    odata[xid] = idata[xid+shift];
}
```

Listing 3.12 Unoptimized data shifts

This copy kernel applies a shift to the global memory location when reading from `idata`, but writes to unshifted global memory locations in `odata`. The amount of shift is specified as a function argument to the kernel. Some degradation of performance occurs when the shift is neither zero nor a multiple of 16 because reading from `idata` will be either uncoalesced (compute capability 1.1 or lower) or result in transactions with wasted bandwidth (compute capability 1.2 or higher). Note that regardless of compute capability, writing to `odata` is fully coalesced.

The version of this code that uses textures to perform the shifted read is shown in Listing 3.13.

```
__global__ void textureShiftCopy(float *odata, float *idata,
                                int shift)
{
    int xid = blockIdx.x * blockDim.x + threadIdx.x;
    odata[xid] = tex1Dfetch(texRef, xid+shift);
}
```

Listing 3.13 Data shifts optimized by use of texture memory

Here, the texture reference `texRef` is bound to the `idata` array in the host code and the function `tex1Dfetch()` reads the shifted memory locations of `idata` via a texture fetch. The results of both kernels (using global memory and textures for loads) on an NVIDIA GeForce GTX 280 and an NVIDIA GeForce GTX 8800 are given in Figure 3.12.

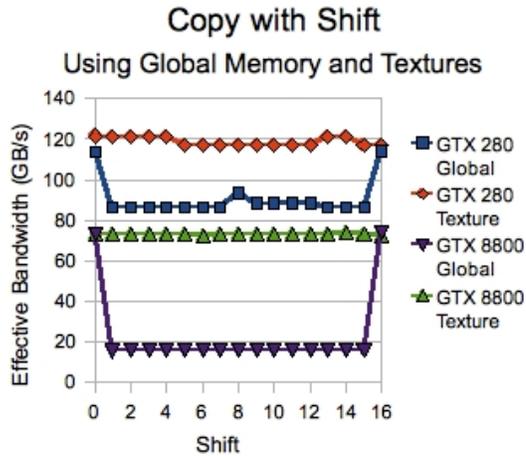


Figure 3.12 Results of Using Texture Memory to Avoid Uncoalesced Global Memory Access

The benefit of using textures for cases that are not optimally coalesced is clear. Textured reads can maintain effective bandwidth of the unshifted, fully coalesced cases within a few percent. Note that shifts that are neither zero nor multiples of 16 show greater effective bandwidth than the `offsetCopy` kernel in Figure 3.7. Because all the stores in the shift kernels are fully coalesced with no wasted bandwidth, the shift applies only to the loads.

3.2.4.2 Additional Texture Capabilities

If textures are fetched using `tex1D()`, `tex2D()`, or `tex3D()` rather than `tex1Dfetch()`, the hardware provides other capabilities that might be useful for some applications, such as image processing. (See Table 3.4.)

Table 3.4 Useful Features for `tex1D()`, `tex2D()`, and `tex3D()` Fetches

Feature	Use	Caveat
Filtering	Fast, low-precision interpolation between texels	Valid only if the texture reference returns floating-point data
Normalized texture coordinates	Resolution-independent coding	
Addressing modes	Automatic handling of boundary cases ¹	Can be used only with normalized texture coordinates

¹The automatic handling of boundary cases in the bottom row of Table 3.4 refers to how a texture coordinate is resolved when it falls outside the valid addressing range. There are two options: *clamp* and *wrap*. If x is the coordinate and N is the number of texels for a one-dimensional texture, then with *clamp*, x is replaced by 0 if $x < 0$ and by $1-1/N$ if $1 \leq x$. With *wrap*, x is replaced by $\text{frac}(x)$ where $\text{frac}(x) = x - \text{floor}(x)$. Floor returns the largest integer less than or equal to x . So, in *clamp* mode where $N = 1$, an x of 1.3 is clamped to 1.0; whereas in *wrap* mode, it is converted to 0.3

Within a kernel call, the texture cache is not kept coherent with respect to global memory writes, so texture fetches from addresses that have been written via global stores in the same kernel call return undefined data. That is, a thread can safely read a memory location via texture if the location has been updated by a previous kernel call or memory copy, but not if it has been previously updated by the same thread or another thread within the same kernel call. This is relevant only when fetching from linear or pitch-linear memory because a kernel cannot write to CUDA arrays.

3.2.4.3 Texture Format Recommendation

For 8-bit texture formats when using OpenGL interoperability, note that interoperating with `GL_RGBA8` textures on devices of compute capability 1.0, 1.1, or 1.3 runs at reduced performance.

3.2.5 Constant Memory

There is a total of 64 KB constant memory on a device. The constant memory space is cached. As a result, a read from constant memory costs one memory read from device memory only on a cache miss; otherwise, it just costs one read from the constant cache.

For all threads of a half warp, reading from the constant cache is as fast as reading from a register as long as all threads read the same address. Accesses to different addresses by threads within a half warp are serialized, so cost scales linearly with the number of different addresses read by all threads within a half warp.

Alternatively, on devices of compute capability 2.x, programs use the Load Uniform (LDU) operation; see Section F.4.4 of the *CUDA C Programming Guide* for details.

3.2.6 Registers

Generally, accessing a register consumes zero extra clock cycles per instruction, but delays may occur due to register read-after-write dependencies and register memory bank conflicts.

The latency of read-after-write dependencies is approximately 24 cycles, but this latency is completely hidden on multiprocessors that have at least 192 active threads (that is, 6 warps) for devices of compute capability 1.x (8 CUDA cores per multiprocessor * 24 cycles of latency = 192 active threads to cover that latency). For devices of compute capability 2.0, which have 32 CUDA cores per multiprocessor, as many as 768 threads might be required to completely hide latency.

