Profiling and Parallelizing with the OpenACC Toolkit

OpenACC Course: Lecture 2 – October 15, 2015

Course Syllabus

Oct 1:	Introduction to OpenACC
Oct 6:	Office Hours
Oct 15:	Profiling and Parallelizing with the OpenACC Toolkit
Oct 20:	Office Hours
Oct 29:	Expressing Data Locality and Optimizations with OpenACC
Nov 3:	Office Hours
Nov 12:	Advanced OpenACC Techniques
Nov 24:	Office Hours

Agenda

Introduction to Accelerated Computing

Identifying Available Parallelism

Expressing Parallelism with OpenACC

Next Steps and Homework

Introduction to Accelerated Computing

Accelerated Computing

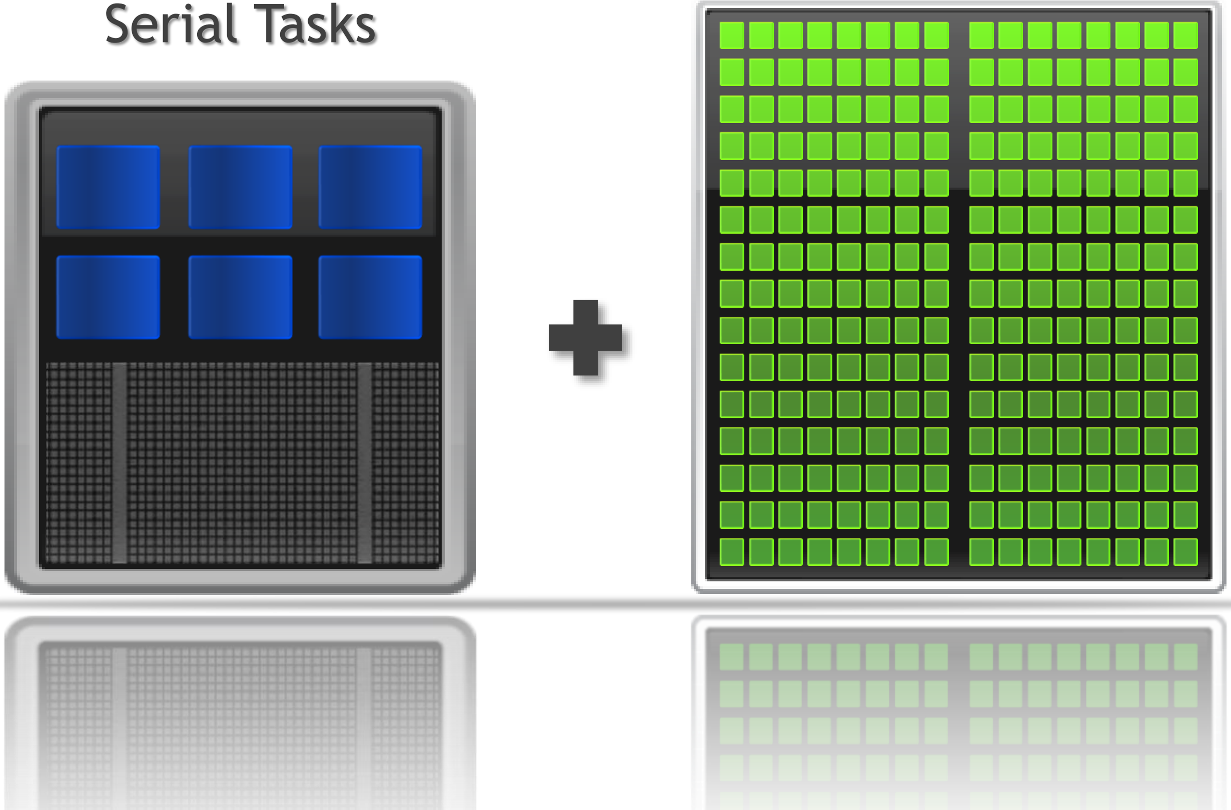
10x Performance & 5x Energy Efficiency for HPC

CPU

Optimized for
Serial Tasks

GPU Accelerator

Optimized for
Parallel Tasks

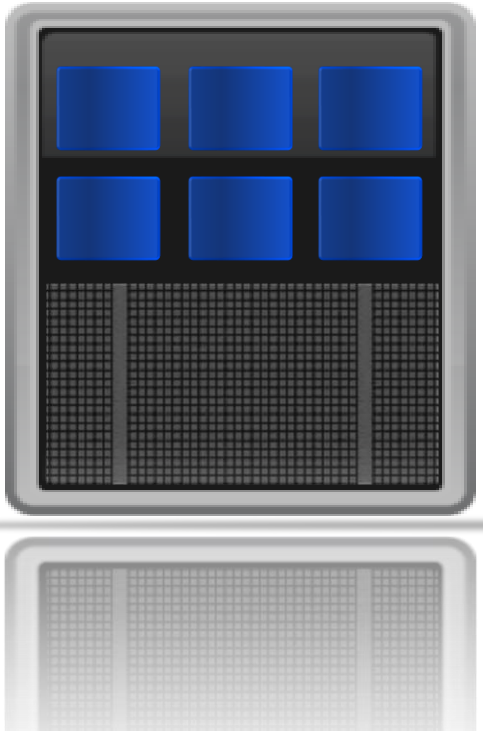


Accelerated Computing

10x Performance & 5x Energy Efficiency for HPC

CPU

Optimized for Serial Tasks



CPU Strengths

- Very large main memory
- Very fast clock speeds
- Latency optimized via large caches
- Small number of threads can run very quickly

CPU Weaknesses

- Relatively low memory bandwidth
- Cache misses very costly
- Low performance/watt

Accelerated Computing

10x Performance & 5x Energy Efficiency for HPC

GPU Strengths

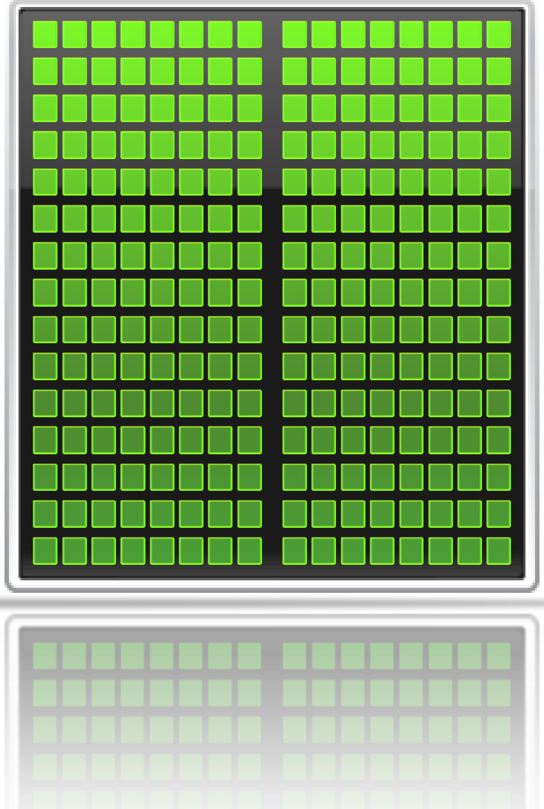
- High bandwidth main memory
- Significantly more compute resources
- Latency tolerant via parallelism
- High throughput
- High performance/watt

