

OpenACC Course

Lecture 1: Introduction to OpenACC

September 2015



Course Objective:

Enable you to accelerate *your* applications
with OpenACC.

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

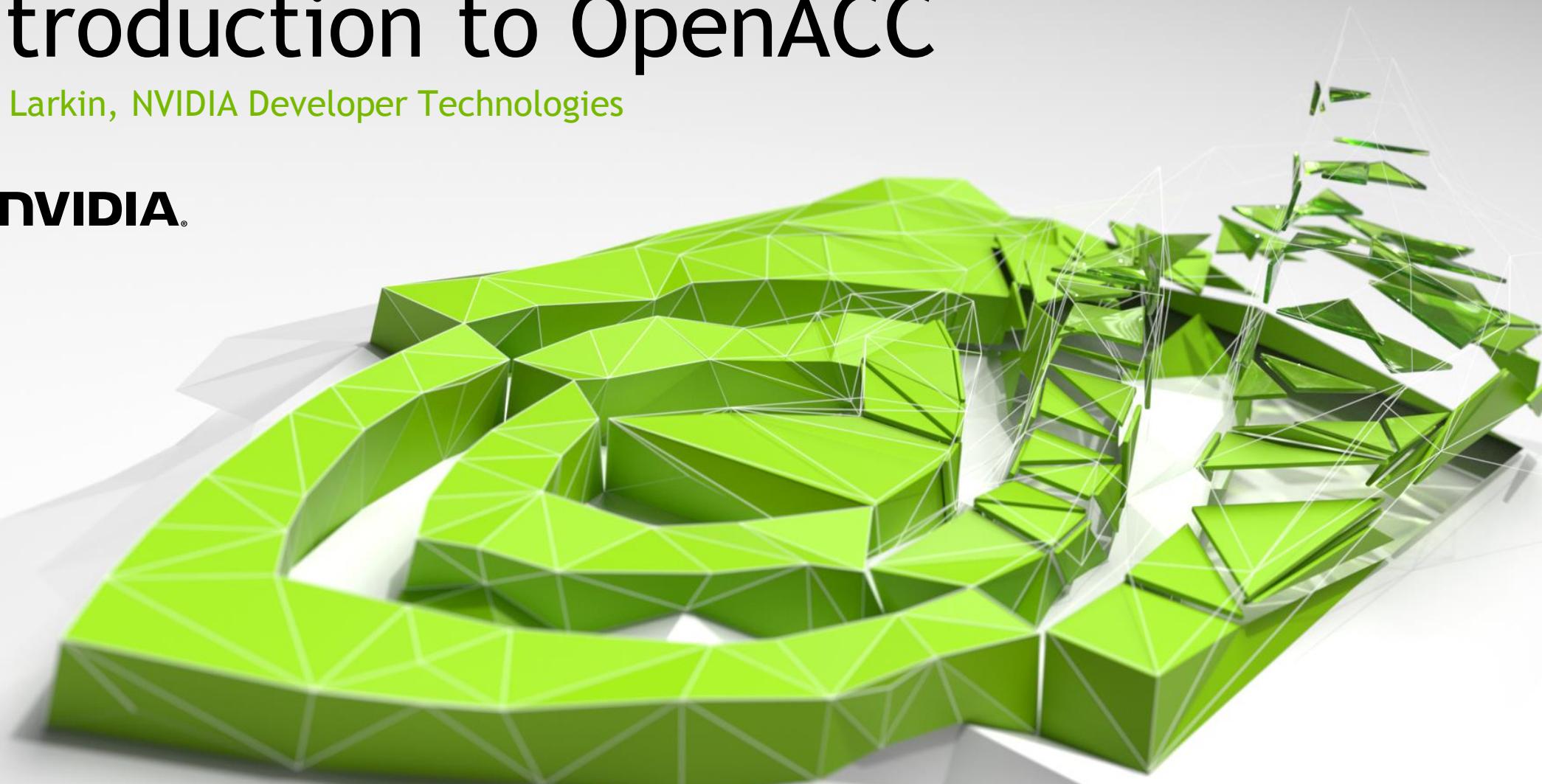
Nov 24: Office Hours

Recordings:

<https://developer.nvidia.com/openacc-course>

Introduction to OpenACC

Jeff Larkin, NVIDIA Developer Technologies



Agenda

Why OpenACC?

Accelerated Computing Fundamentals

OpenACC Programming Cycle

Installing the OpenACC Toolkit

Accessing QwikLabs

Week 1 Homework

Why 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

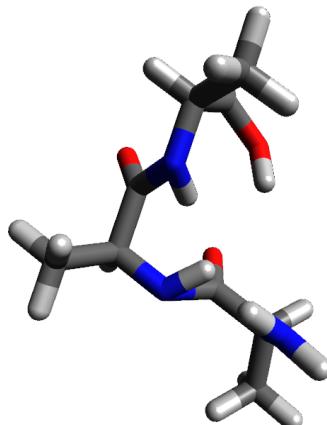


7-8x Speed-Up
5% of Code Modified

8000+
Developers
using OpenACC

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.