The compiler and hardware thread scheduler will schedule instructions as optimally as possible to avoid register memory bank conflicts. They achieve the best results when the number of threads per block is a multiple of 64. Other than following this rule, an

application has no direct control over these bank conflicts. In particular, there is no register-related reason to pack data into `float4` or `int4` types.

3.2.6.1 Register Pressure

Register pressure occurs when there are not enough registers available for a given task. Even though each multiprocessor contains thousands of 32-bit registers (see Section F.1 of the *CUDA C Programming Guide*), these are partitioned among concurrent threads. To prevent the compiler from allocating too many registers, use the `-maxrregcount=N` compiler command-line option (see Section B.1 below) or the launch bounds kernel definition qualifier (see Section B.17 of the *CUDA C Programming Guide*) to control the maximum number of registers to allocated per thread.

3.3 ALLOCATION

Device memory allocation and de-allocation via `cudaMalloc()` and `cudaFree()` (or their Driver API equivalents) are expensive operations, so device memory should be reused and/or sub-allocated by the application wherever possible to minimize the impact of allocations on overall performance.

Chapter 4.

EXECUTION CONFIGURATION OPTIMIZATIONS

One of the keys to good performance is to keep the multiprocessors on the device as busy as possible. A device in which work is poorly balanced across the multiprocessors will deliver suboptimal performance. Hence, it's important to design your application to use threads and blocks in a way that maximizes hardware utilization and to limit practices that impede the free distribution of work. A key concept in this effort is occupancy, which is explained in the following sections.

Another important concept is the management of system resources allocated for a particular task. How to manage this resource utilization is discussed in the final sections of this chapter.

4.1 OCCUPANCY

Thread instructions are executed sequentially in CUDA, and, as a result, executing other warps when one warp is paused or stalled is the only way to hide latencies and keep the hardware busy. Some metric related to the number of active warps on a multiprocessor is therefore important in determining how effectively the hardware is kept busy. This metric is *occupancy*.

Occupancy is the ratio of the number of active warps per multiprocessor to the maximum number of possible active warps. (To determine the latter number, see the `deviceQuery` code sample in the GPU Computing SDK or refer to Appendix F in the *CUDA C Programming Guide*.) Another way to view occupancy is the percentage of the hardware's ability to process warps that is actively in use.

Higher occupancy does not always equate to higher performance—there is a point above which additional occupancy does not improve performance. However, low occupancy always interferes with the ability to hide memory latency, resulting in performance degradation.

4.2 CALCULATING OCCUPANCY

One of several factors that determine occupancy is register availability. Register storage enables threads to keep local variables nearby for low-latency access. However, the set of registers (known as the *register file*) is a limited commodity that all threads resident on a multiprocessor must share. Registers are allocated to an entire block all at once. So, if each thread block uses many registers, the number of thread blocks that can be resident on a multiprocessor is reduced, thereby lowering the occupancy of the multiprocessor. The maximum number of registers per thread can be set manually at compilation time per-file using the `-maxrregcount` option or per-kernel using the `__launch_bounds__` qualifier (see Section 3.2.6.1).

For purposes of calculating occupancy, the number of registers used by each thread is one of the key factors. For example, devices with compute capability 1.0 and 1.1 have 8,192 32-bit registers per multiprocessor and can have a maximum of 768 simultaneous threads resident (24 warps x 32 threads per warp). This means that in one of these devices, for a multiprocessor to have 100% occupancy, each thread can use at most 10 registers. However, this approach of determining how register count affects occupancy does not take into account the register allocation granularity. For example, on a device of compute capability 1.0, a kernel with 128-thread blocks using 12 registers per thread results in an occupancy of 83% with 5 active 128-thread blocks per multiprocessor, whereas a kernel with 256-thread blocks using the same 12 registers per thread results in an occupancy of 66% because only two 256-thread blocks can reside on a multiprocessor. Furthermore, register allocations are rounded up to the nearest 256 registers per block on devices with compute capability 1.0 and 1.1.

The number of registers available, the maximum number of simultaneous threads resident on each multiprocessor, and the register allocation granularity vary over different compute capabilities. Because of these nuances in register allocation and the fact that a multiprocessor's shared memory is also partitioned between resident thread blocks, the exact relationship between register usage and occupancy can be difficult to determine. The `--ptxas-options=-v` option of `nvcc` details the number of registers used per thread for each kernel. See Section 4.2 of the *CUDA C Programming Guide* for the register allocation formulas for devices of various compute capabilities and Section F.1 of the programming guide for the total number of registers available on those devices. Alternatively, NVIDIA provides an occupancy calculator in the form of an Excel spreadsheet that enables developers to hone in on the optimal balance and to test different possible scenarios more easily. This spreadsheet, shown in CUDA GPU

Occupancy Calculator Usage to Project Occupancy, is called `CUDA_occupancy_calculator.xls` and is located in the `tools` directory of the CUDA SDK.

