An (almost) Easy INTRODUCTION TO OPENACC®

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OpenACC
More Science, Less Programming

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Acknowledgements

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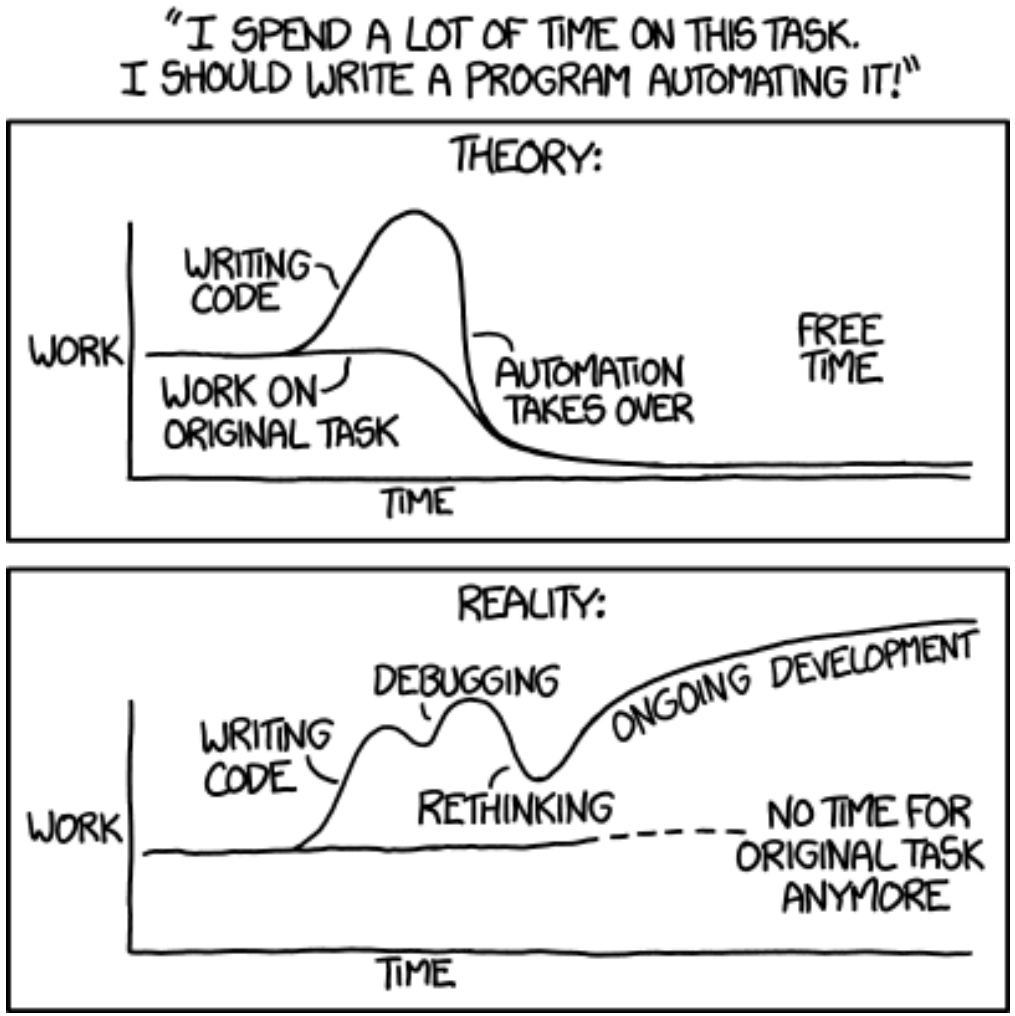
- Fernanda Foertter, Oak Ridge National Laboratory
- Joe Bongo, NVIDIA Deep Learning Institute

GPU Computing is Powerful…

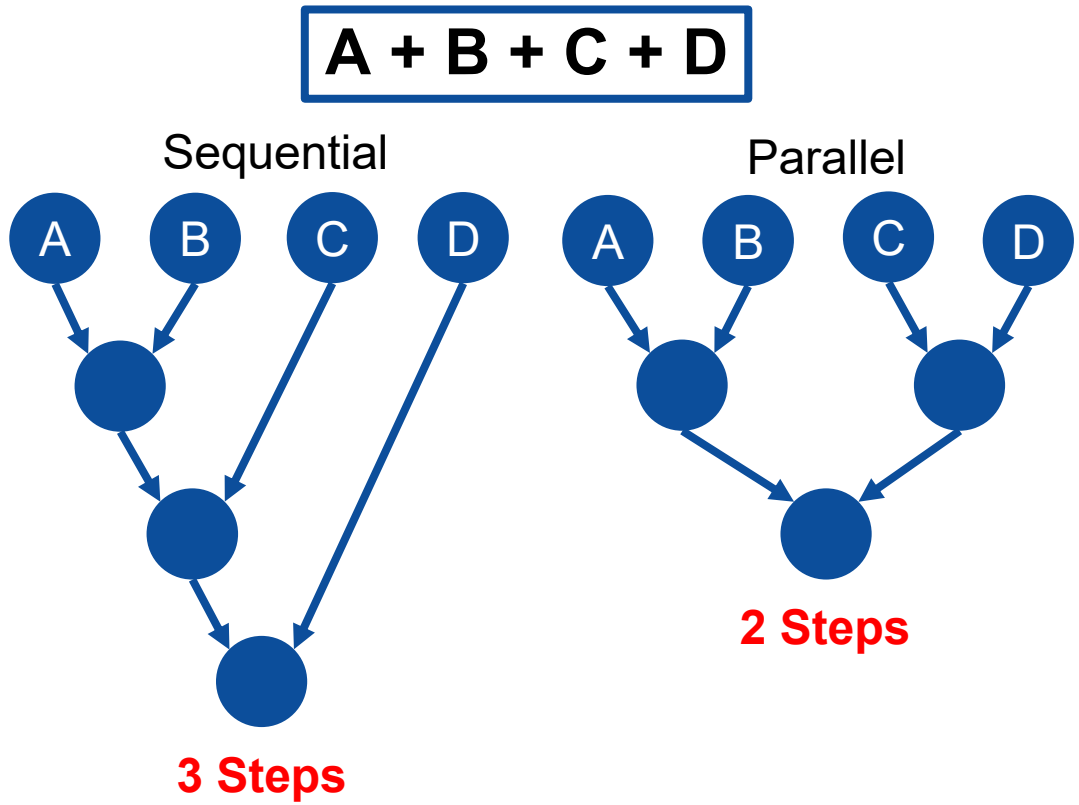


… but it's not simple.

(REMEMBER) INTRODUCTION TO PARALLEL PROGRAMMING

Remember: WHAT IS PARALLEL PROGRAMMING?

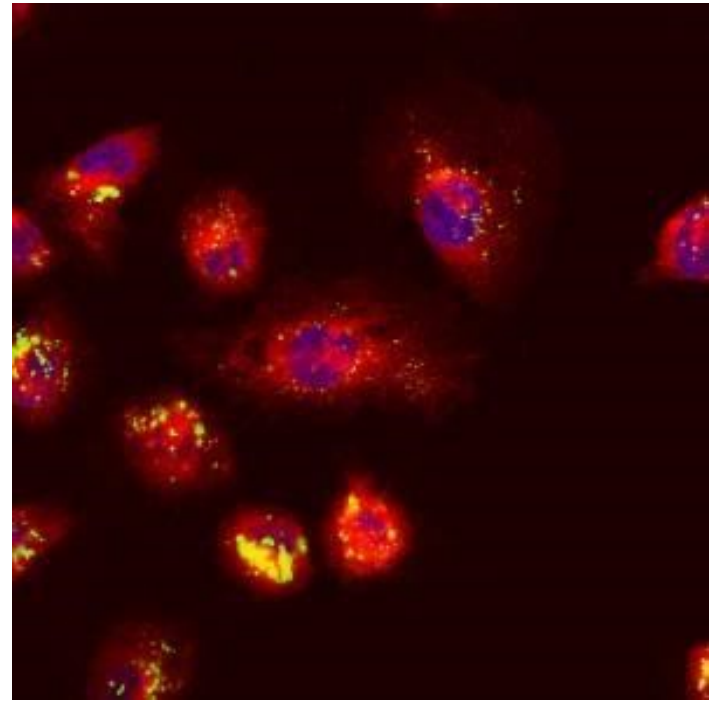
- **“Performance Programming”**
- Parallel programming involves exposing an algorithm’s ability to execute in parallel
- This may involve breaking a large operation into smaller tasks (task parallelism)
- Or doing the same operation on multiple data elements (data parallelism)
- Parallel execution enables better performance on modern hardware



A REAL WORLD CASE STUDY

Modern cancer research

- The Russian Academy of Science created a program to simulate light propagation through human tissue
- This program was used to be able to more accurately detect cancerous cells by simulating **billions** of random paths that the light could take through human tissue
- With parallel programming, they were able to run **thousands** of these paths **simultaneously**
- The sequential program took **2.5 hours** to run
- The parallel version took less than **2 minutes**



Parallel Computing Illuminating a Path to Early Cancer Detection

WHAT IS PARALLEL PROGRAMMING?

A real world example

- A professor and his 3 teaching assistants (TA) are grading 1,000 student exams
- This exam has 8 questions on it
- Let's assume it takes 1 minute to grade 1 question on 1 exam
- To maintain fairness, if someone grades a question (for example, question #1) then they must grade that question on all other exams
- The following is a sequential version of exam grading