GPU Weaknesses

- Relatively low memory capacity
- Low per-thread performance

GPU Accelerator

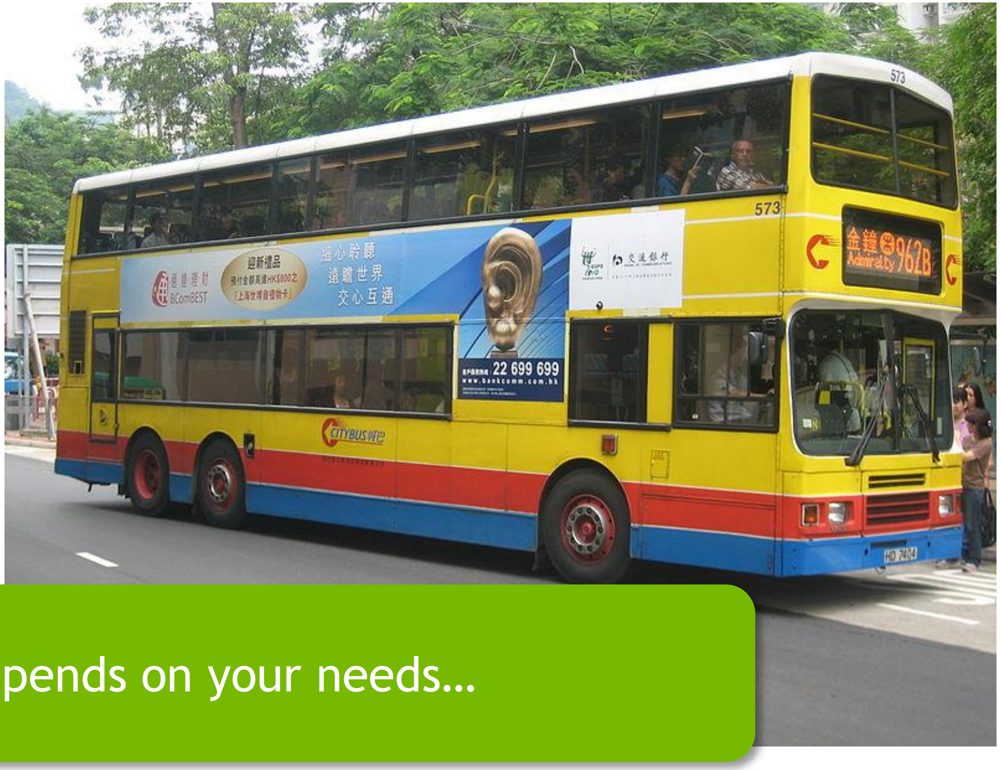
Optimized for
Parallel Tasks



Speed v. Throughput

Speed

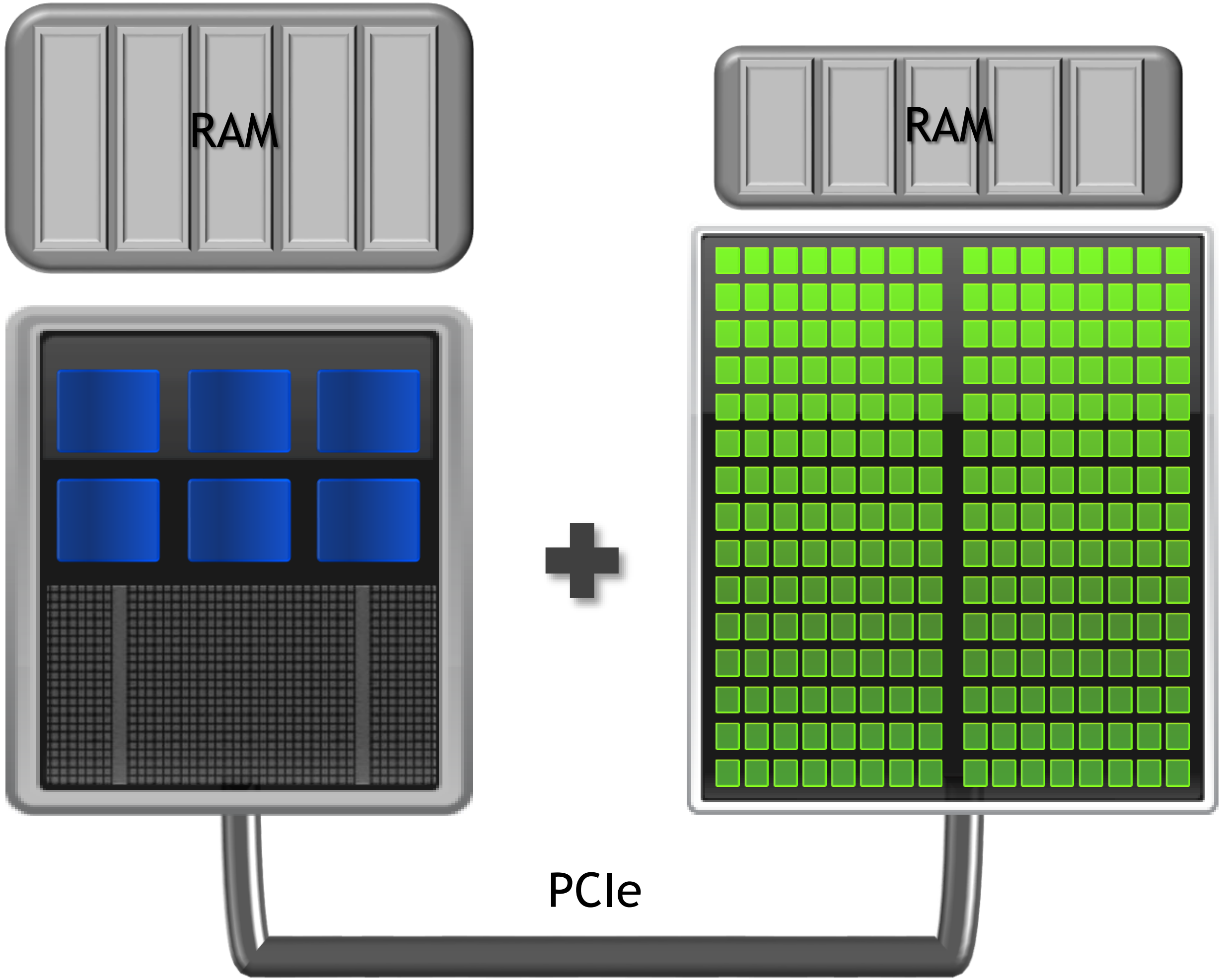
Throughput



Which is better depends on your needs…

*Images from Wikimedia Commons via Creative Commons

Accelerator Nodes



CPU and GPU have distinct memories

- CPU generally larger and slower
- GPU generally smaller and faster

CPU and GPU communicate via PCIe

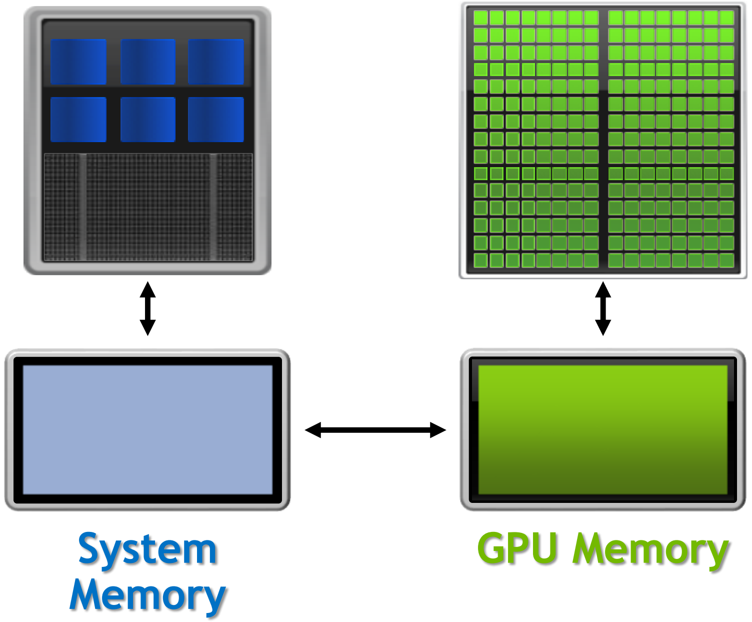
- Data must be copied between these memories over PCIe
- PCIe Bandwidth is much lower than either memories