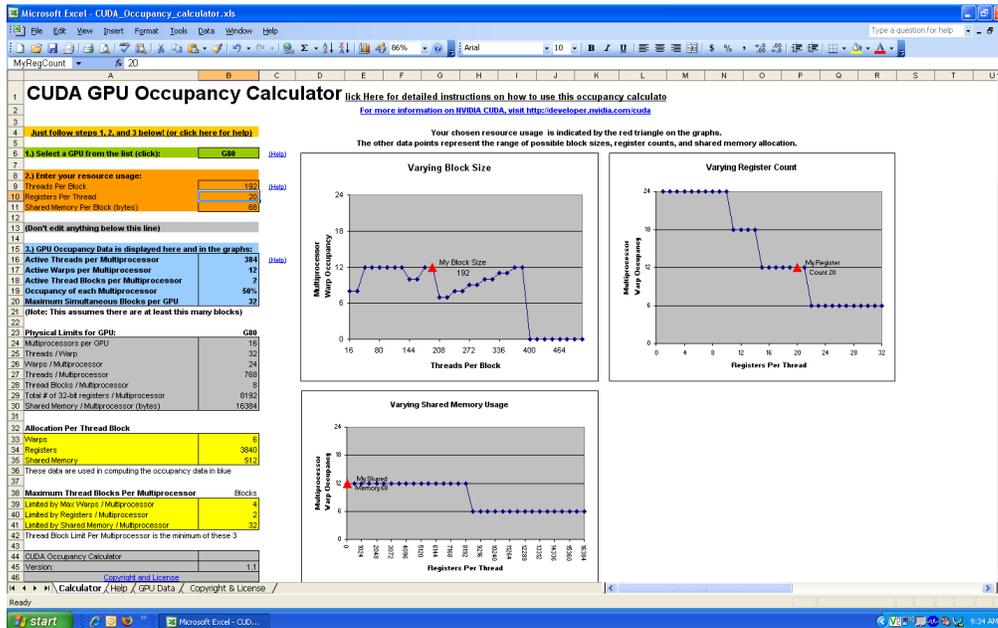


Figure 4.1 CUDA GPU Occupancy Calculator Usage to Project Occupancy

In addition to the calculator spreadsheet, occupancy can be determined using the CUDA profiler.

4.3 HIDING REGISTER DEPENDENCIES

Medium Priority: To hide latency arising from register dependencies, maintain sufficient numbers of active threads per multiprocessor (i.e., sufficient occupancy).

Register dependencies arise when an instruction uses a result stored in a register written by an instruction before it. The latency on current CUDA-enabled GPUs is approximately 24 cycles, so threads must wait 24 cycles before using an arithmetic result. However, this latency can be completely hidden by the execution of threads in other warps. See Section 3.2.6 for details.

4.4 THREAD AND BLOCK HEURISTICS



Medium Priority: The number of threads per block should be a multiple of 32 threads, because this provides optimal computing efficiency and facilitates coalescing.

The dimension and size of blocks per grid and the dimension and size of threads per block are both important factors. The multidimensional aspect of these parameters allows easier mapping of multidimensional problems to CUDA and does not play a role in performance. As a result, this section discusses size but not dimension.

Latency hiding and occupancy depend on the number of active warps per multiprocessor, which is implicitly determined by the execution parameters along with resource (register and shared memory) constraints. Choosing execution parameters is a matter of striking a balance between latency hiding (occupancy) and resource utilization.

Choosing the execution configuration parameters should be done in tandem; however, there are certain heuristics that apply to each parameter individually. When choosing the first execution configuration parameter—the number of blocks per grid, or *grid size*—the primary concern is keeping the entire GPU busy. The number of blocks in a grid should be larger than the number of multiprocessors so that all multiprocessors have at least one block to execute. Furthermore, there should be multiple active blocks per multiprocessor so that blocks that aren't waiting for a `__syncthreads()` can keep the hardware busy. This recommendation is subject to resource availability; therefore, it should be determined in the context of the second execution parameter—the number of threads per block, or *block size*—as well as shared memory usage. To scale to future devices, the number of blocks per kernel launch should be in the thousands.

When choosing the block size, it is important to remember that multiple concurrent blocks can reside on a multiprocessor, so occupancy is not determined by block size alone. In particular, a larger block size does not imply a higher occupancy. For example, on a device of compute capability 1.1 or lower, a kernel with a maximum block size of 512 threads results in an occupancy of 66 percent because the maximum number of threads per multiprocessor on such a device is 768. Hence, only a single block can be active per multiprocessor. However, a kernel with 256 threads per block on such a device can result in 100 percent occupancy with three resident active blocks.

As mentioned in Section 4.1, higher occupancy does not always equate to better performance. For example, improving occupancy from 66 percent to 100 percent generally does not translate to a similar increase in performance. A lower occupancy kernel will have more registers available per thread than a higher occupancy kernel, which may result in less register spilling to local memory. Typically, once an occupancy

of 50 percent has been reached, additional increases in occupancy do not translate into improved performance.

There are many such factors involved in selecting block size, and inevitably some experimentation is required. However, a few rules of thumb should be followed:

- ▶ Threads per block should be a multiple of warp size to avoid wasting computation on under-populated warps and to facilitate coalescing.
- ▶ A minimum of 64 threads per block should be used, but only if there are multiple concurrent blocks per multiprocessor.
- ▶ Between 128 and 256 threads per block is a better choice and a good initial range for experimentation with different block sizes.
- ▶ Use several (3 to 4) smaller thread blocks rather than one large thread block per multiprocessor if latency affects performance. This is particularly beneficial to kernels that frequently call `__syncthreads()`.

Note that when a thread block allocates more registers than are available on a multiprocessor, the kernel launch fails, as it will when too much shared memory or too many threads are requested.

4.5 EFFECTS OF SHARED MEMORY

Shared memory can be helpful in several situations, such as helping to coalesce or eliminate redundant access to global memory. However, it also can act as a constraint on occupancy. In many cases, the amount of shared memory required by a kernel is related to the block size that was chosen, but the mapping of threads to shared memory elements does not need to be one-to-one. For example, it may be desirable to use a 32×32 element shared memory array in a kernel, but because the maximum number of threads per block is 512, it is not possible to launch a kernel with 32×32 threads per block. In such cases, kernels with 32×16 or 32×8 threads can be launched with each thread processing two or four elements, respectively, of the shared memory array. The approach of using a single thread to process multiple elements of a shared memory array can be beneficial even if limits such as threads per block are not an issue. This is because some operations common to each element can be performed by the thread once, amortizing the cost over the number of shared memory elements processed by the thread.

A useful technique to determine the sensitivity of performance to occupancy is through experimentation with the amount of dynamically allocated shared memory, as specified in the third parameter of the execution configuration. By simply increasing this parameter (without modifying the kernel), it is possible to effectively reduce the occupancy of the kernel and measure its effect on performance.