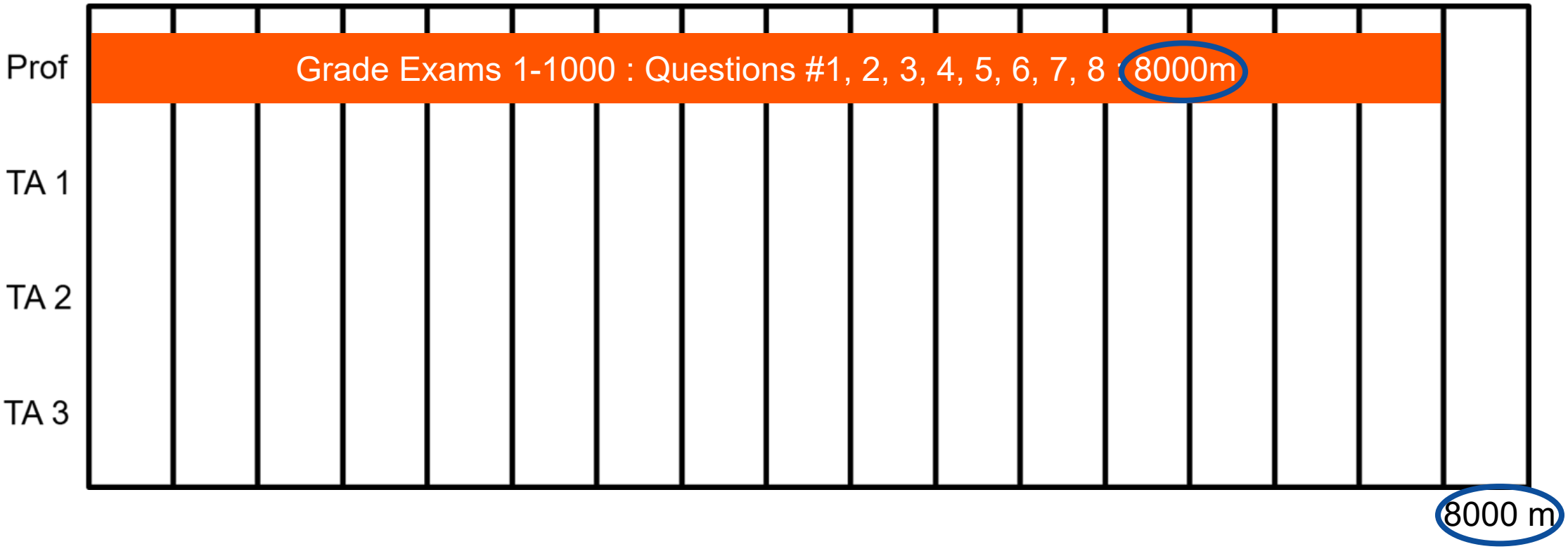
x1000

8 questions per exam

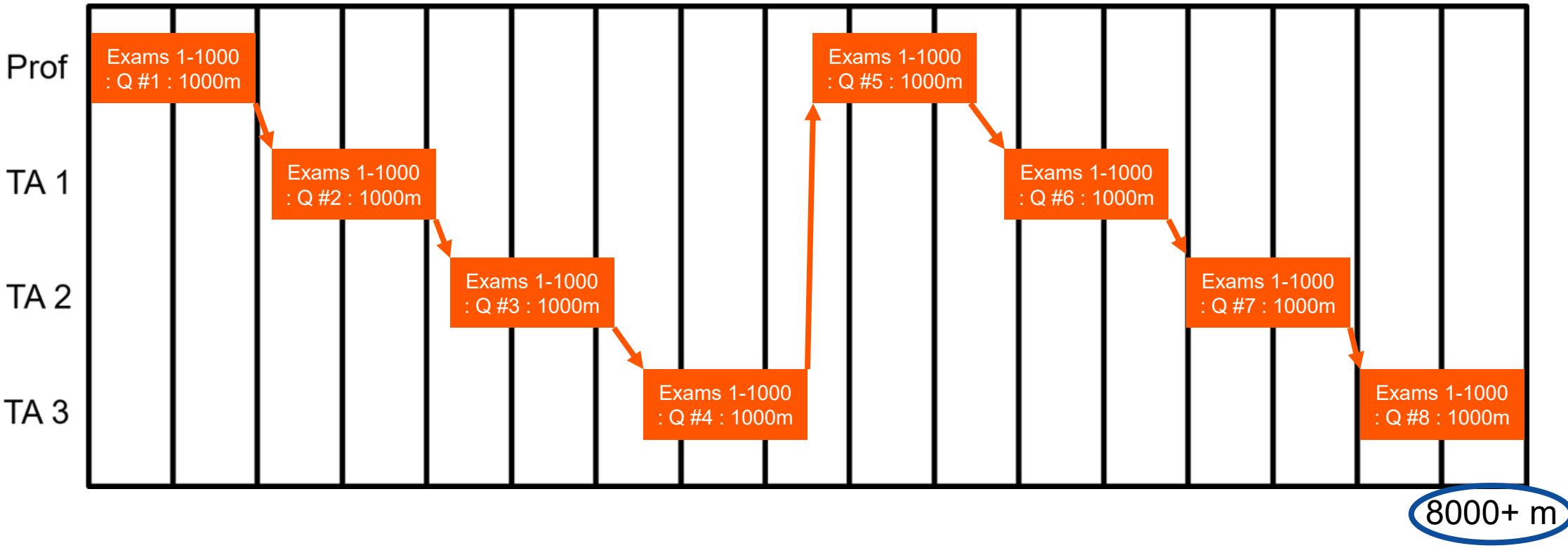
8,000 questions in total

1 minute per question

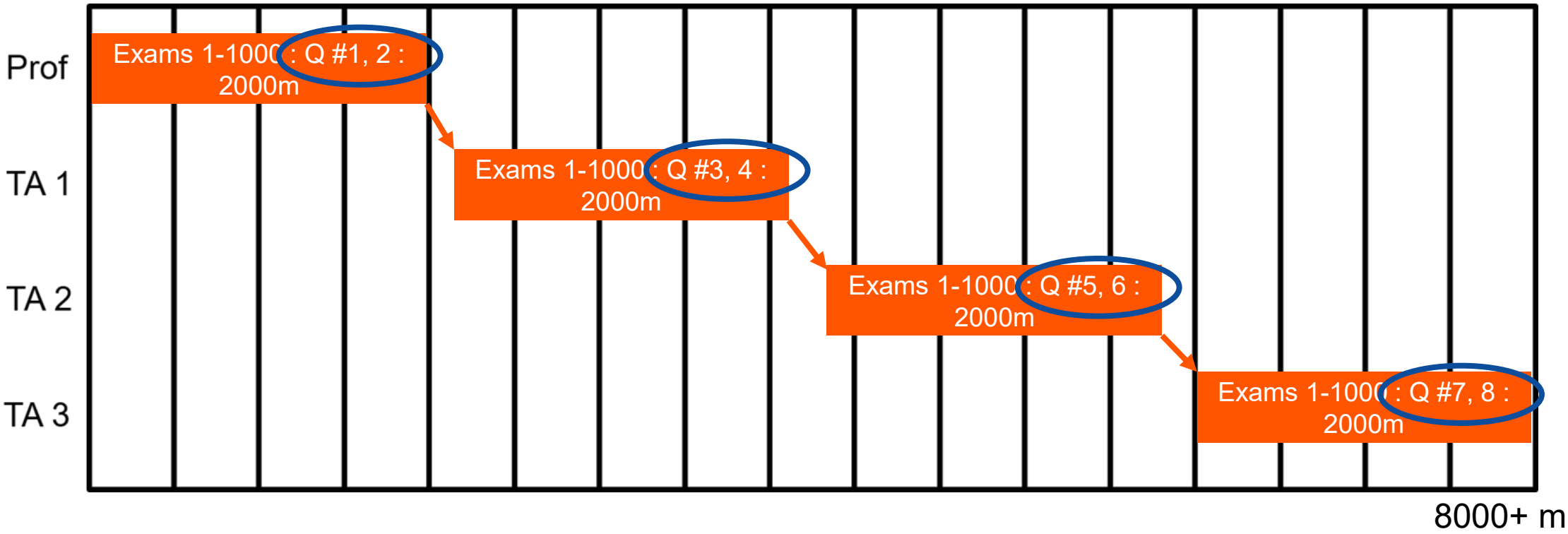
SEQUENTIAL SOLUTION



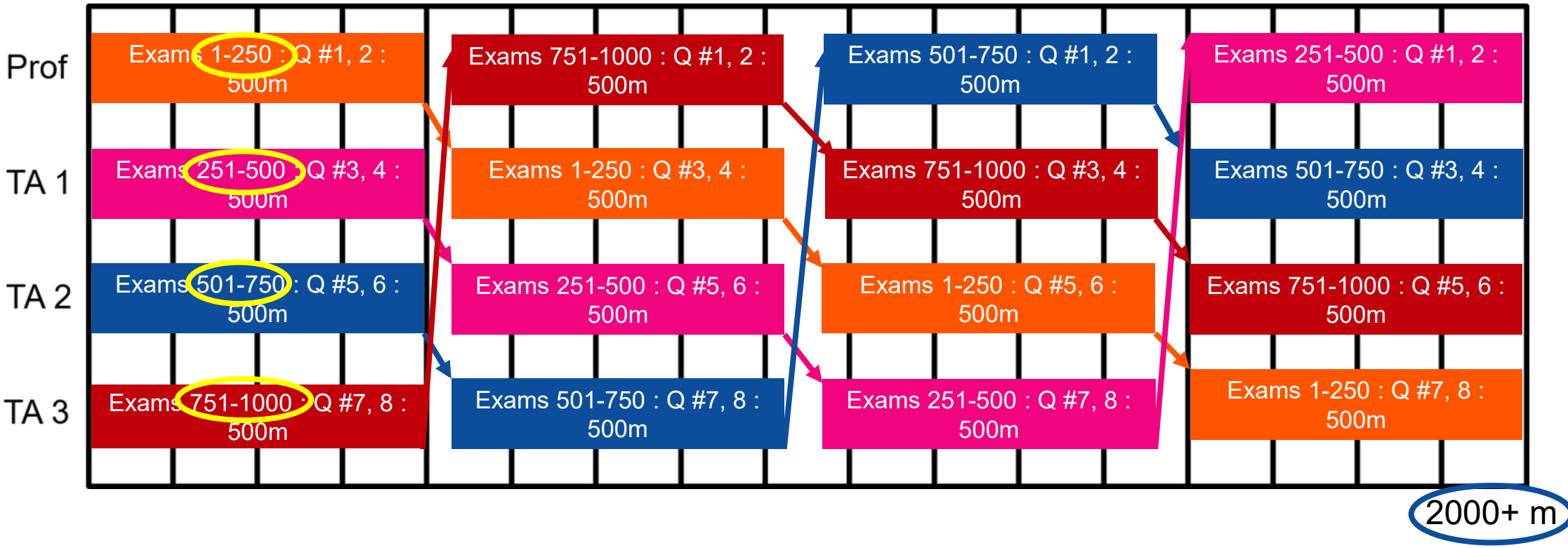
SEQUENTIAL SOLUTION



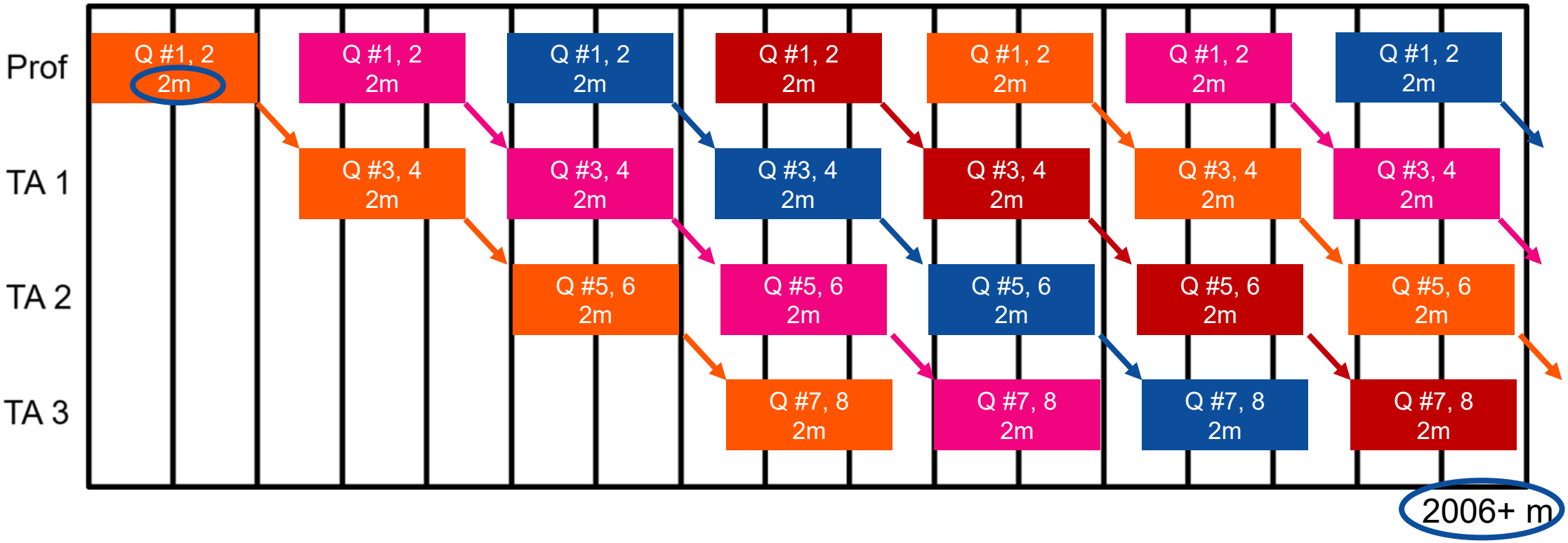
SEQUENTIAL SOLUTION



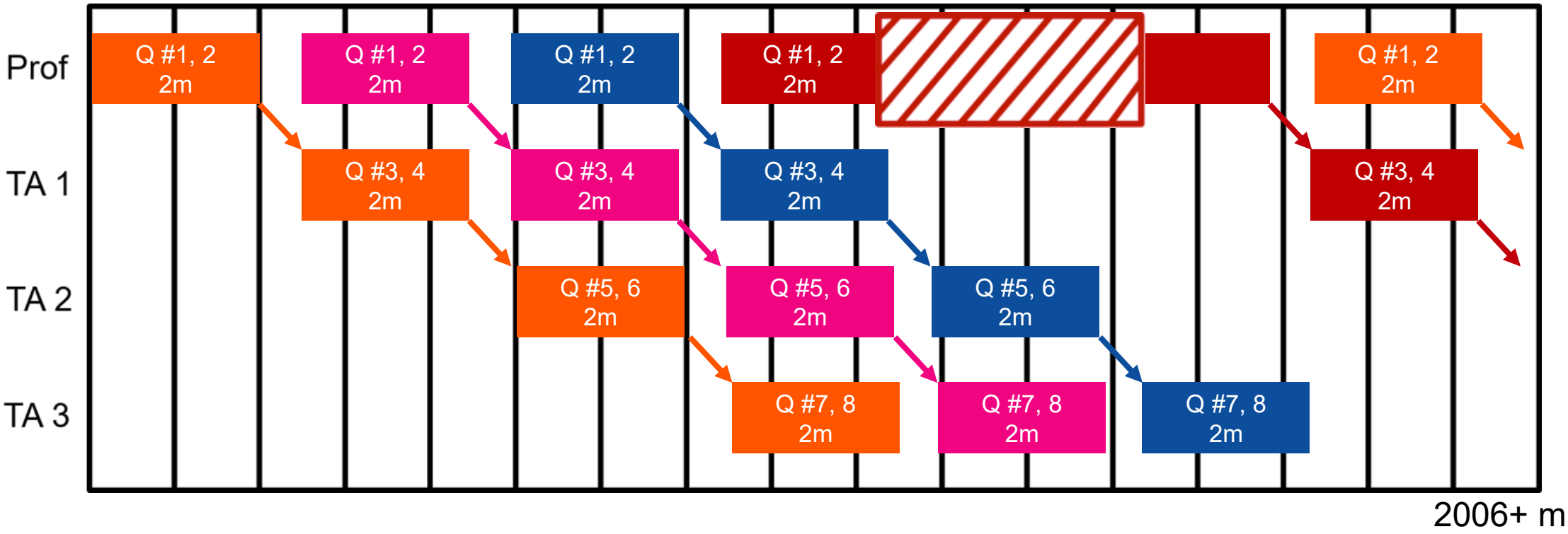
PARALLEL SOLUTION



PIPELINE



PIPELINE STALL



GRADING EXAMPLE SUMMARY

It's critical to understand the problem before trying to parallelize it

- Can the work be done in an arbitrary order, or must it be done in sequential order?
- Does each task take the same amount of time to complete? If not, it may be necessary to *"load balance."*

In our example, the only restriction is that a single question be graded by a single grader, so we could divide the work easily, but had to communicate periodically.