CUDA Unified Memory

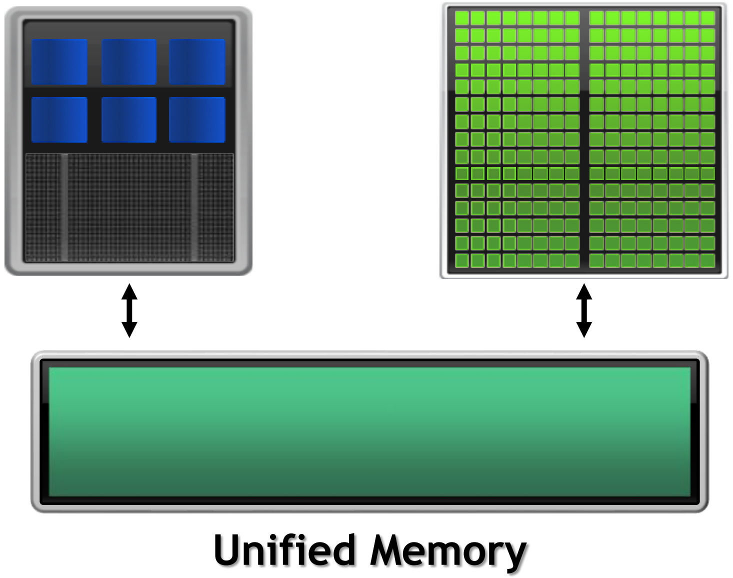
Simplified Developer Effort

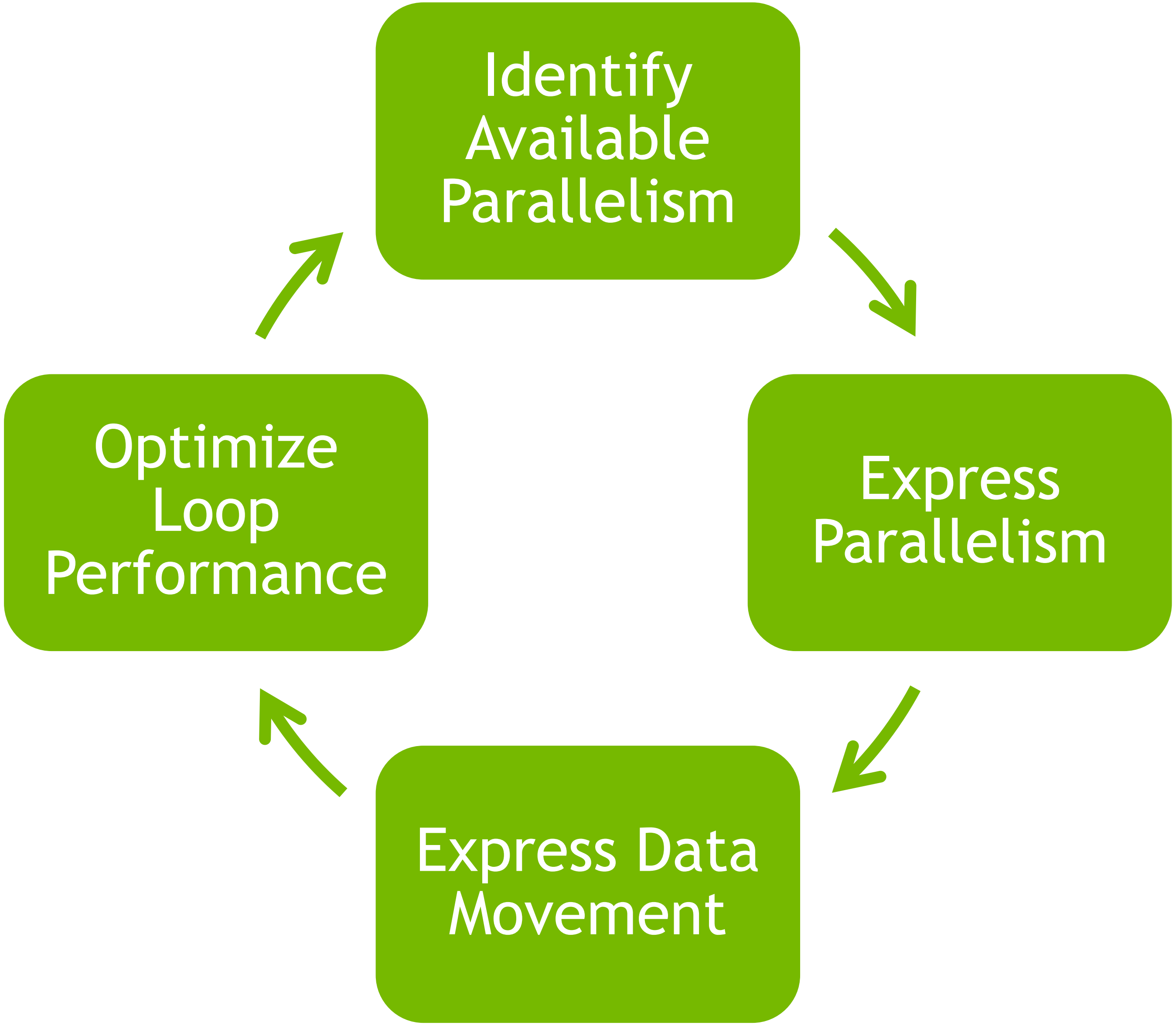
Sometimes referred to as “managed memory.”