As mentioned in the previous section, once an occupancy of more than 50 percent has been reached, it generally does not pay to optimize parameters to obtain higher occupancy ratios. The previous technique can be used to determine whether such a plateau has been reached.

Chapter 5.

INSTRUCTION OPTIMIZATIONS

Awareness of how instructions are executed often permits low-level optimizations that can be useful, especially in code that is run frequently (the so-called hot spot in a program). Best practices suggest that this optimization be performed after all higher-level optimizations have been completed.

5.1 ARITHMETIC INSTRUCTIONS

Single-precision floats provide the best performance, and their use is highly encouraged.

The throughput of individual arithmetic operations on devices of compute capability 1.x is detailed in Section F.3 of the *CUDA C Programming Guide*, and the throughput of these operations on devices of compute capability 2.x is detailed in Section F.4 of the programming guide.

5.1.1 Division and Modulo Operations



Low Priority: Use shift operations to avoid expensive division and modulo calculations.

Integer division and modulo operations are particularly costly and should be avoided or replaced with bitwise operations whenever possible: If n is a power of 2, (i/n) is equivalent to $(i \gg \log_2(n))$ and $(i \% n)$ is equivalent to $(i \& (n-1))$.

The compiler will perform these conversions if n is literal. (For further information, refer to Chapter 5 of the *CUDA C Programming Guide*).

5.1.2 Reciprocal Square Root

The reciprocal square root should always be invoked explicitly as `rsqrtf()` for single precision and `rsqrt()` for double precision. The compiler optimizes `1.0f/sqrtf(x)` into `rsqrtf()` only when this does not violate IEEE-754 semantics.

5.1.3 Other Arithmetic Instructions



Low Priority: Avoid automatic conversion of doubles to floats.

The compiler must on occasion insert conversion instructions, introducing additional execution cycles. This is the case for

- ▶ Functions operating on `char` or `short` whose operands generally need to be converted to an `int`
- ▶ Double-precision floating-point constants (defined without any type suffix) used as input to single-precision floating-point computations

The latter case can be avoided by using single-precision floating-point constants, defined with an `f` suffix such as `3.141592653589793f`, `1.0f`, `0.5f`. This suffix has accuracy implications in addition to its ramifications on performance. The effects on accuracy are discussed in Chapter 7. Note that this distinction is particularly important to performance on devices of compute capability 2.x.

For single-precision code, use of the `float` type and the single-precision math functions are highly recommended. When compiling for devices without native double-precision support such as devices of compute capability 1.2 and earlier, each double-precision floating-point variable is converted to single-precision floating-point format (but retains its size of 64 bits) and double-precision arithmetic is demoted to single-precision arithmetic.

It should also be noted that the CUDA math library's complementary error function, `erfcf()`, is particularly fast with full single-precision accuracy.

5.1.4 Math Libraries



Medium Priority: Use the fast math library whenever speed trumps precision.

Two types of runtime math operations are supported. They can be distinguished by their names: some have names with prepended underscores, whereas others do not (e.g., `__functionName()` versus `functionName()`). Functions following the `__functionName()` naming convention map directly to the hardware level. They are faster but provide

somewhat lower accuracy (e.g., `__sinf(x)` and `__expf(x)`). Functions following `functionName()` naming convention are slower but have higher accuracy (e.g., `sinf(x)` and `expf(x)`). The throughput of `__sinf(x)`, `__cosf(x)`, and `__expf(x)` is much greater than that of `sinf(x)`, `cosf(x)`, `tanf(x)`. The latter become even more expensive (about an order of magnitude slower) if the magnitude of the argument `x` needs to be reduced. Moreover, in such cases, the argument-reduction code uses local memory, which can affect performance even more because of the high latency of local memory. More details are available in the *CUDA C Programming Guide*.

Note also that whenever sine and cosine of the same argument are computed, the `sincos...` family of instructions should be used to optimize performance:

- ▶ `sincosf()` for single-precision fast math (see next paragraph)
- ▶ `sincosf()` for regular single-precision
- ▶ `sincos()` for double precision

The `-use_fast_math` compiler option of `nvcc` coerces every `functionName()` call to the equivalent `__functionName()` call. This switch should be used whenever accuracy is a lesser priority than the performance. This is frequently the case with transcendental functions. Note this switch is effective only on single-precision floating point.



Medium Priority: Prefer faster, more specialized math functions over slower, more general ones when possible.

For small integer powers (e.g., x^2 or x^3), explicit multiplication is almost certainly faster than the use of general exponentiation routines such as `pow()`. While compiler optimization improvements continually seek to narrow this gap, explicit multiplication (or the use of an equivalent purpose-built inline function or macro) can have a significant advantage. This advantage is increased when several powers of the same base are needed (e.g., where both x^2 and x^5 are calculated in close proximity), as this aids the compiler in its common sub-expression elimination (CSE) optimization.

For exponentiation using base 2 or 10, use the functions `exp2()` or `expf2()` and `exp10()` or `expf10()` rather than the functions `pow()` or `powf()`. Both `pow()` and `powf()` are heavy-weight functions in terms of register pressure and instruction count due to the numerous special cases arising in general exponentiation and the difficulty of achieving good accuracy across the entire ranges of the base and the exponent. The functions `exp2()`, `exp2f()`, `exp10()`, and `exp10f()`, on the other hand, are similar to `exp()` and `expf()` in terms of performance, and can be as much as ten times faster than their `pow()/powf()` equivalents.

For exponentiation with an exponent of $1/3$, use the `cbrt()` or `cbrtf()` function rather than the generic exponentiation functions `pow()` or `powf()`, as the former are significantly faster than the latter. Likewise, for exponentiation with an exponent of $-1/3$, use `rcbrt()` or `rcbrtf()`.