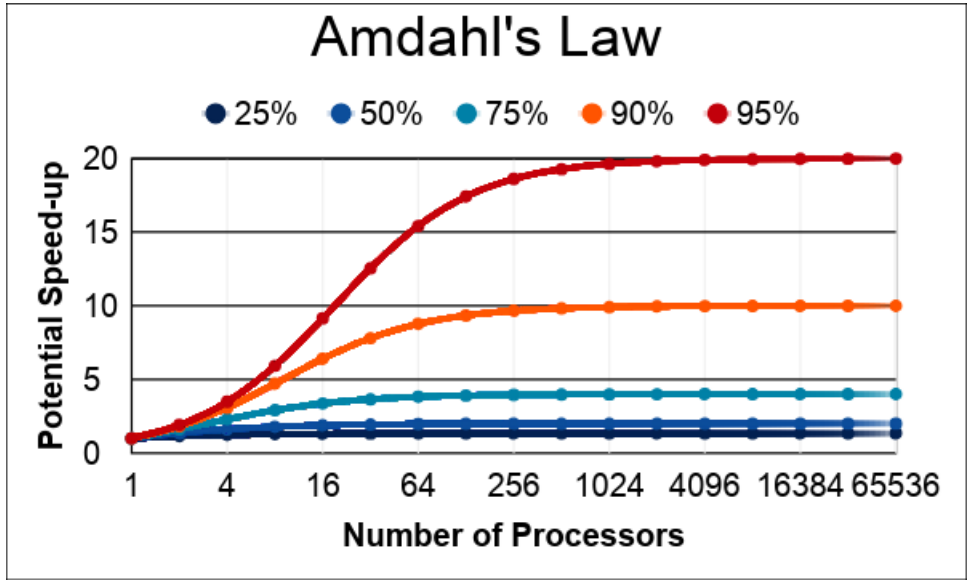
- This case study is an example of task-based parallelism. Each grader is assigned a task like "Grade questions 1 & 2 on the first 500 tests"
- If instead each question could be graded by different graders, then we could have data parallelism: all graders work on Q1 of the following tests, then Q2, etc.

(Remember) AMDAHL'S LAW

AMDAHL'S LAW

Serialization Limits Performance

- Amdahl's law is an observation that how much speed-up you get from parallelizing the code is limited by the remaining serial part.
- Any remaining serial code will reduce the possible speed-up
- This is why it's important to focus on parallelizing the most time consuming parts, not just the easiest.



APPLYING AMDAHL'S LAW

Estimating Potential Speed-up

- What's the maximum speed-up that can be obtained by parallelizing 50% of the code?

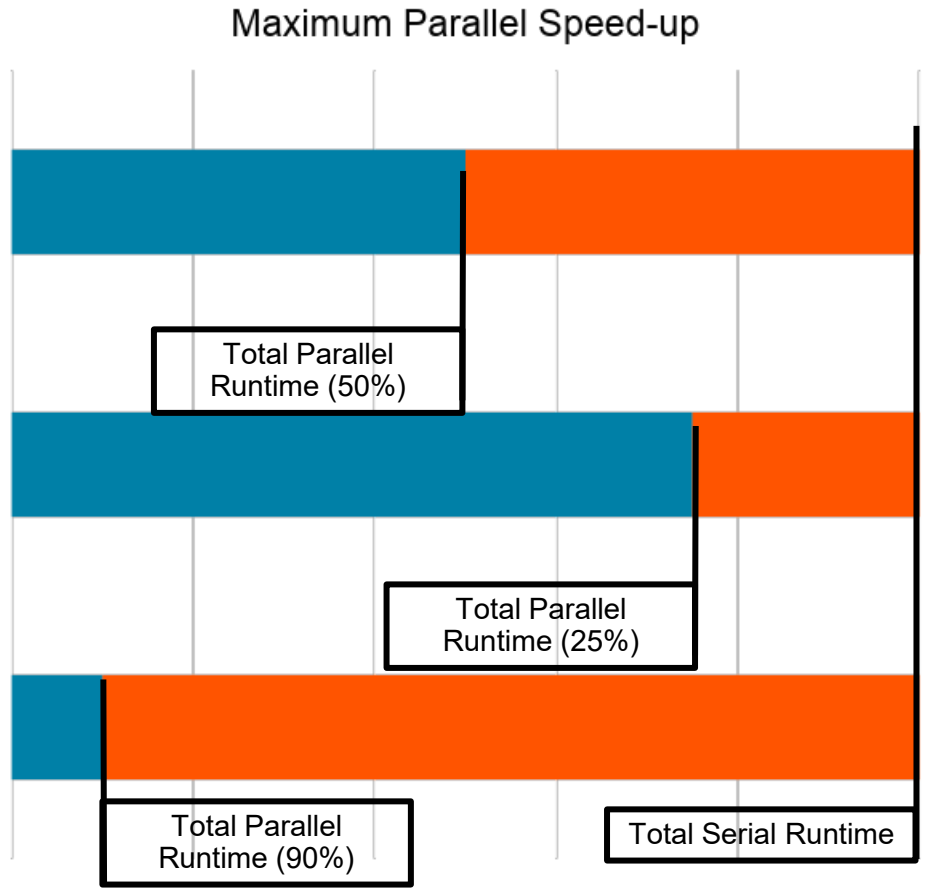
(1 / 100% - 50%) = (1 / 1.0 - 0.50) = 2.0X

- What's the maximum speed-up that can be obtained by parallelizing 25% of the code?

(1 / 100% - 25%) = (1 / 1.0 - 0.25) = 1.3X

- What's the maximum speed-up that can be obtained by parallelizing 90% of the code?

(1 / 100% - 90%) = (1 / 1.0 - 0.90) = 10.0X



(NOW) AN INTRODUCTION TO OPENACC

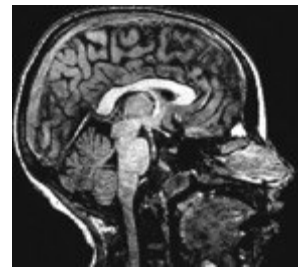
OpenACC

Simple | Powerful | Portable

Fueling the Next Wave of Scientific Discoveries in HPC

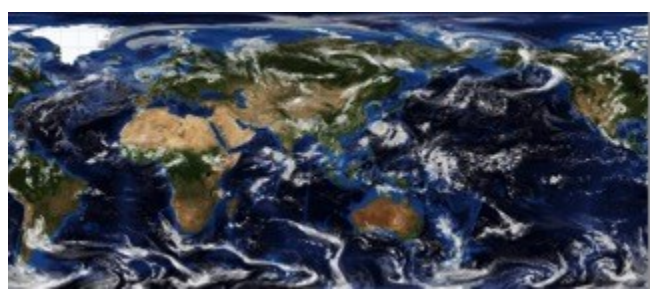

```
main()
{
  <serial code>
  #pragma acc kernels
  //automatically runs on GPU
  {
    <parallel code>
  }
}
```

University of Illinois
PowerGrid- MRI Reconstruction



70x Speed-Up
2 Days of Effort

RIKEN Japan
NICAM- Climate Modeling



7-8x Speed-Up
5% of Code Modified

8000+

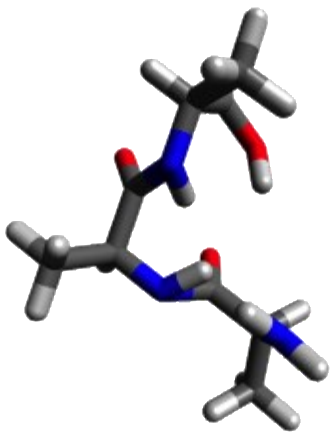
Developers

using OpenACC

http://www.cray.com/sites/default/files/resources/OpenACC_213462.12_OpenACC_Cosmo_CS_FNL.pdf
http://www.hpcwire.com/off-the-wire/first-round-of-2015-hackathons-gets-underway
http://on-demand.gputechconf.com/gtc/2015/presentation/S5297-Hisashi-Yashiro.pdf
http://www.openacc.org/content/experiences-porting-molecular-dynamics-code-gpus-cray-xk7

LS-DALTON

Large-scale application for calculating high-accuracy molecular energies



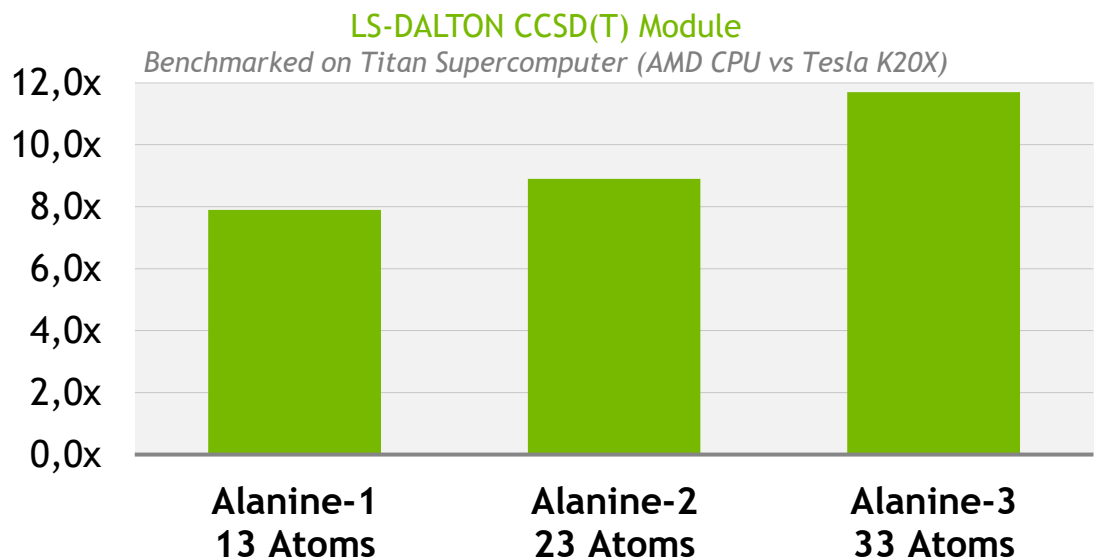
"*OpenACC makes GPU computing approachable for domain scientists. Initial OpenACC implementation required only minor effort, and more importantly, no modifications of our existing CPU implementation.*"

Janus Juul Eriksen, PhD Fellow
qLEAP Center for Theoretical Chemistry, Aarhus University

Minimal Effort

Lines of Code Modified	# of Weeks Required	# of Codes to Maintain
<100 Lines	1 Week	1 Source

Big Performance



OpenACC Directives

Manage Data Movement

Initiate Parallel Execution

Optimize Loop Mappings

```
#pragma acc data copyin(a,b) copyout(c)
{
  ...
  #pragma acc parallel
  {
  #pragma acc loop gang vector
      for (i = 0; i < n; ++i) {
          z[i] = x[i] + y[i];
          ...
      }
  }
  ...
}
```

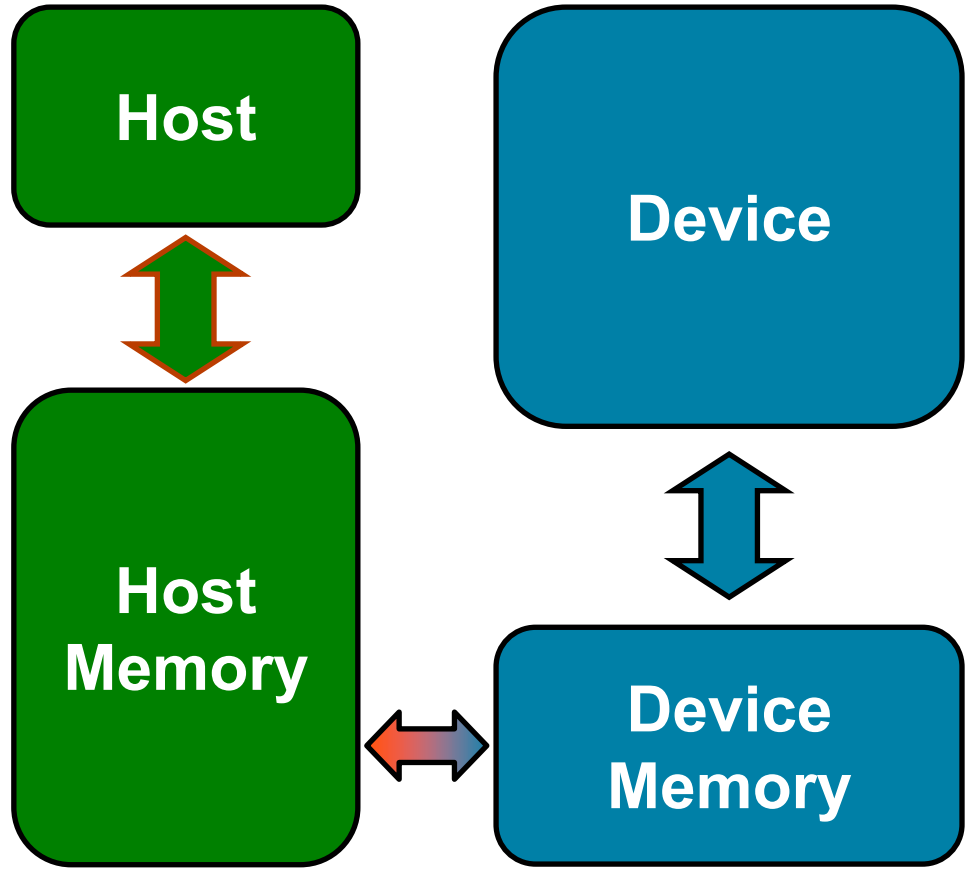
OpenACC
Directives for Accelerators

- Incremental
- Single source
- Interoperable
- Performance portable
- CPU, GPU, MIC

OPENACC PORTABILITY

Describing a generic parallel machine

- OpenACC is designed to be portable to many existing and future parallel platforms
- The programmer need not think about specific hardware details, but rather express the parallelism in generic terms
- An OpenACC program runs on a *host* (typically a CPU) that manages one or more parallel *devices* (GPUs, etc.). The host and device(s) are logically thought of as having separate memories.