Without Unified Memory



With Unified Memory



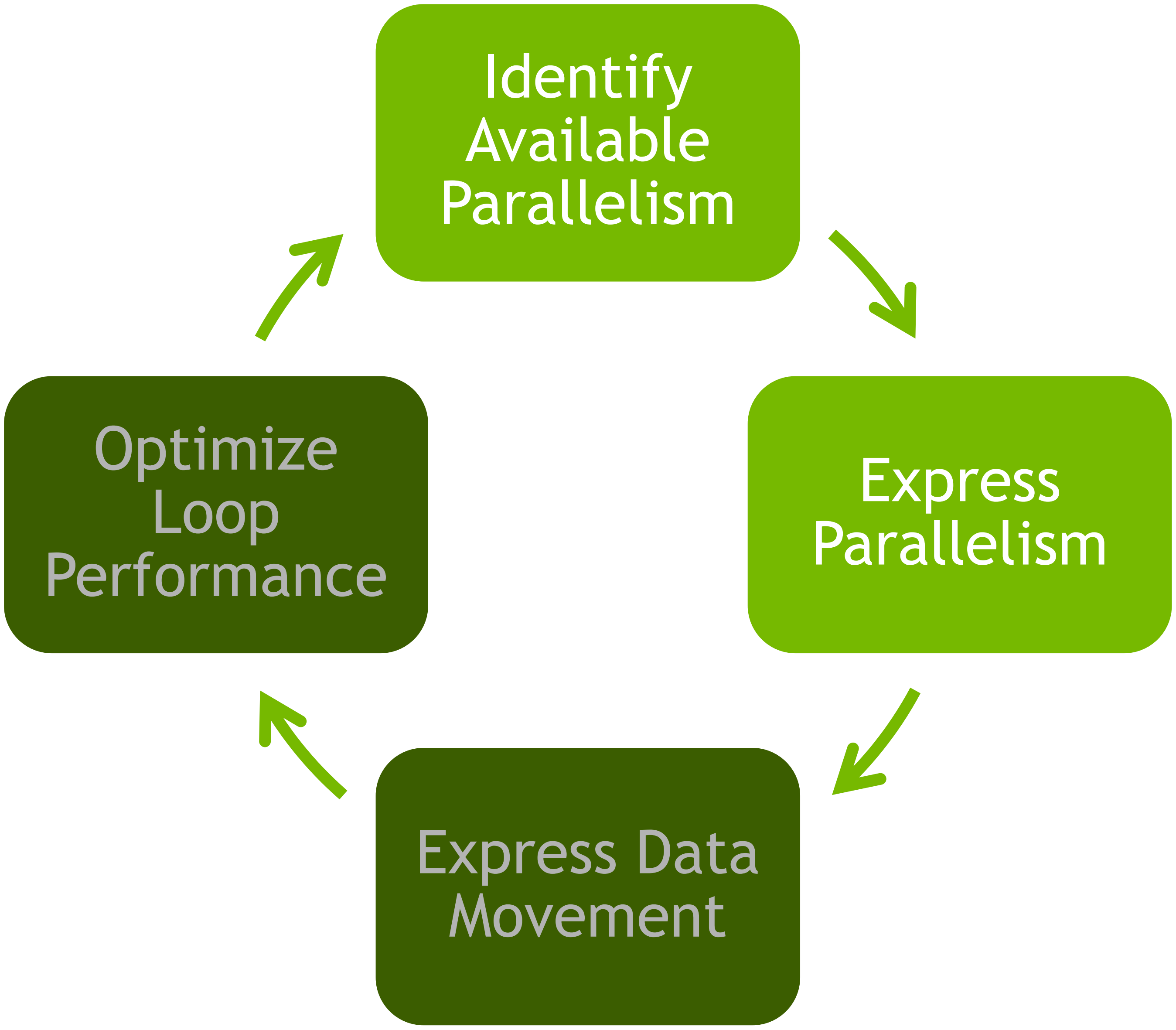


Identify Available Parallelism

Express Parallelism

Express Data Movement

Optimize Loop Performance



Identify Available Parallelism

Express Parallelism

Express Data Movement

Optimize Loop Performance

Case Study

For lectures and labs 2 & 3 we will use an example code that solves a conjugate gradient problem.

- This code is available in C and Fortran, but only C will be shown in the lectures.
- We will be demonstrating OpenACC concepts using this code in the next 2 lectures.
- You will be profiling and accelerating this code in the next 2 labs.
- In addition to the labs, the code is available at https://github.com/NVIDIA-OpenACC-Course/nvidia-openacc-course-sources/tree/master/labs

Identifying Available Parallelism

NVIDIA NVPROF Profiler

NVPROF is a command-line profiler provided in the OpenACC and CUDA Toolkits

- Basic CPU Profiling (New in OpenACC Toolkit & CUDA 7.5)
- GPU Profiling
    - High-level usage statistics
    - Timeline Collection
    - Analysis Metrics
- Used behind-the-scenes by NVIDIA Visual Profiler (nvvp)

NVPROF CPU Profiling

```
$ nvprof --cpu-profiling on --cpu-profiling-mode top-down ./cg
Rows: 8120601, nnz: 218535025
Iteration: 0, Tolerance: 4.0067e+08
Iteration: 10, Tolerance: 1.8772e+07
Iteration: 20, Tolerance: 6.4359e+05
Iteration: 30, Tolerance: 2.3202e+04
Iteration: 40, Tolerance: 8.3565e+02
Iteration: 50, Tolerance: 3.0039e+01
Iteration: 60, Tolerance: 1.0764e+00
Iteration: 70, Tolerance: 3.8360e-02
Iteration: 80, Tolerance: 1.3515e-03
Iteration: 90, Tolerance: 4.6209e-05
Total Iterations: 100 Total Time: 33.926116s

======== CPU profiling result (top down):
99.89% main
| 83.22% matvec(matrix const &, vector const &, vector const &)
| 10.41% waxpby(double, vector const &, double, vector const &, vector const &)
| 3.81% dot(vector const &, vector const &)
| 2.42% allocate_3d_poission_matrix(matrix&, int)
| 0.03% free_matrix(matrix&)
|   0.03% munmap
0.11% __c_mset8

======== Data collected at 100Hz frequency
```

GPROF Profiler

Portable command-line profiler available from GCC.

When used with PGI or GCC, the following steps are required:

1. Add the –pg compiler flag to instrument your code
2. Run the executable (it will produce gmon.out)
3. Run gprof ./executable to analyze the collected data

GPROF Output for Case Study

Add **-pg** to compiler flags, rebuild & rerun, use gprof

```
Each sample counts as 0.01 seconds.
  %   cumulative   self              self     total
 time   seconds   seconds    calls  ms/call  ms/call  name
 77.32     24.82    24.82      101   245.74   245.74  matvec(matrix const&, vector const&,
vector const&)
 15.36     29.75     4.93      302    16.32    16.32  waxpby(double, vector const&, double,
vector const&, vector const&)
  4.24     31.11     1.36      200     6.80     6.80  dot(vector const&, vector const&)
  3.08     32.10     0.99        1   990.00   990.00  allocate_3d_poission_matrix(matrix&,
int)
  0.00     32.10     0.00        5     0.00     0.00  allocate_vector(vector&, unsigned
int)
  0.00     32.10     0.00        4     0.00     0.00  free_vector(vector&)
  0.00     32.10     0.00        2     0.00     0.00  initialize_vector(vector&, double)
  0.00     32.10     0.00        1     0.00     0.00  free_matrix(matrix&)
```

PGI Compiler Feedback

Understanding what the compiler does with your code is critical to understanding the profile.

PGI –Minfo flag, options we’ll use:

- accel – Print compiler operations related to the accelerator
- all – Print (nearly) all compiler output
- intensity – Print loop intensity information
- ccff – Add information to the object files for use by tools

Compiler Feedback for Case Study

Add **-Minfo=all,intensity** to compiler flags and rebuild

```
$ pgc++ -fast -Minfo=all,intensity main.cpp -o cg
waxpby(double, const vector &, double, const vector &, const vector &):
      5, include "vector_functions.h"
          24, Intensity = 1.00
              Generated 4 alternate versions of the loop
              Generated vector and scalar versions of the loop; pointer
conflict tests determine which is executed
              Generated 2 prefetch instructions for the loop
              Loop unrolled 4 times
matvec(const matrix &, const vector &, const vector &):
      7, include "matrix_functions.h"
          14, Intensity = (num_rows*((row_end-row_start)*
2))/(num_rows+(num_rows+(num_rows+((row_end-row_start)+(row_end-row_start)))))
          18, Intensity = 1.00
              Unrolled inner loop 4 times
              Generated 2 prefetch instructions for the loop
```

Computational Intensity

Computational Intensity of a loop is a measure of how much work is being done compared to memory operations.

Computation Intensity = Compute Operations / Memory Operations

Computational Intensity of 1.0 or greater is often a clue that something might run well on a GPU.

Analyzing the Code: Matvec

```
for(int i=0;i<num_rows;i++) {
   double sum=0;
   int row_start=row_offsets[i];
   int row_end=row_offsets[i+1];
   for(int j=row_start;
           j<row_end;j++) {
     unsigned int Acol=cols[j];
     double Acoef=Acoefs[j];
     double xcoef=xcoefs[Acol];
     sum+=Acoef*xcoef;
   }
   ycoefs[i]=sum;
 }
```

Look for data dependencies:

- Does one loop iteration affect other loop iterations?
- Do loop iterations read from and write to different places in the same array?
- Is sum a data dependency? No, it’s a reduction.