Replace `sin(π *<expr>)` with `sinpi(<expr>)` and `cos(π *<expr>)` with `cospi(<expr>)`. This is advantageous with regard to both accuracy and performance. As a particular example, to evaluate the sine function in degrees instead of radians, use `sinpi(x/180.0)`. Similarly, the single-precision functions `sinpif()` and `cospif()` should replace calls to `sinf()` and `cosf()` when the function argument is of the form `π *<expr>`. (The performance advantage `sinpi()` has over `sin()` is due to simplified argument reduction; the accuracy advantage is because `sinpi()` multiplies by π only implicitly, effectively using an infinitely precise mathematical π rather than a single- or double-precision approximation thereof.)

5.2 MEMORY INSTRUCTIONS



High Priority: Minimize the use of global memory. Prefer shared memory access where possible.

Memory instructions include any instruction that reads from or writes to shared, local, or global memory. When accessing uncached local or global memory, there are 400 to 600 clock cycles of memory latency.

As an example, the assignment operator in the following sample code has a high throughput, but, crucially, there is a latency of 400 to 600 clock cycles to read data from global memory:

```
__shared__ float shared[32];  
__device__ float device[32];  
shared[threadIdx.x] = device[threadIdx.x];
```

Much of this global memory latency can be hidden by the thread scheduler if there are sufficient independent arithmetic instructions that can be issued while waiting for the global memory access to complete. However, it is best to avoid accessing global memory whenever possible.

Chapter 6.

CONTROL FLOW

6.1 BRANCHING AND DIVERGENCE



High Priority: Avoid different execution paths within the same warp.

Any flow control instruction (`if`, `switch`, `do`, `for`, `while`) can significantly affect the instruction throughput by causing threads of the same warp to diverge; that is, to follow different execution paths. If this happens, the different execution paths must be serialized, increasing the total number of instructions executed for this warp. When all the different execution paths have completed, the threads converge back to the same execution path.

To obtain best performance in cases where the control flow depends on the thread ID, the controlling condition should be written so as to minimize the number of divergent warps.

This is possible because the distribution of the warps across the block is deterministic as mentioned in Section 4.1 of the *CUDA C Programming Guide*. A trivial example is when the controlling condition depends only on $(\text{threadIdx} / \text{WSIZE})$ where `WSIZE` is the warp size.

In this case, no warp diverges because the controlling condition is perfectly aligned with the warps.

6.2 BRANCH PREDICATION

Low Priority: Make it easy for the compiler to use branch predication in lieu of loops or control statements.

Sometimes, the compiler may unroll loops or optimize out `if` or `switch` statements by using branch predication instead. In these cases, no warp can ever diverge. The programmer can also control loop unrolling using

```
#pragma unroll
```

For more information on this pragma, refer to the *CUDA C Programming Guide*.

When using branch predication, none of the instructions whose execution depends on the controlling condition is skipped. Instead, each such instruction is associated with a per-thread condition code or predicate that is set to true or false according to the controlling condition. Although each of these instructions is scheduled for execution, only the instructions with a true predicate are actually executed. Instructions with a false predicate do not write results, and they also do not evaluate addresses or read operands.

The compiler replaces a branch instruction with predicated instructions only if the number of instructions controlled by the branch condition is less than or equal to a certain threshold: If the compiler determines that the condition is likely to produce many divergent warps, this threshold is 7; otherwise it is 4.

6.3 LOOP COUNTERS SIGNED VS. UNSIGNED

Medium Priority: Use signed integers rather than unsigned integers as loop counters.

In the C language standard, unsigned integer overflow semantics are well defined, whereas signed integer overflow causes undefined results. Therefore, the compiler can optimize more aggressively with signed arithmetic than it can with unsigned arithmetic. This is of particular note with loop counters: since it is common for loop counters to have values that are always positive, it may be tempting to declare the counters as unsigned. For slightly better performance, however, they should instead be declared as signed.

For example, consider the following code:

```
for (i = 0; i < n; i++) {
    out[i] = in[offset + stride*i];
}
```

Here, the sub-expression `stride*i` could overflow a 32-bit integer, so if `i` is declared as unsigned, the overflow semantics prevent the compiler from using some optimizations that might otherwise have applied, such as strength reduction. If instead `i` is declared as signed, where the overflow semantics are undefined, the compiler has more leeway to use these optimizations.

Chapter 7.

GETTING THE RIGHT ANSWER

Obtaining the right answer is clearly the principal goal of all computation. On parallel systems, it is possible to run into difficulties not typically found in traditional serial-oriented programming. These include threading issues, unexpected values due to the way floating-point values are computed, and challenges arising from differences in the way CPU and GPU processors operate. This chapter examines issues that can affect the correctness of returned data and points to appropriate solutions.

7.1 DEBUGGING

The CUDA debugger, CUDA-GDB, is a valuable debugging tool. It is a port of the GNU Debugger version 6.6 and runs on 32-bit and 64-bit Linux. See the *CUDA-GDB User Manual* for more details.

For Microsoft Windows Vista and 7, the NVIDIA Parallel Nsight debugging and profiling tool is available as a free plugin for Microsoft Visual Studio. See <http://developer.nvidia.com/object/nsight.html> for more details.

7.2 NUMERICAL ACCURACY AND PRECISION

Incorrect or unexpected results arise principally from issues of floating-point accuracy due to the way floating-point values are computed and stored. The following sections explain the principal items of interest. Other peculiarities of floating-point arithmetic are presented in Section F.2 of the *CUDA C Programming Guide*.