OPENACC

Three major strengths

Incremental	Single Source	Low Learning Curve

OPENACC

Incremental

- Maintain existing sequential code
- Add annotations to expose parallelism
- After verifying correctness, annotate more of the code

Enhance Sequential Code

```
#pragma acc parallel loop
for( i = 0; i < N; i++ )
{
   < loop code >
}

#pragma acc parallel loop
for( i = 0; i < N; i++ )
{
   < loop code >
}
```

Begin with a working sequential code.

Parallelize it with OpenACC.

Rerun the code to verify correct behavior, remove/alter OpenACC code as needed.

OPENACC

Incremental

- Maintain existing sequential code
- Add annotations to expose parallelism
- After verifying correctness, annotate more of the code

Single Source

Low Learning Curve

OPENACC

Supported Platforms

POWER

Sunway

x86 CPU

x86 Xeon Phi

NVIDIA GPU

PEZY-SC

Single Source

- Rebuild the same code on multiple architectures
- Compiler determines how to parallelize for the desired machine
- Sequential code is maintained

The compiler can **ignore** your OpenACC code additions, so the same code can be used for **parallel** or **sequential** execution.

```
int main(){

:::

            #pragma acc
parallel loop
            for(int i = 0; i <
N; i++)
                        < loop
code >

}
```

OPENACC

Incremental

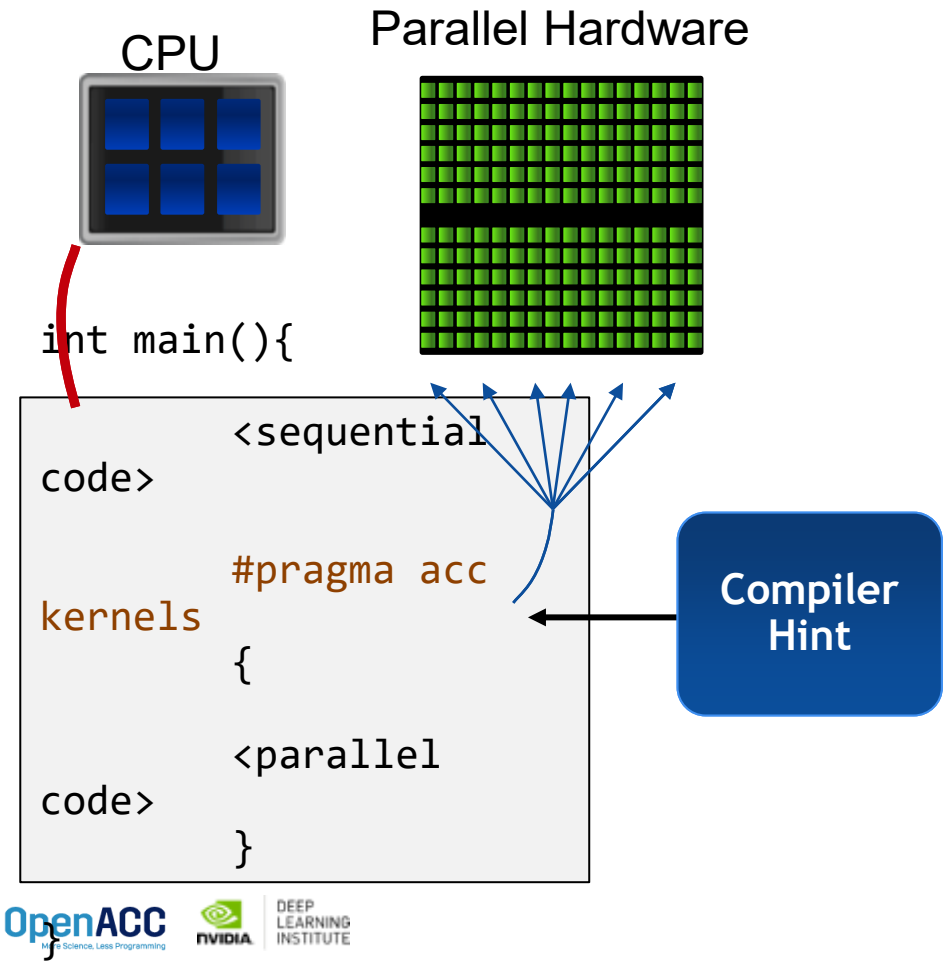
- Maintain existing sequential code
- Add annotations to expose parallelism
- After verifying correctness, annotate more of the code

Single Source

- Rebuild the same code on multiple architectures
- Compiler determines how to parallelize for the desired machine
- Sequential code is maintained

Low Learning Curve

OPENACC



The programmer will give hints to the compiler about which parts of the code to parallelize.

The compiler will then generate parallelism for the target parallel hardware.

Low Learning Curve

- OpenACC is meant to be easy to use, and easy to learn
- Programmer remains in familiar C, C++, or Fortran
- No reason to learn low-level details of the hardware.

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OPENACC

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Single Source

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OPENACC RESOURCES

Guides ● Talks ● Tutorials ● Videos ● Books ● Spec ● Code Samples ● Teaching Materials ● Events ● Success Stories ● Courses ● Slack ● Stack Overflow

FREE Compilers

slack

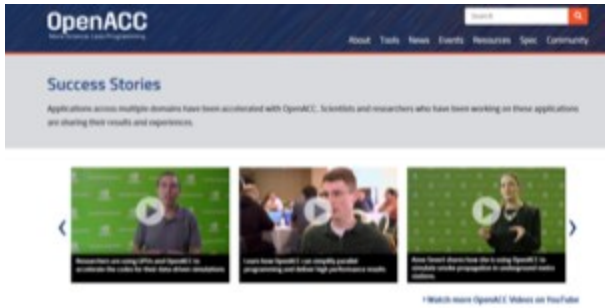
https://www.openacc.org/community#slack

Resources

https://www.openacc.org/resources

Success Stories

https://www.openacc.org/success-stories



Compilers and Tools

https://www.openacc.org/tools

Events

https://www.openacc.org/events

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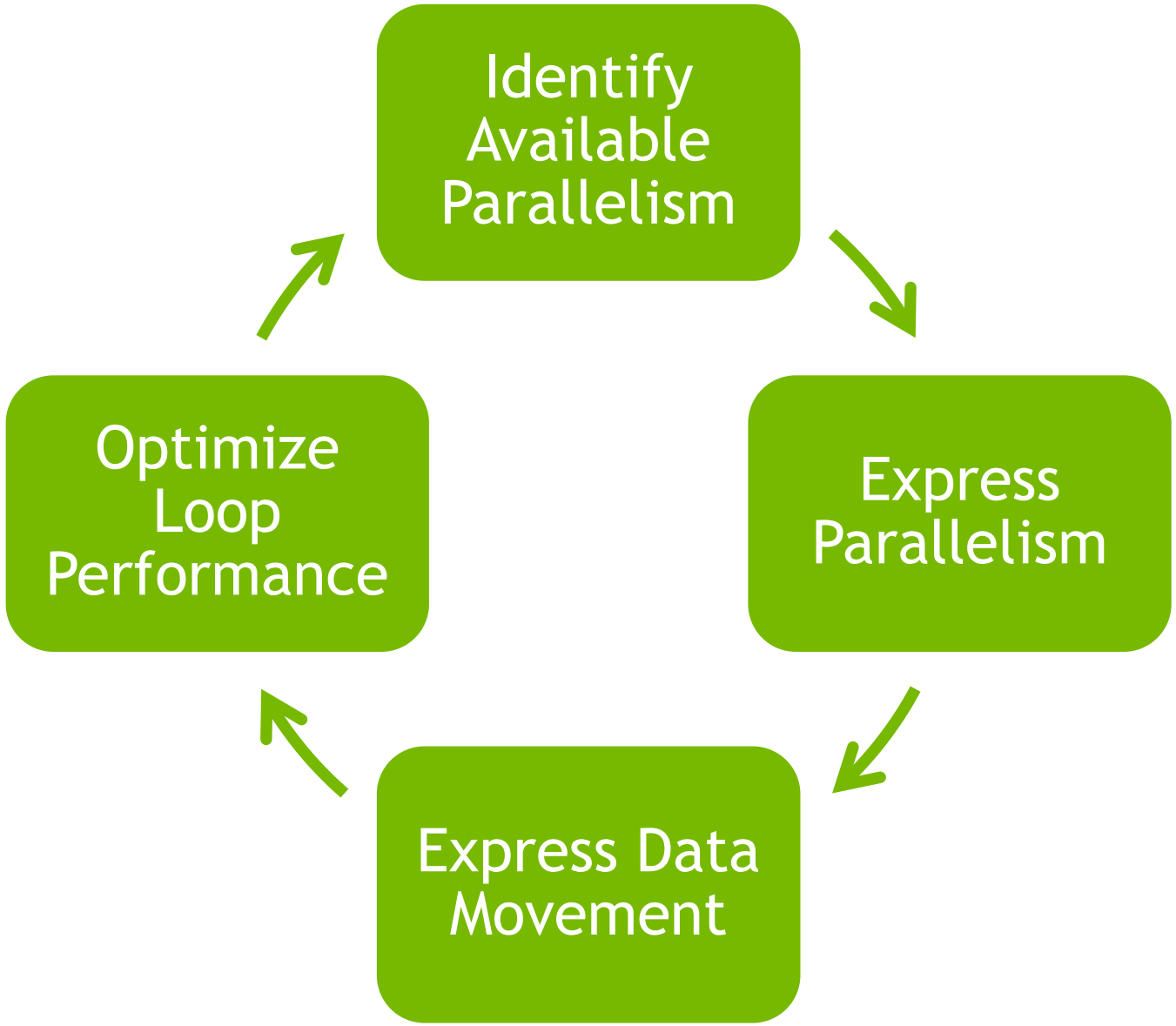
OpenACC Programming Cycle

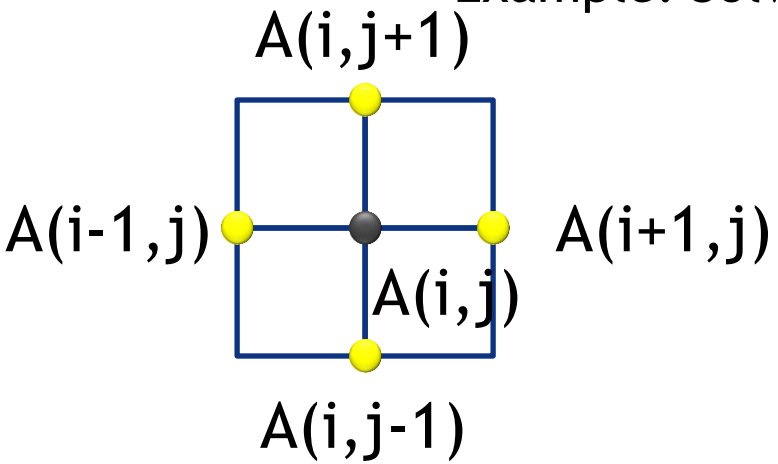

Identify Available Parallelism
Express Parallelism
Express Data Movement
Optimize Loop Performance

Example: Jacobi Iteration

Iteratively converges to correct value (e.g. Temperature), by computing new values at each point from the average of neighboring points.