Analyzing the Code: Waxpy and Dot

```
for(int i=0;i<n;i++) {
   wcoefs[i] =
     alpha*xcoefs[i] +
     beta*ycoefs[i];
}

for(int i=0;i<n;i++) {
  sum+=xcoefs[i]*ycoefs[i];
}
```

Look for data dependencies:

- Does one loop iteration affect other loop iterations?
- Do loop iterations read from and write to different places in the same array?

Expressing Parallelism

OpenACC kernels Directive

Identifies a region of code where I think the compiler can turn *loops* into *kernels*

```
#pragma acc kernels
{
for(int i=0; i<N; i++)
{
  x[i] = 1.0;
  y[i] = 2.0;
}

for(int i=0; i<N; i++)
{
  y[i] = a*x[i] + y[i];
}
}
```

kernel 1

kernel 2

The compiler identifies 2 parallel loops and generates 2 kernels.

OpenACC kernels Directive (Fortran)

Identifies a region of code where I think the compiler can turn *loops* into *kernels*

```
!$acc kernels
do i=1,N
  x(i) = 1.0
  y(i) = 2.0
end do


y(:) = a*x(:) + y(:)

!$acc end kernels
```

kernel 1

kernel 2

The compiler identifies 2 parallel loops and generates 2 kernels.

Loops vs. Kernels

```
for (int i = 0; i < 16384; i++)
{
  C[i] = A[i] + B[i];
}
```

```
function loopBody(A, B, C, i)
{
  C[i] = A[i] + B[i];
}
```

Loops vs. Kernels

```
for (int i = 0; i < 16384; i++)
{
  C[i] = A[i] + B[i];
}
```

Calculate 0 -16383 in order.

```
function loopBody(A, B, C, i)
{
  C[i] = A[i] + B[i];
}
```

Loops vs. Kernels

```
for (int i = 0; i < 16384; i++)
{
  C[i] = A[i] + B[i];
}
```

Calculate 0 -16383 in order.

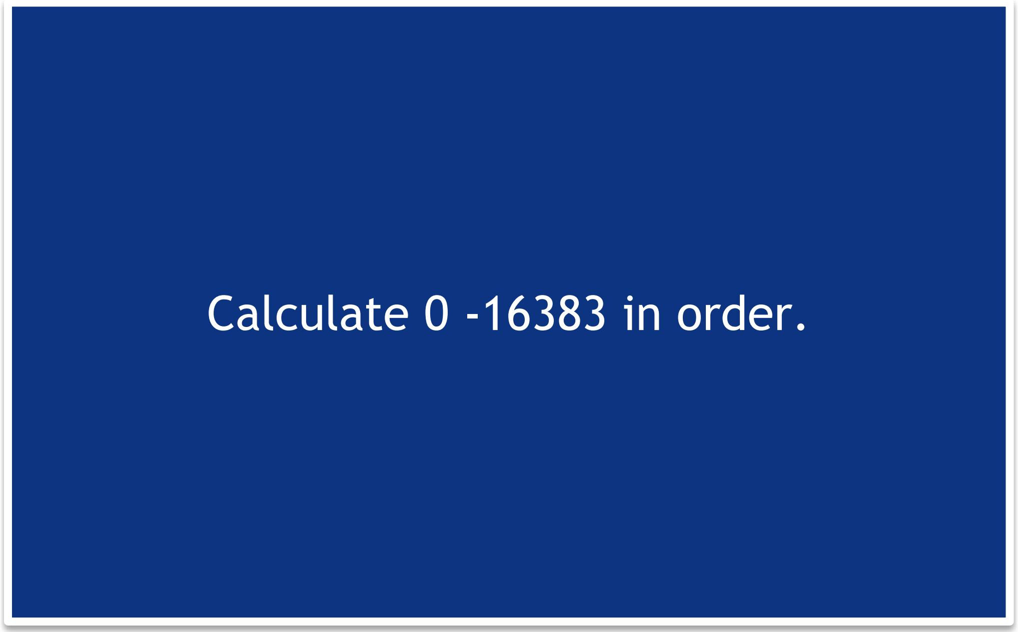
```
function loopBody(A, B, C, i)
{
  C[i] = A[i] + B[i];
}
```

Calculate 0

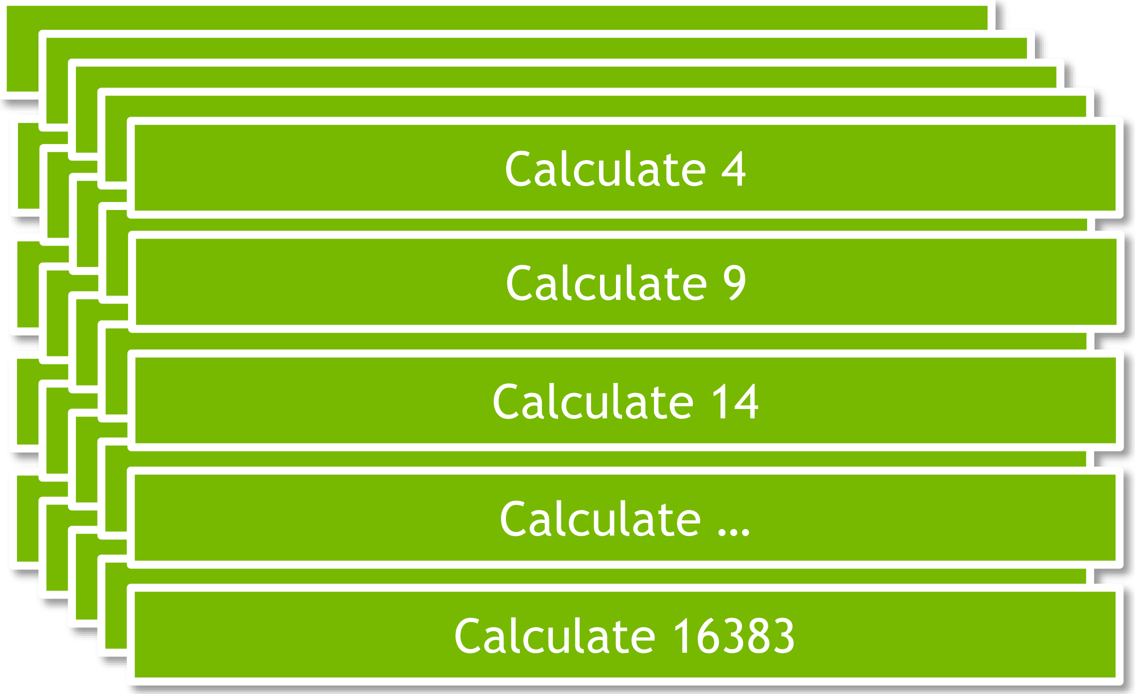
Loops vs. Kernels

```
for (int i = 0; i < 16384; i++)
{
  C[i] = A[i] + B[i];
}
```

```
function loopBody(A, B, C, i)
{
  C[i] = A[i] + B[i];
}
```



Calculate 0 -16383 in order.



Calculate 4

Calculate 9

Calculate 14

Calculate …

Calculate 16383

The Kernels Directive

Identifies a region of code where I think the compiler can turn *loops* into *kernels*

```
#pragma acc kernels
{
for (int i = 0; i < 16384;
              i++)
{
  C[i] = A[i] + B[i];
}
}
```

The Compiler will…

1. Analyze the code to determine if it contains parallelism
2. Identify data that needs to be moved to/from the GPU memory
3. Generate kernels
4. Run on the GPU

Parallelizing the Code: Matvec

```
#pragma acc kernels
{
for(int i=0;i<num_rows;i++) {
  double sum=0;
  int row_start=row_offsets[i];
  int row_end=row_offsets[i+1];
  for(int j=row_start;
          j<row_end;j++) {
    unsigned int Acol=cols[j];
    double Acoef=Acoefs[j];
    double xcoef=xcoefs[Acol];
    sum+=Acoef*xcoef;
  }
  ycoefs[i]=sum;
}
}
```

Let’s tell the compiler where we think it can turn *loops* into *kernels*.