7.2.1 Single vs. Double Precision

Devices of compute capability 1.3 and higher provide native support for double-precision floating-point values (that is, values 64 bits wide). Results obtained using double-precision arithmetic will frequently differ from the same operation performed via single-precision arithmetic due to the greater precision of the former and due to rounding issues. Therefore, it is important to be sure to compare like with like and to express the results within a certain tolerance rather than expecting them to be exact.

Whenever doubles are used, use at least the `-arch=sm_13` switch on the `nvcc` command line; see Sections 3.1.3 and 3.1.4 of the *CUDA C Programming Guide* for more details.

7.2.2 Floating-Point Math Is Not Associative

Each floating-point arithmetic operation involves a certain amount of rounding. Consequently, the order in which arithmetic operations are performed is important. If *A*, *B*, and *C* are floating-point values, $(A+B)+C$ is not guaranteed to equal $A+(B+C)$ as it is in symbolic math. When you parallelize computations, you potentially change the order of operations and therefore the parallel results might not match sequential results. This limitation is not specific to CUDA, but an inherent part of parallel computation on floating-point values.

7.2.3 Promotions to Doubles and Truncations to Floats

When comparing the results of computations of float variables between the host and device, make sure that promotions to double precision on the host do not account for different numerical results. For example, if the code segment

```
float a;  
...  
a = a*1.02;
```

were performed on a device of compute capability 1.2 or less, or on a device with compute capability 1.3 but compiled without enabling double precision (as mentioned above), then the multiplication would be performed in single precision. However, if the code were performed on the host, the literal `1.02` would be interpreted as a double-precision quantity and `a` would be promoted to a double, the multiplication would be performed in double precision, and the result would be truncated to a float—thereby yielding a slightly different result. If, however, the literal `1.02` were replaced with `1.02f`, the result would be the same in all cases because no promotion to doubles would occur. To ensure that computations use single-precision arithmetic, always use float literals.

In addition to accuracy, the conversion between doubles and floats (and vice versa) has a detrimental effect on performance, as discussed in Chapter 5.

7.2.4 IEEE 754 Compliance

All CUDA compute devices follow the IEEE 754 standard for binary floating-point representation, with some small exceptions. These exceptions, which are detailed in Section F.2 of the *CUDA C Programming Guide*, can lead to results that differ from IEEE 754 values computed on the host system.

One of the key differences is the fused multiply-add (FMAD) instruction, which combines multiply-add operations into a single instruction execution and truncates the intermediate result of the multiplication. Its result will differ at times from results obtained by doing the two operations separately.

7.2.5 x86 80-bit Computations

x86 processors can use an 80-bit “double extended precision” math when performing floating-point calculations. The results of these calculations can frequently differ from pure 64-bit operations performed on the CUDA device. To get a closer match between values, set the x86 host processor to use regular double or single precision (64 bits and 32 bits, respectively). This is done with the `FLDCW` assembly instruction or the equivalent operating system API.

Chapter 8.

MULTI-GPU PROGRAMMING

8.1 INTRODUCTION TO MULTI-GPU

Programming a multi-GPU application is no different from programming an application to utilize multiple cores or sockets because CUDA is completely orthogonal to CPU thread management or message passing APIs. The only new concept is selecting the correct GPU, which in most cases is an available GPU (one without an existing context). In fact, GPU acceleration can be added straightforwardly to existing multi-threaded CPU code, whether it uses lightweight or heavyweight threads – all one has to do is port the compute-intensive portions of the code to GPU and add calls to transfer data between CPU and GPU, leaving the inter-CPU-thread communication code unchanged.

8.2 MULTI-GPU PROGRAMMING

In order to issue work to a GPU, a context (view of a GPU) is established between a CPU thread (or group of threads) and the GPU. The context contains all of the driver state that refers to that GPU – the virtual address space, streams, events, allocated blocks of memory, etc. Only one context can be active on a GPU at any particular instant; similarly, a CPU thread can execute commands (perform memory allocations, launch kernels, etc.) in only one context at any particular instant.

A context is established automatically by the CUDA Runtime during the program's first call to a function that changes state (such as `cudaMalloc()`, etc.), so one can force the creation of a context by calling `cudaFree(0)`. Note that a context is created on GPU 0 by default, unless another GPU is selected explicitly prior to context creation with a `cudaSetDevice()` call. The context is destroyed either by calling `cudaDeviceReset()` or when the controlling CPU process exits.

In order to issue work to p GPUs concurrently, a program can either use p CPU threads, each with its own context, or it can use one CPU thread that swaps among several contexts, or some combination thereof. CPU threads can be lightweight (pthreads, OpenMP, etc.) or heavyweight (MPI). Note that any CPU multi-threading or message-passing API or library can be used, as CPU thread management is completely orthogonal to CUDA. For example, one can add GPU processing to an existing MPI application by porting the compute-intensive portions of the code without changing the communication structure.

Even though a GPU can execute calls from one context at a time, it can belong to multiple contexts. For example, it is possible for several CPU threads to establish separate contexts with the same GPU (though multiple CPU threads within the same process accessing the same GPU would normally share the same context by default). The CUDA driver manages the GPU's switching among those contexts (switching to the next waiting context whenever the GPU goes idle) as well as partitioning memory among the contexts (GPU memory allocated in one context cannot be accessed from another context since the allocations are in separate virtual address spaces).

8.3 SELECTING A GPU

In many cases, the intent is for each CPU thread to control a different GPU. Achieving this is straightforward if a program spawns as many lightweight threads as there are GPUs – one can derive GPU index from thread ID. For example, OpenMP thread ID can be readily used to select GPUs.

MPI rank can be used to choose a GPU reliably as long as all MPI processes are launched on a single host node. However, when MPI processes are launched across several cluster nodes, the assignment of processes to host nodes depends on the MPI implementation and launch configuration (hostfile), preventing reliable selection of a unique GPU. To address this issue, one could implement a negotiation protocol among MPI processes running on the same host (using `MPI_Get_processor_name()` call), so that each one claims a unique GPU. A less robust option is for the GPU selection to rely on a specific allocation MPI processes to nodes (for example, allocating consecutive processes to the same node).