Common, useful algorithm

Example: Solve Laplace equation in 2D: $\nabla^2 f(x, y) = 0$



Jacobi Iteration: C Code

```
while ( err > tol && iter < iter_max ) {
  err=0.0;


  for( int j = 1; j < n-1; j++) {
    for(int i = 1; i < m-1; i++) {

      Anew[j][i] = 0.25 * (A[j][i+1] + A[j][i-1] +
                           A[j-1][i] + A[j+1][i]);

      err = max(err, abs(Anew[j][i] - A[j][i]));
    }
  }


  for( int j = 1; j < n-1; j++) {
    for( int i = 1; i < m-1; i++ ) {
      A[j][i] = Anew[j][i];
    }
  }

  iter++;
}
```

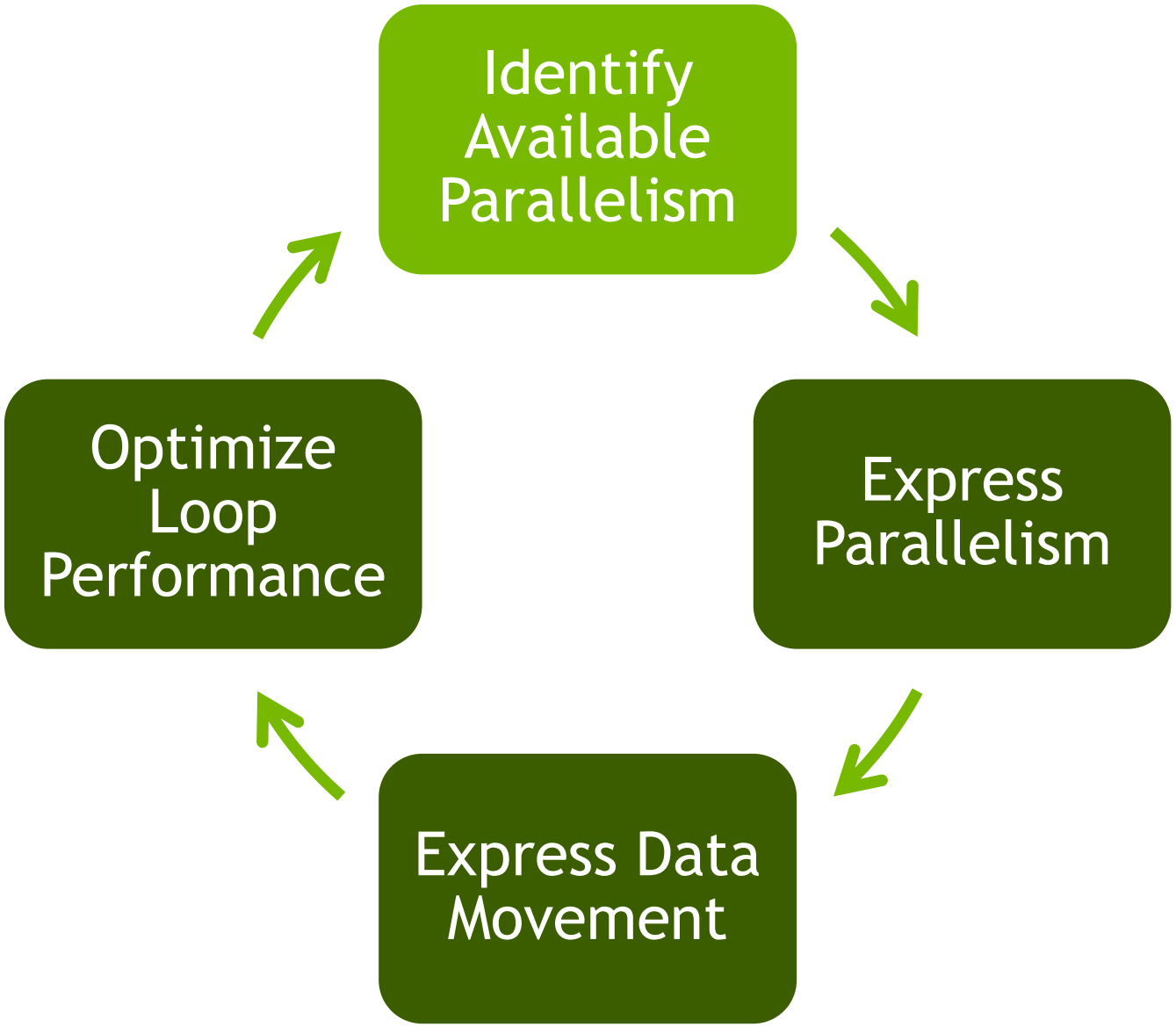
Iterate until converged

Iterate across matrix elements

Calculate new value from neighbors

Compute max error for convergence

Swap input/output arrays


Identify Available Parallelism
Express Parallelism
Express Data Movement
Optimize Loop Performance

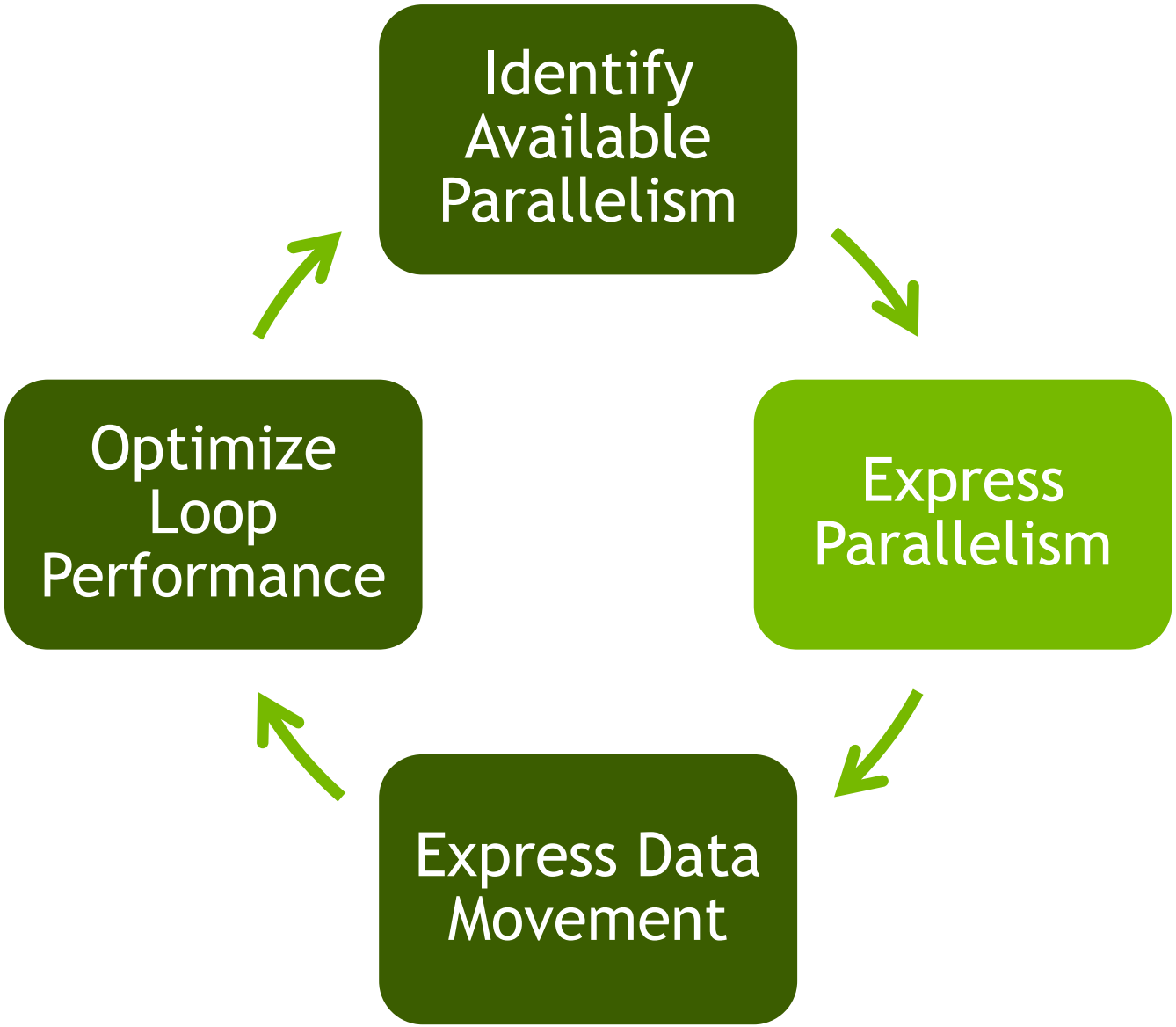
Identify Parallelism

```
while ( err > tol && iter < iter_max ) {
  err=0.0;


  for( int j = 1; j < n-1; j++) {
    for(int i = 1; i < m-1; i++) {

      Anew[j][i] = 0.25 * (A[j][i+1] + A[j][i-1] +
                           A[j-1][i] + A[j+1][i]);

      err = max(err, abs(Anew[j][i] - A[j][i]));
    }
  }


  for( int j = 1; j < n-1; j++) {
    for( int i = 1; i < m-1; i++ ) {
      A[j][i] = Anew[j][i];
    }
  }

  iter++;
}
```

Data dependency between iterations.

Independent loop iterations

Independent loop iterations


Identify Available Parallelism
Express Parallelism
Express Data Movement
Optimize Loop Performance

OpenACC kernels Directive

The kernels directive identifies a region that may contain *loops* that the compiler can turn into parallel *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.