Don’t worry about your data or how to parallelize these loops, let the compiler decide.

Building with OpenACC

Enable OpenACC with the `–ta` (target accelerator) flag.

Target Accelerator:

- `tesla` – NVIDIA Tesla GPU
- `managed` – Use CUDA Managed Memory (simplifies the process)

Building with OpenACC - Feedback

```
$ pgc++ -fast -Minfo=accel -ta=tesla:managed main.cpp -o challenge
matvec(const matrix &, const vector &, const vector &):
      7, include "matrix_functions.h"
          15, Generating copyout(ycoefs[:num_rows])
              Generating
copyin(xcoefs[:],Acoefs[:],cols[:],row_offsets[:num_rows+1])
          16, Complex loop carried dependence of row_offsets-> prevents
parallelization
              Loop carried dependence of ycoefs-> prevents parallelization
              Loop carried backward dependence of ycoefs-> prevents
vectorization
              Complex loop carried dependence of cols->,Acoefs->,xcoefs->
prevents parallelization
              Accelerator kernel generated
              Generating Tesla code
              20, #pragma acc loop vector(128) /* threadIdx.x */
              24, Sum reduction generated for sum
          20, Loop is parallelizable
```

False Loop Dependencies

Aliasing prevents parallelization.

The compiler things there's a *carried dependency* in our loop iterations, but we thought they were parallel. Only the innermost loop was parallelized.

In C/C++, the arrays are simply pointers, so they may be aliased (two pointers accessing the same memory differently). If the compiler doesn't know pointers aren't aliased, it must assume they are.

This is not a problem with Fortran arrays.

C99: restrict Keyword

- Promise given by the programmer to the compiler that pointer will not alias with another pointer
  - Applied to a pointer, e.g.

    `float *restrict ptr`
  - Meaning: “for the lifetime of `ptr`, only it or a value directly derived from it (such as `ptr + 1`) will be used to access the object to which it points”*
- Parallelizing compilers often require `restrict` to determine independence
  - Otherwise the compiler can’t parallelize loops that access `ptr`
  - Note: if programmer violates the declaration, behavior is undefined

⚠ ~~`float restrict *ptr`~~

`float *restrict ptr`

http://en.wikipedia.org/wiki/Restrict

Loop independent clause

Specifies that loop iterations are data independent. This overrides any compiler dependency analysis. This is implied for *parallel loop*.

```
#pragma acc kernels
{
```

```
#pragma acc loop independent
for(int i=0; i<N; i++)
{
  a[i] = 0.0;
  b[i] = 1.0;
  c[i] = 2.0;
}
```

kernel 1

```
#pragma acc loop independent
for(int i=0; i<N; i++)
{
  a[i] = b[i] + c[i]
}
```

kernel 2

```
}
```

Informs the compiler that both loops are safe to parallelize so it will generate both kernels.

Fixing False Aliasing

```
unsigned int num_rows=A.num_rows;
unsigned int *restrict  \
        row_offsets=A.row_offsets;
unsigned int *restrict  \
        cols=A.cols;
double *restrict Acoefs=A.coefs;
double *restrict xcoefs=x.coefs;
double *restrict ycoefs=y.coefs;
```

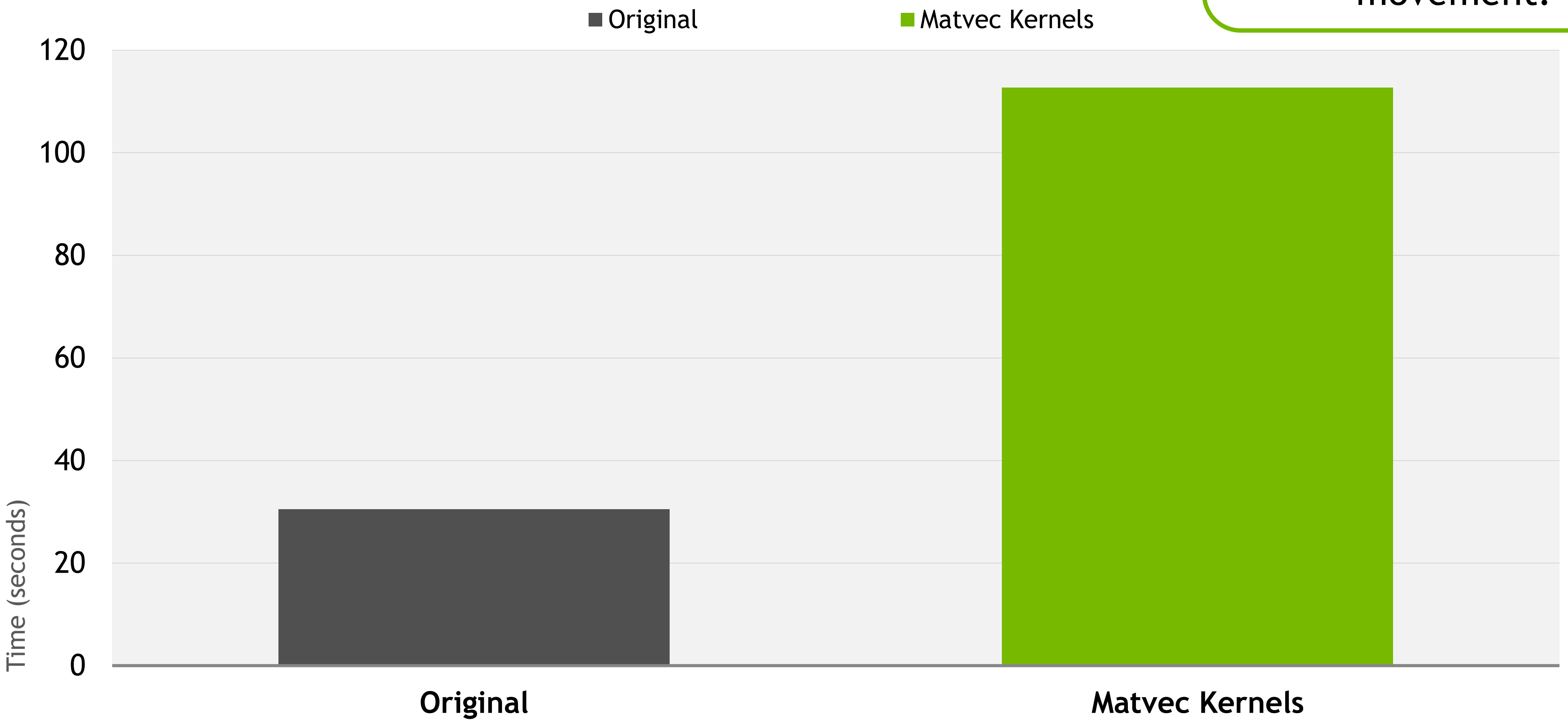
- By declaring our pointers with the restrict keyword, we've promised the compiler they will not alias.
- We could also use loop independent on our loops, but restrict fixes the underlying issue.