Starting with CUDA 2.2, Linux drivers provide an alternative and much simpler way to ensure that each GPU is assigned to at most one context – the administrator can select exclusive mode via the SMI (System Management Interface) tool that comes with the driver. In exclusive mode, if the application does not specify a GPU with a `cudaSetDevice()` call, the context is no longer created on GPU 0, but on a GPU without an active context. If there are no available GPUs, or if `cudaSetDevice()` specifies a GPU already having an active context, the first CUDA call that attempts to change the device state will fail and return an error.

8.4 INTER-GPU COMMUNICATION

All inter-GPU communication takes place via host nodes. GPU and the controlling CPU thread communicate via memcpy, while CPU threads exchange data using the same methods as applications not accelerated with GPUs. Thus, best performance is achieved when one follows best practices for the CPU-GPU communication as well as CPU-CPU communication. Note that the two are independent and orthogonal.

Communication between CPU and GPU is most efficient when using pinned memory on the CPU. Pinned memory enables asynchronous memory copies (allowing for overlap with both CPU and GPU execution), as well as improves PCIe throughput on FSB systems. Please refer to the *CUDA C Programming Guide* for more details and examples of pinned memory usage.

Lightweight CPU threads exchange data most efficiently via shared memory. Note that in order for a pinned memory region to be viewed as pinned by CPU threads other than the one that allocated it, one must call `cudaHostAlloc()` with the `cudaHostAllocPortable` flag. A common communication pattern will be for one CPU thread to copy data from its GPU to a shared host memory region, after which another CPU thread will copy the data to its GPU. Users of NUMA systems will have to follow the same best practices as for communication between non-GPU accelerated CPU threads.

Communication between heavy-weight processes takes place via message passing, for example MPI. Once data has been copied from GPU to CPU it is transferred to another process by calling one of the MPI functions. For example, one possible pattern when exchanging data between two GPUs is for a CPU thread to call a device-to-host `cudaMemcpy()`, then `MPI_Sendrecv()`, then a host-to-device `cudaMemcpy()`. Note that performance of the MPI function is not dependent on the fact that data originated at or is destined for a GPU. Since MPI provides several variations for most of its communication functions, the choice of a function should be dictated by the best practices guide for the MPI implementation as well as the system and network.

8.5 COMPILING MULTI-GPU APPLICATIONS

Code that includes GPU kernels or CUDA runtime kernel launch syntax must be compiled with `nvcc`, the compiler driver. `nvcc` invokes either `gcc` (on Linux) or Microsoft Visual C++ compiler (on Windows) for non-GPU code. One can pass options to the host C/C++ compiler through `nvcc` by using `-Xcompiler` option (for more details please refer to `nvcc` documentation included in the CUDA toolkit). For example, one would specify `nvcc -Xcompiler /openmp` in order to pass the `-fopenmp` option to the host `gcc` compiler (the same option for MSVC compiler is `/openmp`).

MPI applications are typically compiled using `mpicc`, the MPI compiler driver. While it is possible to pass all the necessary flags through `nvcc`, it is often simpler to compile MPI code and CUDA kernel code into separate object files. This approach also fits many larger projects well, since they separate the communication and computation source code already.

8.6 INFINIBAND

NVIDIA GPUDirect™ technology allows the sharing of CUDA pinned host memory with other devices. This allows accelerated transfers of GPU data to other devices, such as supported Infiniband network adapters. If GPUDirect support is not available for your network device, network transfer throughput can be reduced. A possible workaround is to disable RDMA. For the OpenMPI implementation, this can be achieved by passing the flag `-mca btl_openib_flags 1` to `mpirun`.

Appendix A.

RECOMMENDATIONS AND BEST PRACTICES

This appendix contains a list of all the recommendations for optimization and the list of best practices that are explained in this document.

A.1 Overall Performance Optimization Strategies

Performance optimization revolves around three basic strategies:

- ▶ Maximizing parallel execution
- ▶ Optimizing memory usage to achieve maximum memory bandwidth
- ▶ Optimizing instruction usage to achieve maximum instruction throughput

Maximizing parallel execution starts with structuring the algorithm in a way that exposes as much data parallelism as possible. Once the parallelism of the algorithm has been exposed, it needs to be mapped to the hardware as efficiently as possible. This is done by carefully choosing the execution configuration of each kernel launch. The application should also maximize parallel execution at a higher level by explicitly exposing concurrent execution on the device through streams, as well as maximizing concurrent execution between the host and the device.

Optimizing memory usage starts with minimizing data transfers between the host and the device because those transfers have much lower bandwidth than internal device data transfers. Kernel access to global memory also should be minimized by maximizing the use of shared memory on the device. Sometimes, the best optimization might even be to avoid any data transfer in the first place by simply recomputing the data whenever it is needed.

The effective bandwidth can vary by an order of magnitude depending on the access pattern for each type of memory. The next step in optimizing memory usage is therefore to organize memory accesses according to the optimal memory access patterns. This optimization is especially important for global memory accesses, because latency of access costs hundreds of clock cycles. Shared memory accesses, in counterpoint, are usually worth optimizing only when there exists a high degree of bank conflicts.

As for optimizing instruction usage, the use of arithmetic instructions that have low throughput should be avoided. This suggests trading precision for speed when it does not affect the end result, such as using intrinsics instead of regular functions or single precision instead of double precision. Finally, particular attention must be paid to control flow instructions due to the SIMT (single instruction multiple thread) nature of the device.