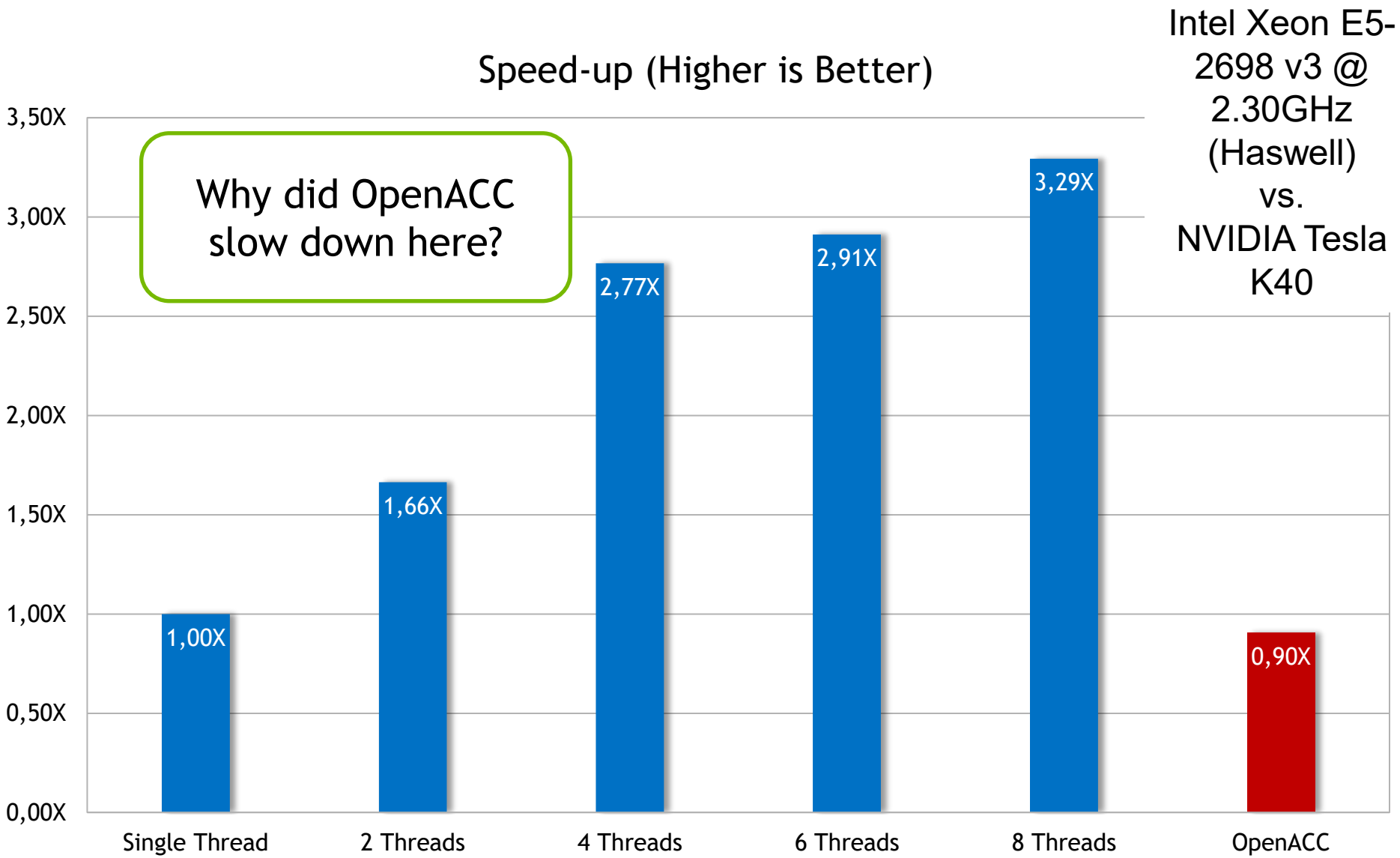
Parallelize with OpenACC kernels

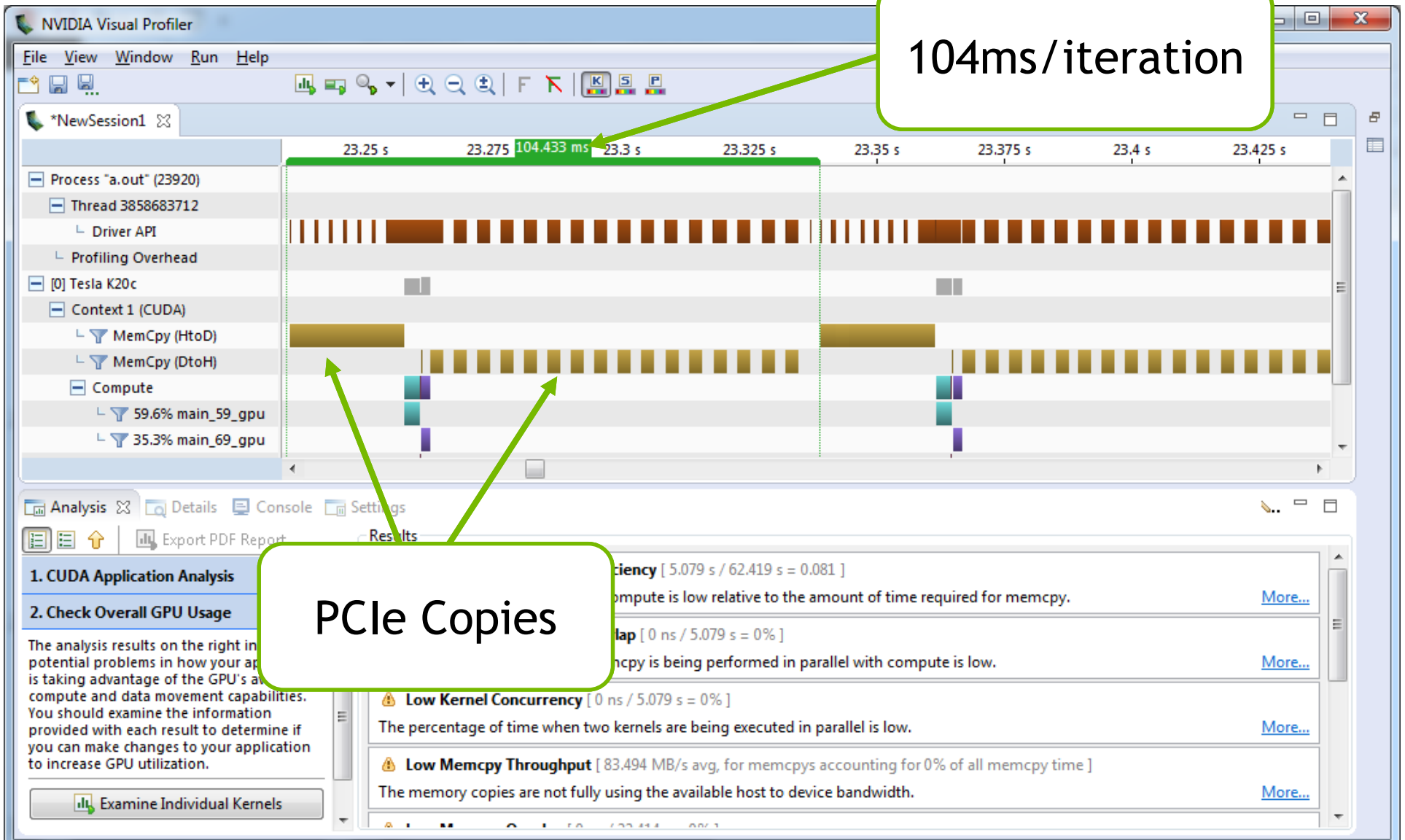
```
while ( err > tol && iter < iter_max ) {
  err=0.0;

#pragma acc kernels
{
  for( int j = 1; j < n-1; j++) {
    for(int i = 1; i < m-1; i++) {

      Anew[j][i] = 0.25 * (A[j][i+1] + A[j][i-1] +
                           A[j-1][i] + A[j+1][i]);

      err = max(err, abs(Anew[j][i] - A[j][i]));
    }
  }

  for( int j = 1; j < n-1; j++) {
    for( int i = 1; i < m-1; i++ ) {
      A[j][i] = Anew[j][i];
    }
  }
}
  iter++;
}
```

Look for parallelism within this region.

Building the code

```
$ pgcc -fast -ta=tesla -Minfo=all laplace2d.c
main:
     40, Loop not fused: function call before adjacent loop
         Generated vector sse code for the loop
     51, Loop not vectorized/parallelized: potential early exits
     55, Generating copyout(Anew[1:4094][1:4094])
         Generating copyin(A[:][:])
         Generating copyout(A[1:4094][1:4094])
         Generating Tesla code
     57, Loop is parallelizable
     59, Loop is parallelizable
         Accelerator kernel generated
         57, #pragma acc loop gang /* blockIdx.y */
         59, #pragma acc loop gang, vector(128) /* blockIdx.x threadIdx.x */
         63, Max reduction generated for error
     67, Loop is parallelizable
     69, Loop is parallelizable
         Accelerator kernel generated
         67, #pragma acc loop gang /* blockIdx.y */
         69, #pragma acc loop gang, vector(128) /* blockIdx.x threadIdx.x */
```


Speed-up (Higher is Better)
Intel Xeon E5-2698 v3 @ 2.30GHz (Haswell) vs. NVIDIA Tesla K40
Why did OpenACC slow down here?
3,50X
3,00X
2,50X
2,00X
1,50X
1,00X
0,50X
0,00X
1,00X
1,66X
2,77X
2,91X
3,29X
0,90X
Single Thread
2 Threads
4 Threads
6 Threads
8 Threads
OpenACC


NVIDIA Visual Profiler
File View Window Run Help
*NewSession1
104ms/iteration
23.25 s
23.275
104.433 ms
23.3 s
23.325 s
23.35 s
23.375 s
23.4 s
23.425 s
Process "a.out" (23920)
Thread 3858683712
Driver API
Profiling Overhead
[0] Tesla K20c
Context 1 (CUDA)
MemCpy (HtoD)
MemCpy (DtoH)
Compute
59.6% main_59_gpu
35.3% main_69_gpu
Analysis
Details
Console
Export PDF Report
Results
PCIe Copies
1. CUDA Application Analysis
2. Check Overall GPU Usage
The analysis results on the right in
potential problems in how your ap
is taking advantage of the GPU's a
compute and data movement capabilities.
You should examine the information
provided with each result to determine if
you can make changes to your application
to increase GPU utilization.
Examine Individual Kernels
ciency [5.079 s / 62.419 s = 0.081]
mpute is low relative to the amount of time required for memcpy.
More...
lap [0 ns / 5.079 s = 0%]
ncpy is being performed in parallel with compute is low.
More...
Low Kernel Concurrency [0 ns / 5.079 s = 0%]
The percentage of time when two kernels are being executed in parallel is low.
More...
Low Memcpy Throughput [83.494 MB/s avg, for memcpys accounting for 0% of all memcpy time]
The memory copies are not fully using the available host to device bandwidth.
More...

Excessive Data Transfers

```
while ( err > tol && iter < iter_max )
{
  err=0.0;
```

A, Anew resident on host

Copy

A, Anew resident on accelerator

```
#pragma acc kernels
for( int j = 1; j < n-1; j++) {
  for(int i = 1; i < m-1; i++) {
    Anew[j][i] = 0.25 * (A[j][i+1] +
                 A[j][i-1] + A[j-1][i] +
                 A[j+1][i]);
    err = max(err, abs(Anew[j][i] -
                       A[j][i]);
  }
}
...
```

These copies happen every iteration of the outer while loop!

Copy

A, Anew resident on host

A, Anew resident on accelerator

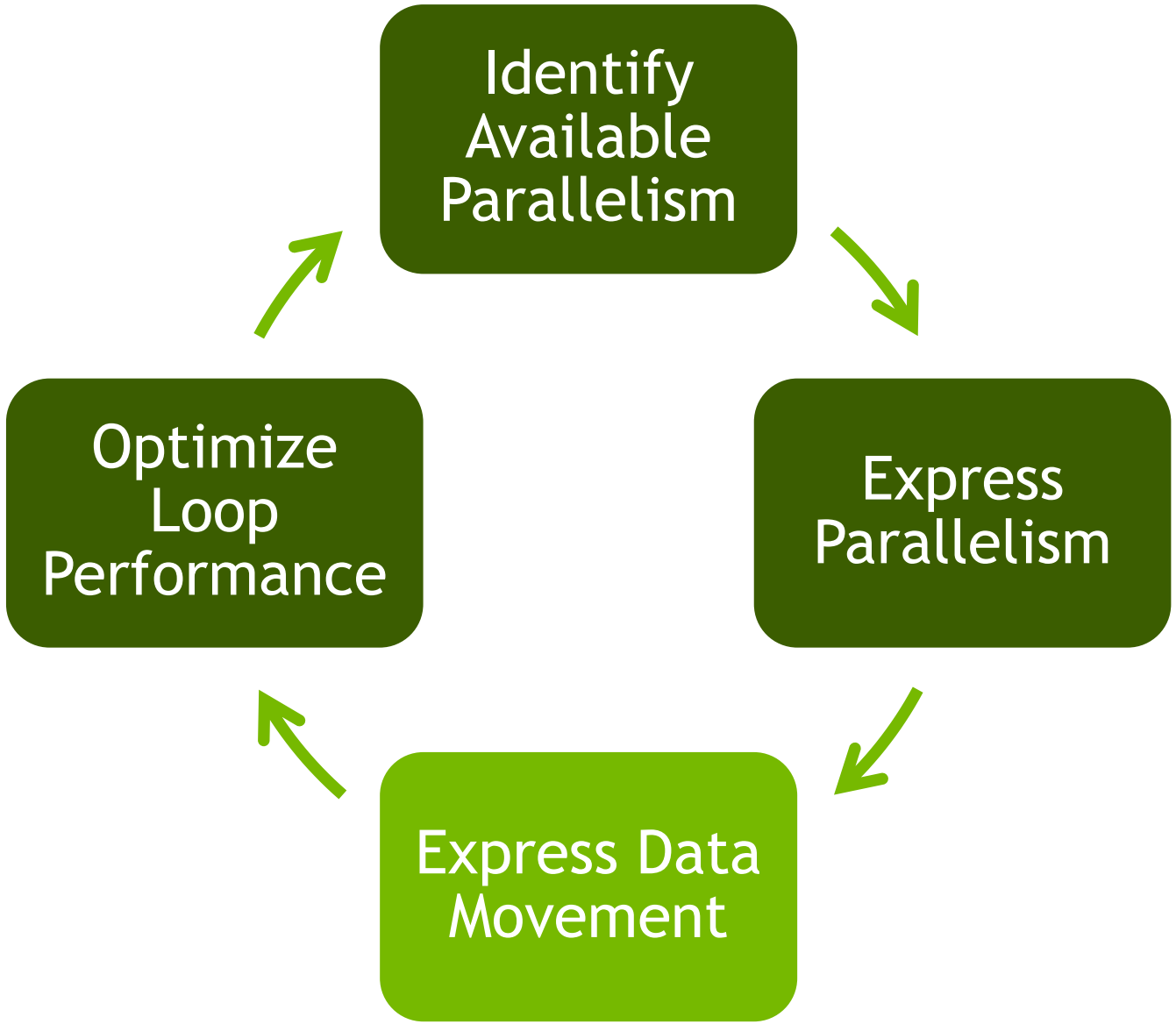
```
  ...
}
```

Identifying Data Locality

```
while ( err > tol && iter < iter_max ) {
  err=0.0;

#pragma acc kernels
  {
  for( int j = 1; j < n-1; j++) {
    for(int i = 1; i < m-1; i++) {

      Anew[j][i] = 0.25 * (A[j][i+1] + A[j][i-1] +
                           A[j-1][i] + A[j+1][i]);

      err = max(err, abs(Anew[j][i] - A[j][i]));
    }
  }

  for( int j = 1; j < n-1; j++) {
    for( int i = 1; i < m-1; i++ ) {
      A[j][i] = Anew[j][i];
    }
  }
  }

  iter++;
}
```

Does the CPU need the data between these loop nests?

Does the CPU need the data between iterations of the convergence loop?


Identify Available Parallelism
Express Parallelism
Express Data Movement
Optimize Loop Performance

Data regions

The **`data`** directive defines a region of code in which GPU arrays remain on the GPU and are shared among all kernels in that region.

```
#pragma acc data
{
#pragma acc kernels
...

#pragma acc kernels
...
}
```

Data Region

Arrays used within the data region will remain on the GPU until the end of the data region.

Data Clauses

`copy ( list )`	Allocates memory on GPU and copies data from host to GPU when entering region and copies data to the host when exiting region.
`copyin ( list )`	Allocates memory on GPU and copies data from host to GPU when entering region.
`copyout ( list )`	Allocates memory on GPU and copies data to the host when exiting region.
`create ( list )`	Allocates memory on GPU but does not copy.
`present ( list )`	Data is already present on GPU from another containing data region.
`deviceptr( list )`	The variable is a device pointer (e.g. CUDA) and can be used directly on the device.