Rebuilding with OpenACC - Feedback

```
$ pgc++ -fast -Minfo=accel -ta=tesla:managed main.cpp -o challenge
matvec(const matrix &, const vector &, const vector &):
      7, include "matrix_functions.h"
          15, Generating copyout(ycoefs[:num_rows])
              Generating
copyin(xcoefs[:],Acoefs[:],cols[:],row_offsets[:num_rows+1])
          16, Loop is parallelizable
              Accelerator kernel generated
              Generating Tesla code
              16, #pragma acc loop gang, vector(128) /* blockIdx.x
threadIdx.x */
          20, Loop is parallelizable
```

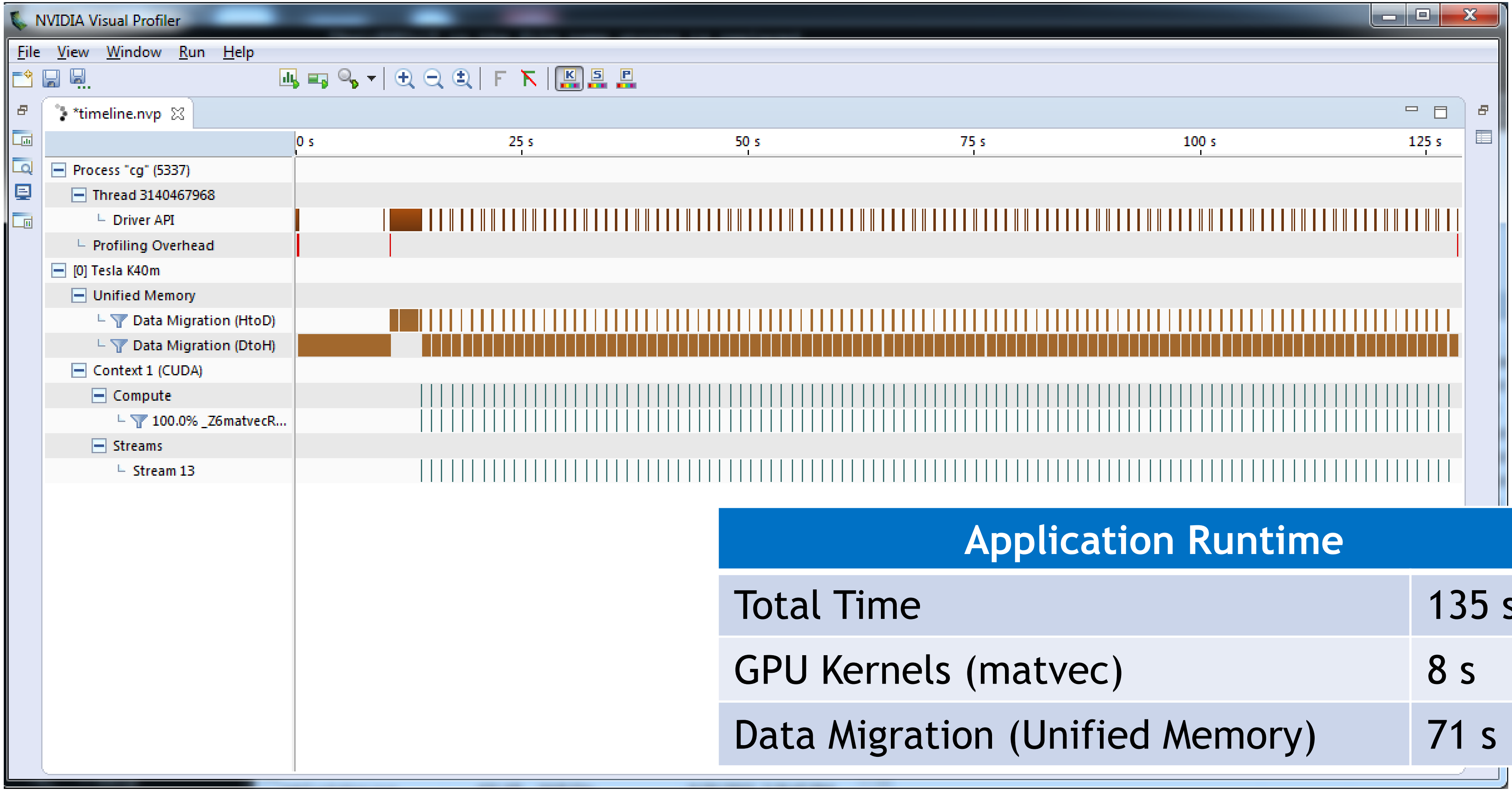
Performance Now

Remember, a slow-down is expected at this point due to excess data movement.



Put specs here…

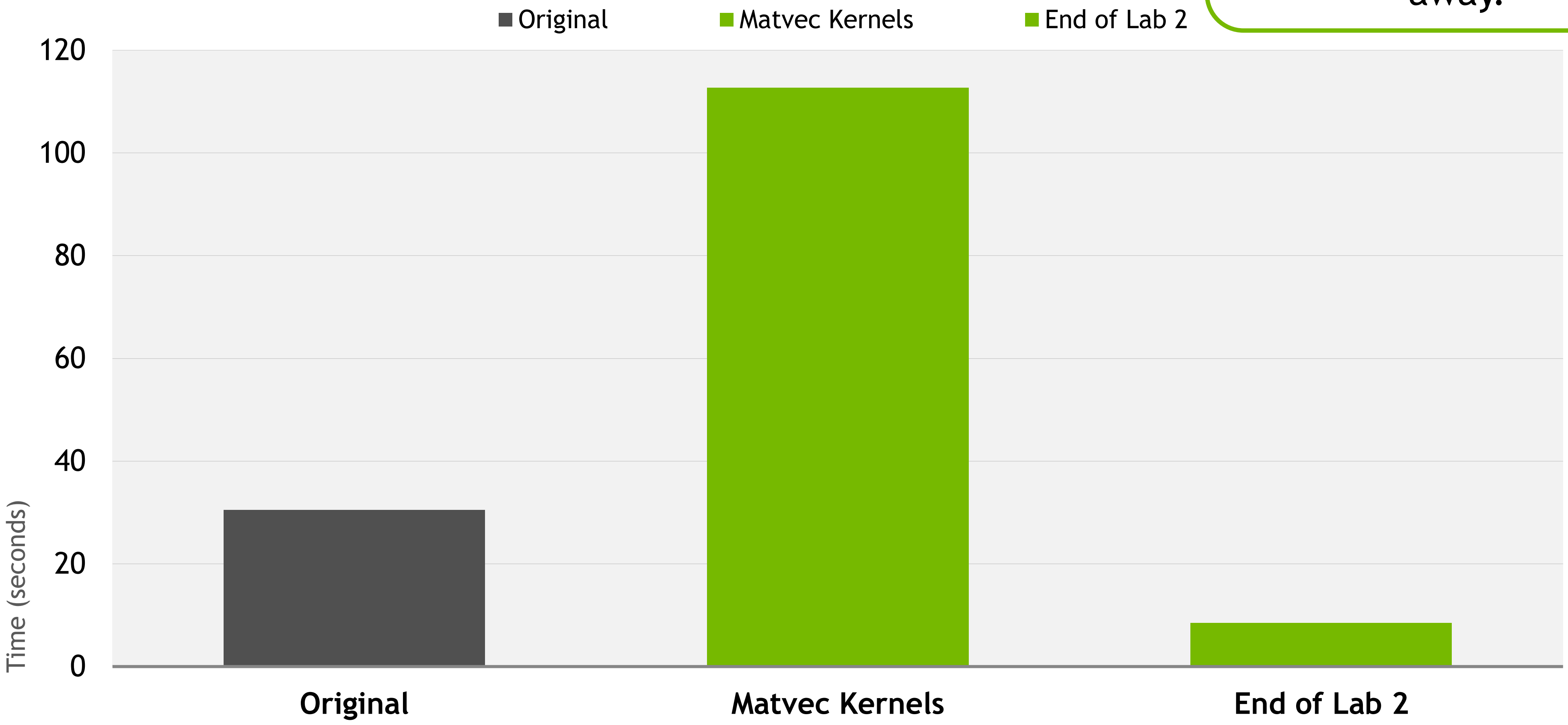
Re-profiling the code



Application Runtime	
Total Time	135 s
GPU Kernels (matvec)	8 s
Data Migration (Unified Memory)	71 s

Performance After Lab 2

Once you've moved all 3 functions to the GPU, data movement will go away.