A.2 High-Priority Recommendations

- ▶ To get the maximum benefit from CUDA, focus first on finding ways to parallelize sequential code. (Section 0)
- ▶ Use the effective bandwidth of your computation as a metric when measuring performance and optimization benefits. (Section 2.2)
- ▶ Minimize data transfer between the host and the device, even if it means running some kernels on the device that do not show performance gains when compared with running them on the host CPU. (Section 3.1)
- ▶ Ensure global memory accesses are coalesced whenever possible. (Section 3.2.1)
- ▶ Minimize the use of global memory. Prefer shared memory access where possible. (Section 5.2)
- ▶ Avoid different execution paths within the same warp. (Section 6.1)

A.3 Medium-Priority Recommendations

- ▶ Accesses to shared memory should be designed to avoid serializing requests due to bank conflicts. (Section 3.2.2.1)
- ▶ Use shared memory to avoid redundant transfers from global memory. (Section 3.2.2.2)
- ▶ To hide latency arising from register dependencies, maintain sufficient numbers of active threads per multiprocessor (i.e., sufficient occupancy). (Sections 3.2.6 and 4.3)
- ▶ The number of threads per block should be a multiple of 32 threads, because this provides optimal computing efficiency and facilitates coalescing. (Section 4.4)
- ▶ Use the fast math library whenever speed trumps precision. (Section 5.1.4)

- ▶ Prefer faster, more specialized math functions over slower, more general ones when possible. (Section 5.1.4)
- ▶ Use signed integers rather than unsigned integers as loop counters. (Section 6.3)

A.4 Low-Priority Recommendations

- ▶ On version 2.2 of the CUDA Toolkit (and later), use zero-copy operations on integrated GPUs. (Section 3.1.3)
- ▶ For kernels with long argument lists, place some arguments into constant memory to save shared memory. (Section 3.2.2.4)
- ▶ Use shift operations to avoid expensive division and modulo calculations. (Section 5.1.1)
- ▶ Avoid automatic conversion of doubles to floats. (Section 5.1.3)
- ▶ Make it easy for the compiler to use branch predication in lieu of loops or control statements. (Section 6.2)

Appendix B.

NVCC COMPILER SWITCHES

B.1 NVCC

The NVIDIA `nvcc` compiler driver converts `.cu` files into C for the host system and CUDA assembly or binary instructions for the device. It supports a spate of switches, of which the following are especially useful for optimization and related best practices:

- ▶ `-arch=sm_13` or higher is required for double precision. See Section 7.2.1.
- ▶ `-maxrregcount=N` specifies the maximum number of registers kernels can use at a per-file level. See Section 3.2.6.1. (See also the `__launch_bounds__` qualifier discussed in Section B.17 of the *CUDA C Programming Guide* to control the number of registers used on a per-kernel basis.)
- ▶ `--ptxas-options=-v` or `-Xptxas=-v` lists per-kernel register, shared, and constant memory usage.
- ▶ `-use_fast_math` compiler option of `nvcc` coerces every `functionName()` call to the equivalent `__functionName()` call. This makes the code run faster at the cost of slightly diminished precision and accuracy. See Section 5.1.4.

Appendix C.

REVISION HISTORY

C.1 Version 3.0

- ▶ Added compute capability 2.0.
- ▶ Devices of compute capability 2.0 have an L1 cache of configurable size for global and local memory (see Section F.4.1 of the *CUDA C Programming Guide*). Note that the L1 cache has higher bandwidth than the texture cache and therefore obviates some of the benefits of texture fetch seen in devices of compute capability 1.x. See Section 3.2.4.1.
- ▶ Removed references to device emulation mode, which is deprecated in CUDA Toolkit 3.0 and will be removed in CUDA Toolkit 3.1.
- ▶ The CUFFT and CUBLAS libraries can now interoperate with applications that use the Driver API.
- ▶ Added a recommendation for the use of `exp2()` or `exp10()` in preference to `pow()` to Section 5.1.4.
- ▶ The `__launch_bounds__` kernel definition qualifier can now be used to control register usage on a per-kernel basis (in contrast to the `-maxrregcount` command-line option of `nvcc`, which controls this on a per-file basis). See Section 3.2.6.1 of this guide and Section B.17 of the *CUDA C Programming Guide*.
- ▶ Note importance of distinguishing single-precision floating-point constants and arithmetic from double-precision constants and arithmetic for performance on devices of compute capability 2.0 in Section 5.1.3.
- ▶ Devices of compute capability 2.0 can multicast shared memory accesses in addition to the broadcast mechanism in devices of compute capability 1.x.
- ▶ Added Chapter 8 on multi-GPU programming.

C.2 Version 3.1

- ▶ Added Section 3.3 on memory allocation.
- ▶ Added fourth bullet to rules of thumb for block size selection in Section 4.4.
- ▶ Added Section 6.3 on signed versus unsigned loop counters.

C.3 Version 3.2

- ▶ `CUdeviceptr` is now a 64-bit value in 64-bit applications, so it is no longer necessary to cast `CUdeviceptr` values with `(void*)(size_t)` when passing them as arguments to kernels using the CUDA Driver API; this casting is now effectively a no-op. As such, the type casts have been removed from the example code in Section 1.3.4.
- ▶ Corrected discussion in Section 3.2.6 of the necessary numbers of active threads per multiprocessor to hide latency on devices of compute capability 2.0.

C.4 Version 4.0

- ▶ Added recommendation for the use of explicit multiplication in place of `pow()` for small integer powers in Section 5.1.4.
- ▶ Added recommendations for the use (when applicable) of `sinpi()`, `cospi()`, `cbrt()`, and `rcbrt()` in Section 5.1.4.
- ▶ Modified API recommendation in Section 1.3: most applications should now prefer the CUDA Runtime API over the CUDA Driver API.
- ▶ Revised Chapter 8 to better reflect the multi-GPU features of CUDA Toolkit 4.0.
- ▶ Minor clarifications.

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