Array Shaping

Compiler sometimes cannot determine size of arrays

Must specify explicitly using data clauses and array “shape”

C/C++

```
#pragma acc data copyin(a[0:nelem]) copyout(b[s/4:3*s/4])
```

Fortran

```
!$acc data copyin(a(1:end)) copyout(b(s/4:3*s/4))
```

Note: data clauses can be used on `data`, `parallel`, or `kernels`

Express Data Locality

```
#pragma acc data copy(A) create(Anew)
while ( err > tol && iter < iter_max ) {
  err=0.0;
#pragma acc kernels
{
  for( int j = 1; j < n-1; j++) {
    for(int i = 1; i < m-1; i++) {

      Anew[j][i] = 0.25 * (A[j][i+1] + A[j][i-1] +
                           A[j-1][i] + A[j+1][i]);

      err = max(err, abs(Anew[j][i] - A[j][i]));
    }
  }

  for( int j = 1; j < n-1; j++) {
    for( int i = 1; i < m-1; i++ ) {
      A[j][i] = Anew[j][i];
    }
  }
}
  iter++;
}
```

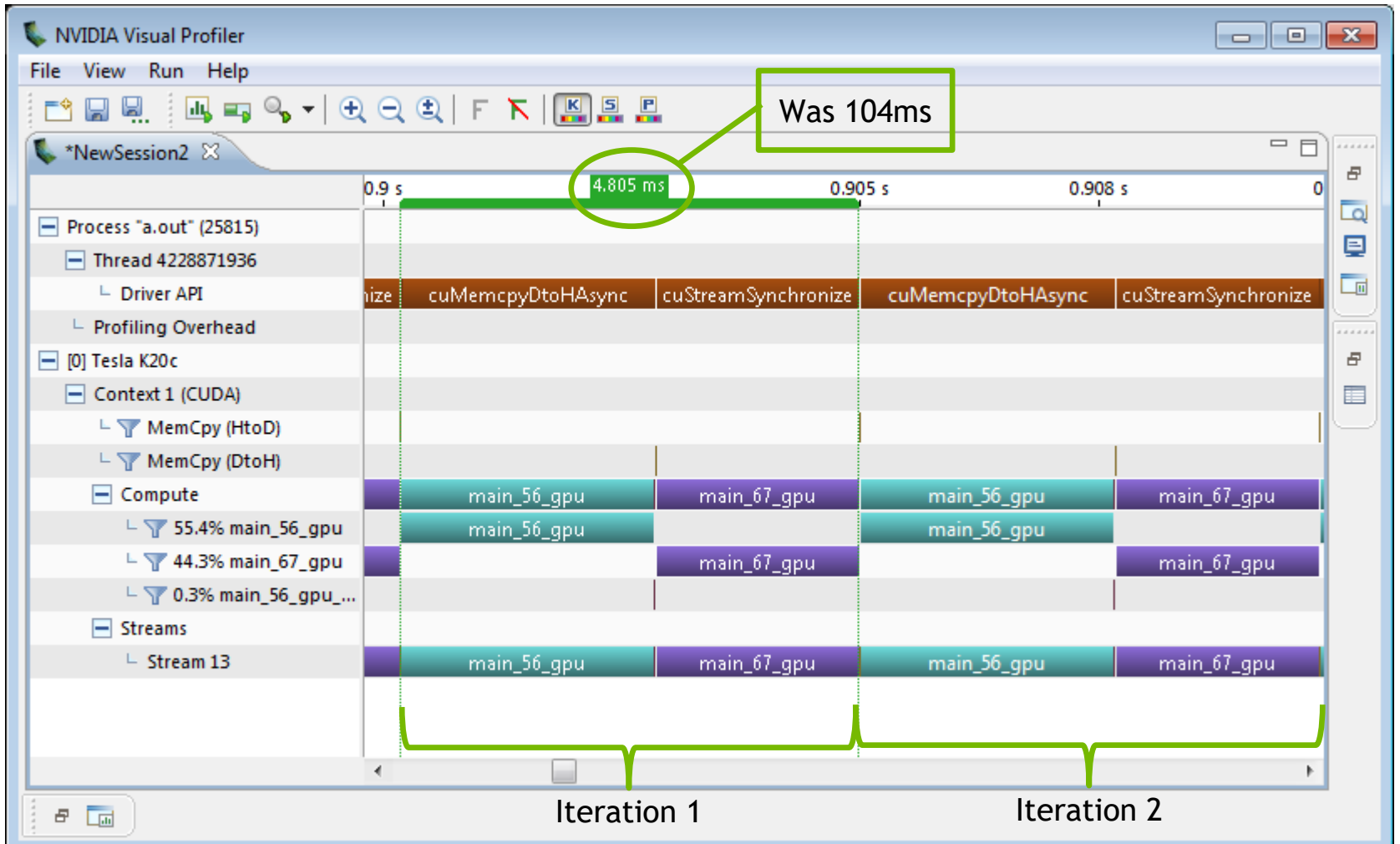
Copy A to/from the accelerator only when needed.

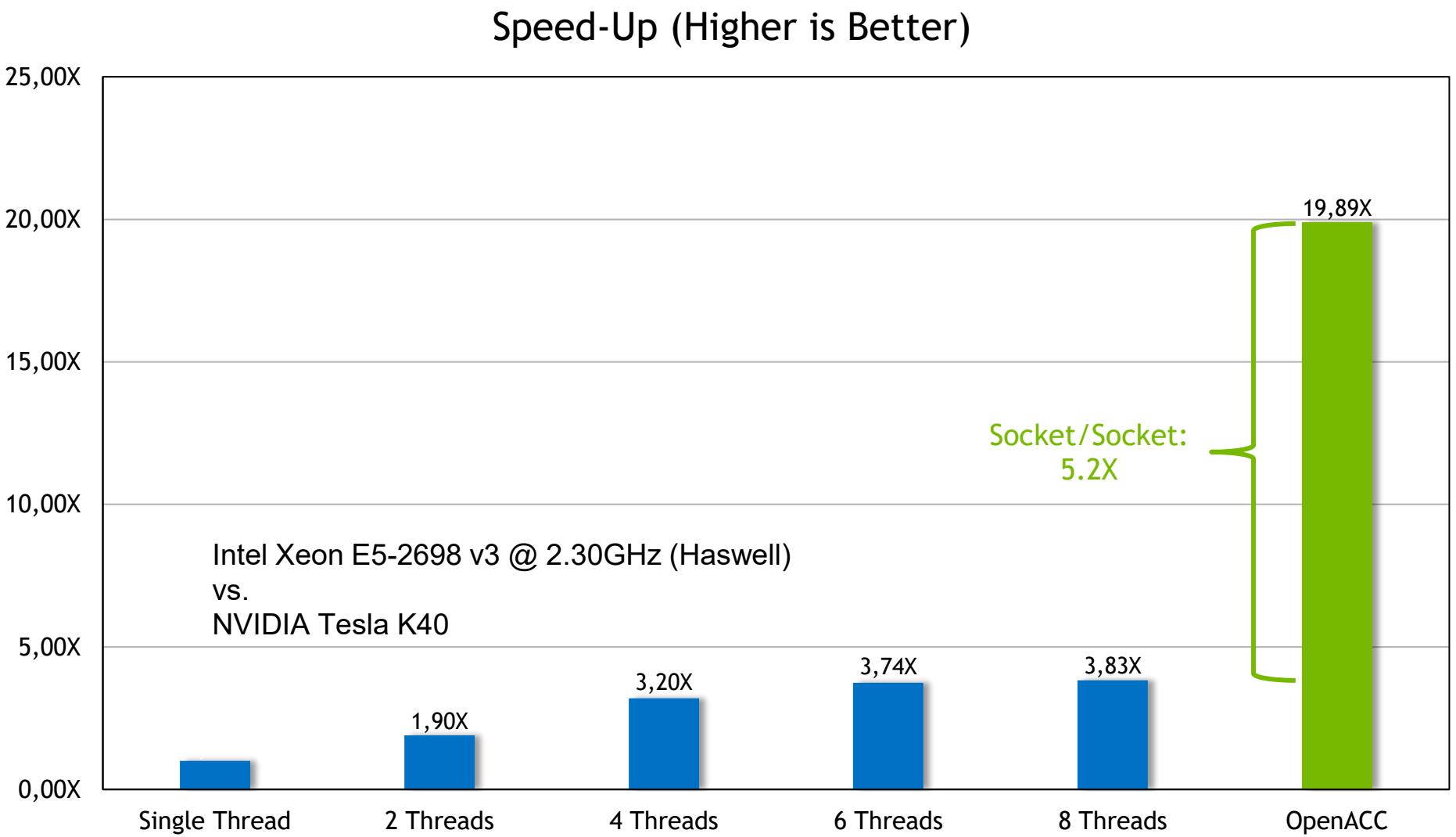
Create Anew as a device temporary.

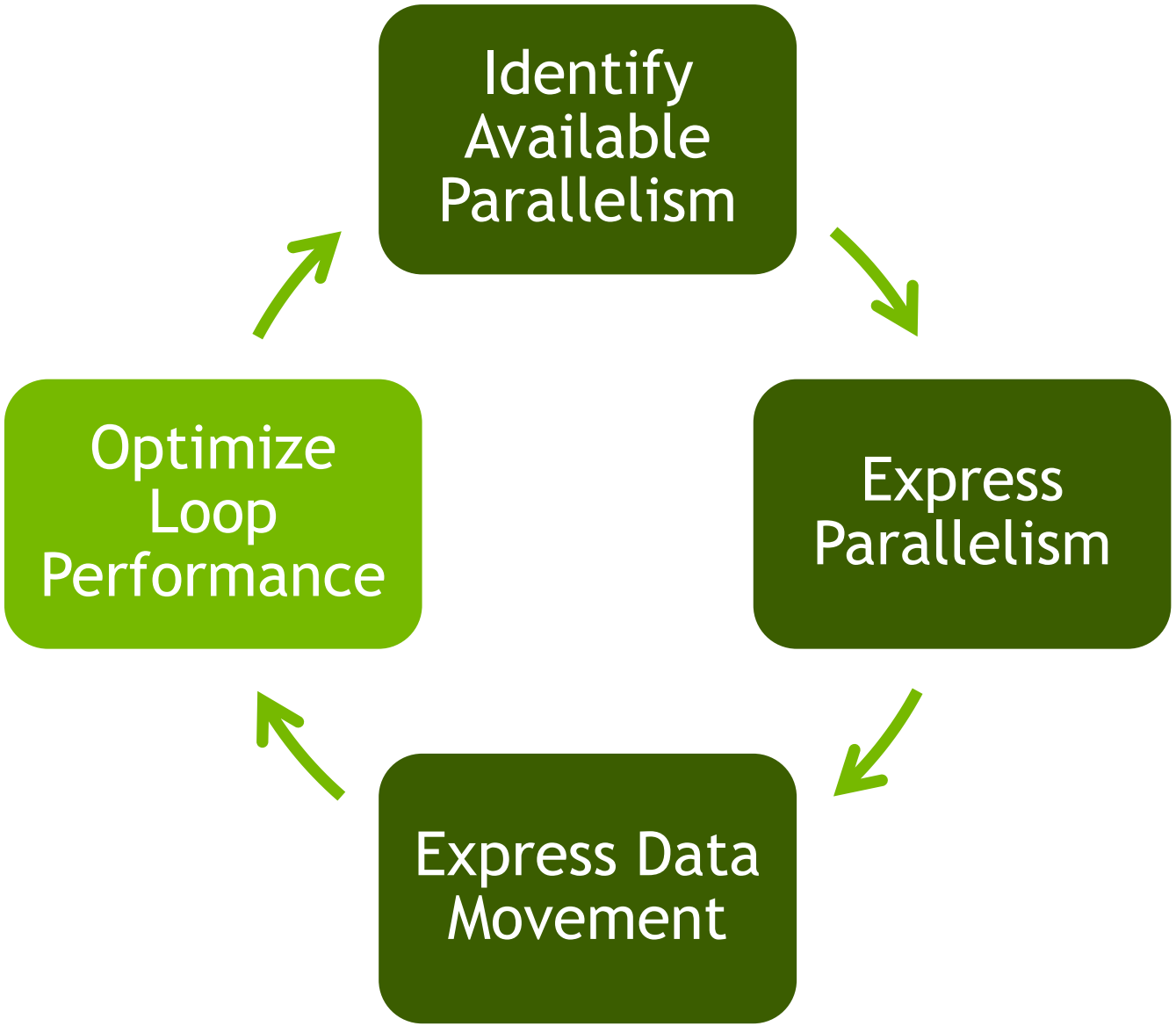
Rebuilding the code

```
$ pgcc -fast -acc -ta=tesla -Minfo=all laplace2d.c
main:
     40, Loop not fused: function call before adjacent loop
         Generated vector sse code for the loop
     51, Generating copy(A[:][:])
         Generating create(Anew[:][:])
         Loop not vectorized/parallelized: potential early exits
     56, Accelerator kernel generated
         56, Max reduction generated for error
         57, #pragma acc loop gang /* blockIdx.x */
         59, #pragma acc loop vector(256) /* threadIdx.x */
     56, Generating Tesla code
     59, Loop is parallelizable
     67, Accelerator kernel generated
         68, #pragma acc loop gang /* blockIdx.x */
         70, #pragma acc loop vector(256) /* threadIdx.x */
     67, Generating Tesla code
     70, Loop is parallelizable
```

Visual Profiler: Data Region




Speed-Up (Higher is Better)
25,00X
20,00X
15,00X
10,00X
5,00X
0,00X
Intel Xeon E5-2698 v3 @ 2.30GHz (Haswell)
vs.
NVIDIA Tesla K40
1,90X
3,20X
3,74X
3,83X
19,89X
Socket/Socket:
5.2X
Single Thread
2 Threads
4 Threads
6 Threads
8 Threads
OpenACC


Identify Available Parallelism
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Express Data Movement
Optimize Loop Performance

The loop Directive

The `loop` directive gives the compiler additional information about the *next* loop in the source code through several clauses.