Intel(R) Xeon(R) CPU E5-2698 v3 @ 2.30GHz and NVIDIA Tesla K40 GPU

OpenACC parallel loop Directive

`parallel` - Programmer identifies a block of code containing parallelism. Compiler generates a *kernel*.

`loop` - Programmer identifies a loop that can be parallelized within the kernel.

NOTE: parallel & loop are often placed together

```
#pragma acc parallel loop

for(int i=0; i<N; i++)

{

  y[i] = a*x[i]+y[i];

}
```

Generates a Parallel Kernel

NOTE: The independent clause to loop is implied when used within a parallel region.

OpenACC loop directive: private & reduction

The `private` and `reduction` clauses are not optimization clauses, they may be required for correctness.

- `private` – A copy of the variable is made for each loop iteration
- `reduction` – A reduction is performed on the listed variables.
  - Supports +, *, max, min, and various logical operations

Note: The kernels directive will generally handle these for you.

Using Parallel Loop

```
#pragma acc parallel loop
for(int i=0;i<num_rows;i++) {
  double sum=0;
  int row_start=row_offsets[i];
  int row_end=row_offsets[i+1];
#pragma acc loop reduction(+:sum)
  for(int j=row_start;
          j<row_end;j++) {
    unsigned int Acol=cols[j];
    double Acoef=Acoefs[j];
    double xcoef=xcoefs[Acol];
    sum+=Acoef*xcoef;
  }
  ycoefs[i]=sum;
}
```

- Instead of letting the compiler analyze the loops, let’s tell the compiler they’re parallel.
- Adding a loop directive to inner loops will tell the compiler they’re also independent.
- We must specify the reduction on sum for correctness.

Rebuilding with Parallel Loop - Feedback

```
$ pgc++ -fast -Minfo=accel -ta=tesla:managed main.cpp -o challenge
matvec(const matrix &, const vector &, const vector &):
      8, include "matrix_functions.h"
          12, Accelerator kernel generated
              Generating Tesla code
              15, #pragma acc loop gang /* blockIdx.x */
              20, #pragma acc loop vector(128) /* threadIdx.x */
                  Sum reduction generated for sum
          12, Generating copyout(ycoefs[:num_rows])
              Generating
copyin(xcoefs[:],Acoefs[:],cols[:],row_offsets[:num_rows+1])
          20, Loop is parallelizable
```

OpenACC parallel loop vs. kernels

PARALLEL LOOP

- Programmer's responsibility to ensure safe parallelism
- Will parallelize what a compiler may miss
- Straightforward path from OpenMP

KERNELS

- Compiler's responsibility to analyze the code an parallelize what is safe.
- Can cover larger area of code with single directive
- Gives compiler additional leeway to optimize.

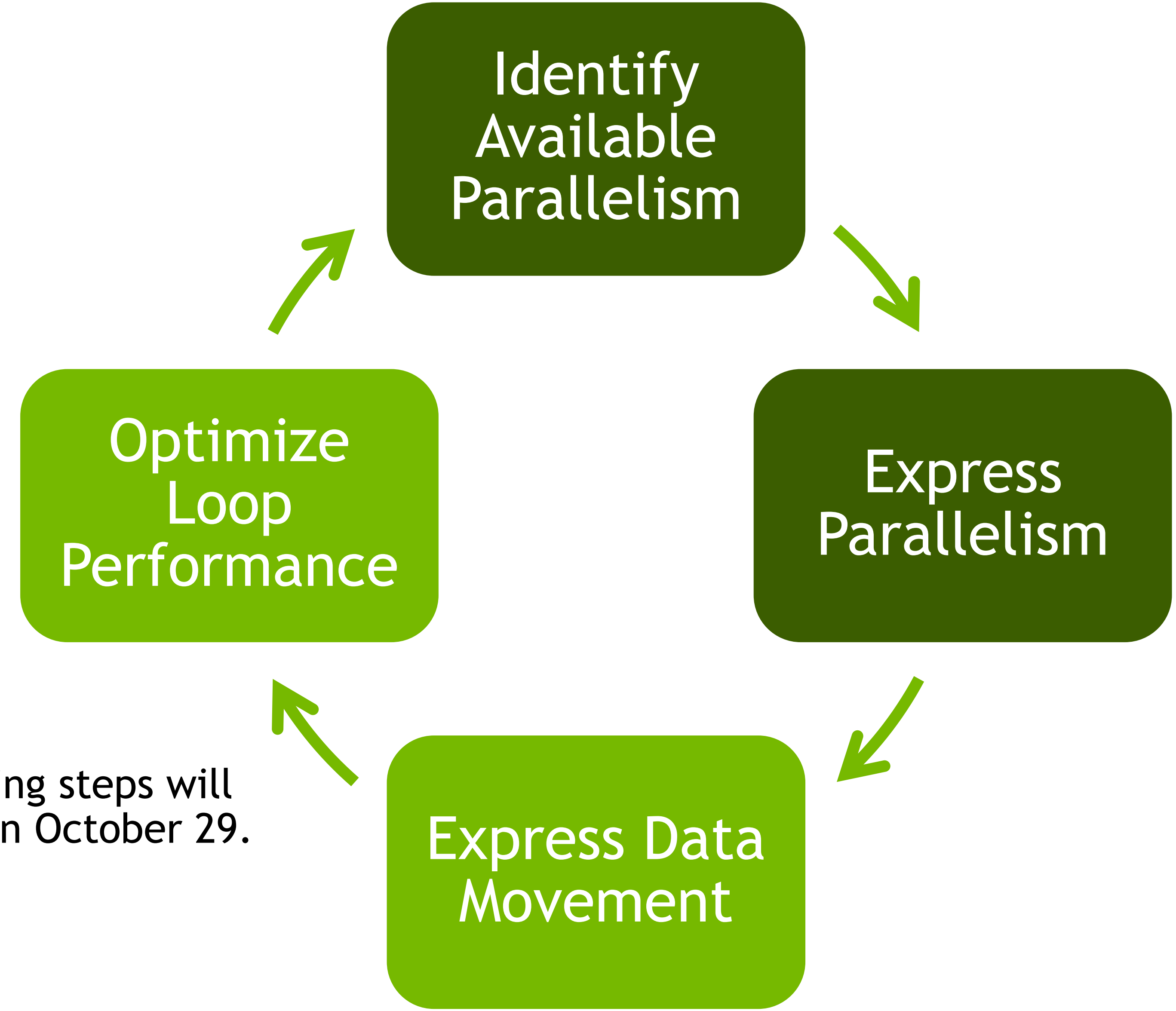
Both approaches are equally valid and can perform equally well.

Review

Today we discussed:

- Tools that can be used to profile a code and identify important routines and loops where there is available parallelism
- How to analyze the code for parallelism blockers
- How to use the kernels and parallel loop directives to express the available parallelism to the compiler
- How to build with PGI and OpenACC
- How to re-profile the accelerated code

Next Steps & Homework



The remaining steps will be covered on October 29.

Homework

Go to http://bit.ly/nvoacclab2

Build and profile the example code using the PGI compiler and gprof.

Complete the acceleration of the example code by accelerating the matvec, waxpy, and dot functions using either kernels or parallel loop.

Periodically use nvprof and/or Visual Profiler to obtain accelerated profiles and observed the results of your changes.

Note: The GPUs provided via Qwiklabs will provide a much smaller speed-up than shown here (10-15%). This is expected. Lab 3 will improve upon this.

Office Hours Next Week

Next week’s session will be an office hours session.

Bring your questions from this week’s lecture and homework to next week’s session.

If you can’t wait until then, post a question on StackOverflow tagged with openacc.

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