- `independent` – all iterations of the loop are independent
- `collapse(N)` – turn the next N loops into one, flattened loop
- `tile(N[,M,…])` - break the next 1 or more loops into *tiles* based on the provided dimensions.

These clauses and more will be discussed in greater detail in a later class.

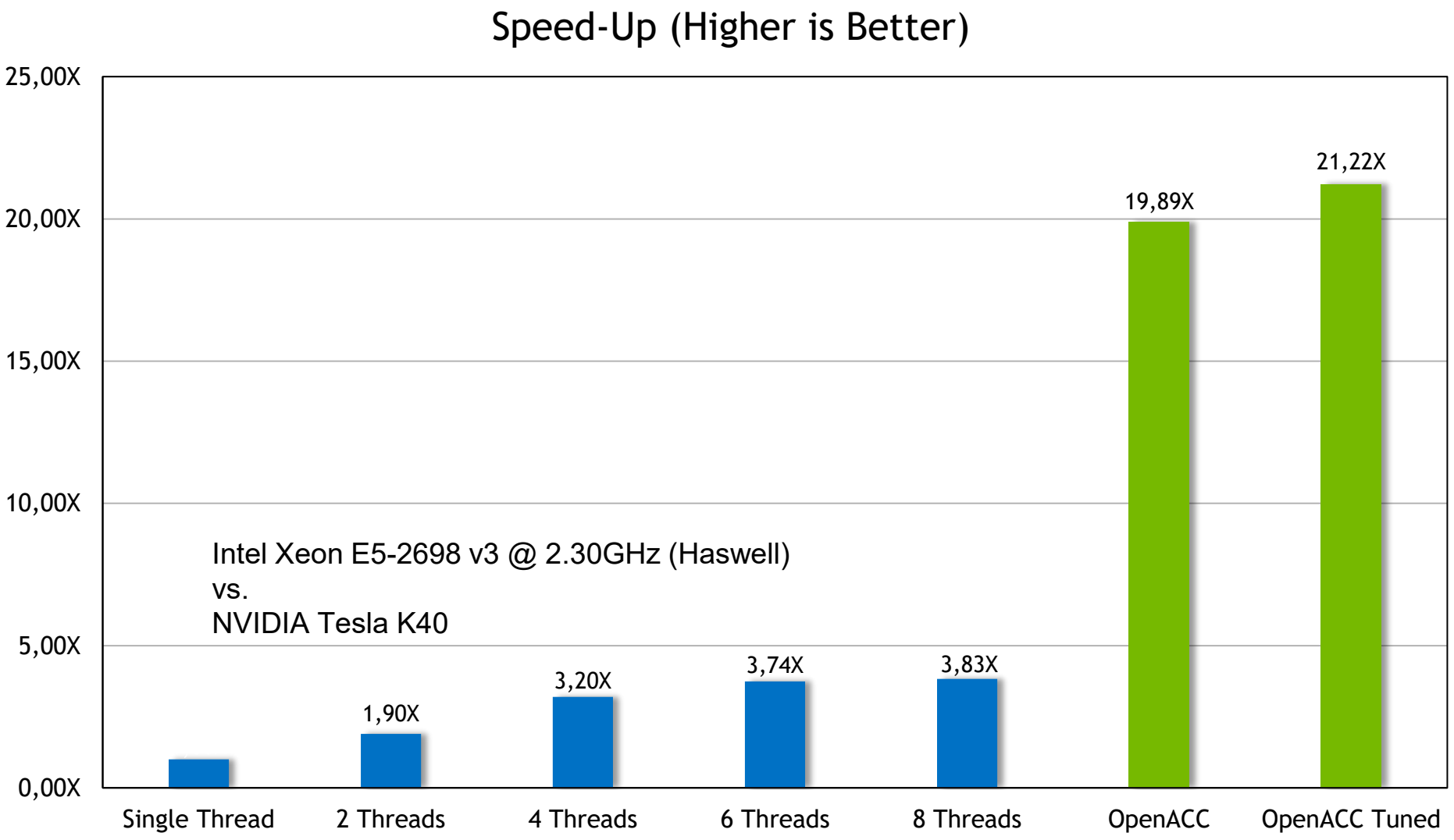
Optimize Loop Performance

```
#pragma acc data copy(A) create(Anew)
while ( err > tol && iter < iter_max ) {
  err=0.0;
#pragma acc kernels
{
#pragma acc loop device_type(nvidia) tile(32,4)
  for( int j = 1; j < n-1; j++) {
    for(int i = 1; i < m-1; i++) {

      Anew[j][i] = 0.25 * (A[j][i+1] + A[j][i-1] +
                           A[j-1][i] + A[j+1][i]);

      err = max(err, abs(Anew[j][i] - A[j][i]));
    }
  }
#pragma acc loop device_type(nvidia) tile(32,4)
  for( int j = 1; j < n-1; j++) {
    for( int i = 1; i < m-1; i++ ) {
      A[j][i] = Anew[j][i];
    }
  }
}
  iter++;
}
```

"Tile" the next two loops into 32x4 blocks, but only on NVIDIA GPUs.


Speed-Up (Higher is Better)
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Intel Xeon E5-2698 v3 @ 2.30GHz (Haswell)
vs.
NVIDIA Tesla K40
1,90X
3,20X
3,74X
3,83X
19,89X
21,22X
Single Thread
2 Threads
4 Threads
6 Threads
8 Threads
OpenACC
OpenACC Tuned

The OpenACC Toolkit

Introducing the New OpenACC Toolkit

Free Toolkit Offers Simple & Powerful Path to Accelerated Computing

http://developer.nvidia.com/openacc

PGI Compiler
Free OpenACC compiler for academia

NVProf Profiler
Easily find where to add compiler directives

GPU Wizard
Identify which GPU libraries can jumpstart code

Code Samples
Learn from examples of real-world algorithms

Documentation
Quick start guide, Best practices, Forums

Download the OpenACC Toolkit

- Go to https://developer.nvidia.com/openacc

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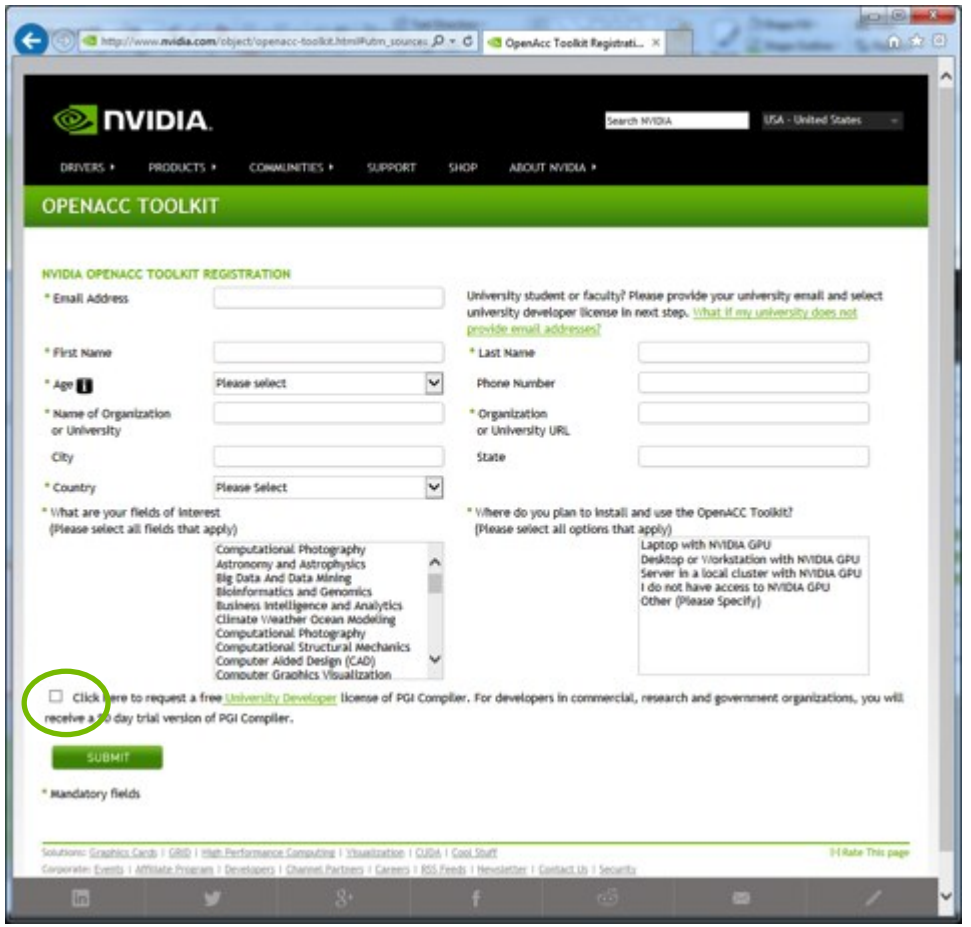
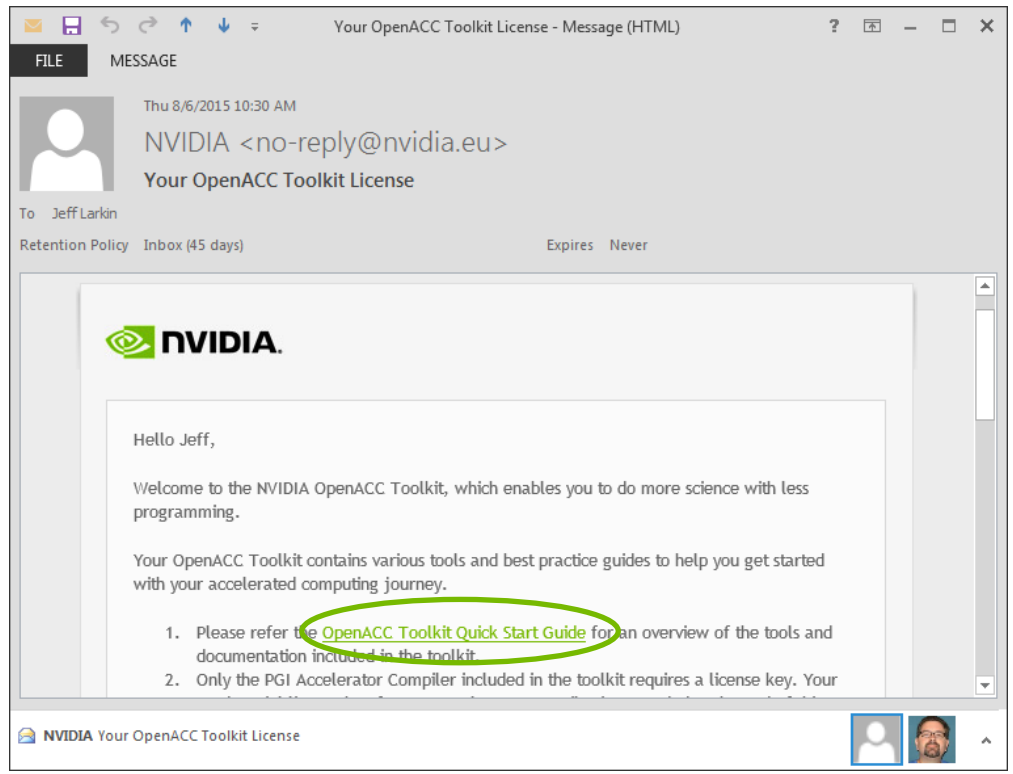
- Go to https://developer.nvidia.com/openacc
- Register for the toolkit
  - If you are an academic developer, be sure to click the check box at the bottom.



Download the OpenACC Toolkit

- Go to https://developer.nvidia.com/openacc
- Register for the toolkit
  - If you are an academic developer, be sure to click the check box at the bottom.
- You will receive an email from NVIDIA
  - Be sure to read the Quick Start Guide



Windows/Mac Developers

- The OpenACC Toolkit is only available on Linux, however…
- The PGI compiler is available on Mac and Windows from http://www.pgroup.com/support/trial.htm
  - You should still register for the OpenACC Toolkit to get the 90 day license.
- The CUDA Toolkit contains the libraries and profiling tools that will be used in this course.
  - https://developer.nvidia.com/cuda-zone
- The OpenACC Programming Guide is available from http://bit.ly/openacc-guide
  - Obtaining all examples and guides from the toolkit will still require downloading the full OpenACC toolkit.

Install the OpenACC Toolkit

- Go to developer.nvidia.com/openacc
- Register for the OpenACC Toolkit
- Install on your **personal machine. (Linux Only)**

Where to find help

- OpenACC Course Recordings - https://developer.nvidia.com/openacc-course
- OpenACC on StackOverflow - http://stackoverflow.com/questions/tagged/openacc
- OpenACC Toolkit - http://developer.nvidia.com/openacc

Additional Resources:

- Parallel Forall Blog - http://devblogs.nvidia.com/parallelforall/
- GPU Technology Conference - http://www.gputechconf.com/
- OpenACC Website - http://openacc.org/

Get Started

OpenACC is a user-driven directive-based performance-portable parallel programming model. It is designed for scientists and engineers interested in porting their codes to a wide-variety of heterogeneous HPC hardware platforms and architectures with significantly less programming effort than required with a low-level model.

Then, follow the exercises of the OpenAcc tutorial: https://www.openacc.org/get-started

THANK YOU

@carlosjaimebh