”

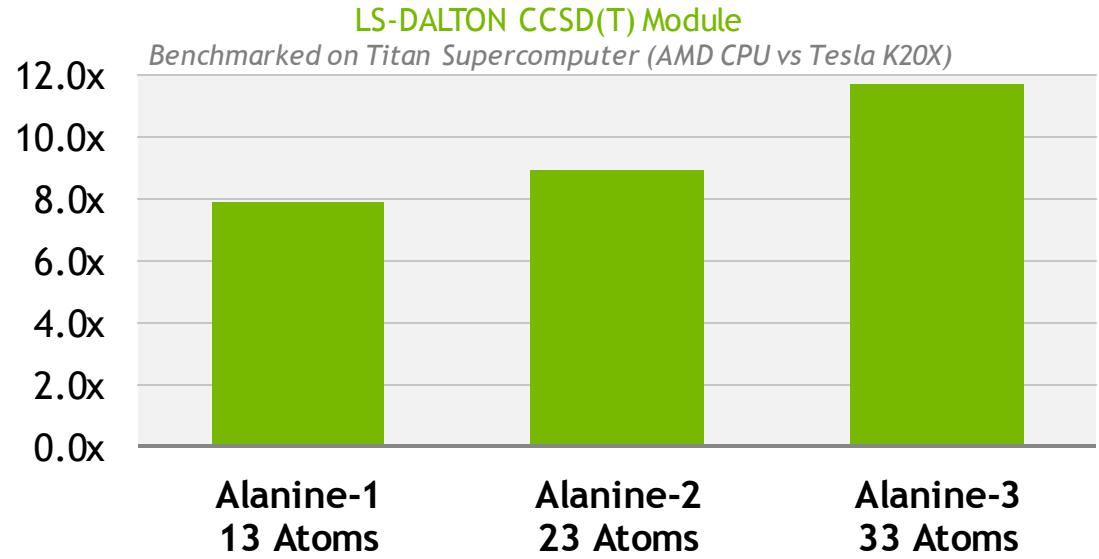
Janus Juul Eriksen, PhD Fellow
qLEAP Center for Theoretical Chemistry, Aarhus University



Minimal Effort

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

Big Performance



OpenACC Directives

The diagram illustrates the use of OpenACC directives in a C-like code snippet. Three green arrows point from text labels on the left to specific code elements:

- A green arrow labeled "Manage Data Movement" points to the first `#pragma acc data` directive.
- A green arrow labeled "Initiate Parallel Execution" points to the first `#pragma acc parallel` directive.
- A green arrow labeled "Optimize Loop Mappings" points to the `#pragma acc loop` directive and the nested `for` loop below it.

```
#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

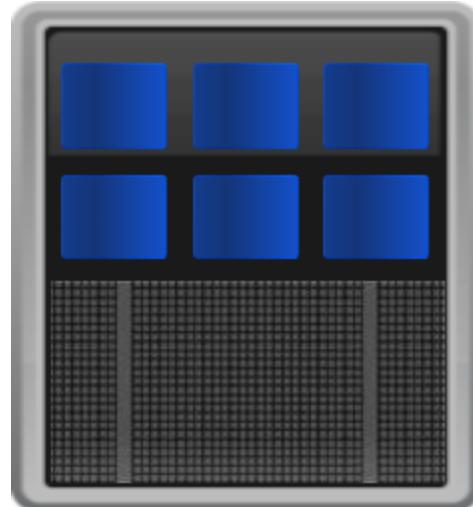
Accelerated Computing Fundamentals

Accelerated Computing

10x Performance & 5x Energy Efficiency for HPC

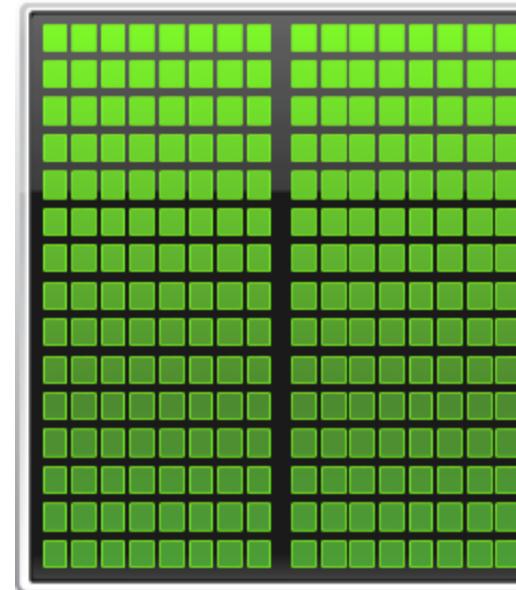
CPU

Optimized for
Serial Tasks

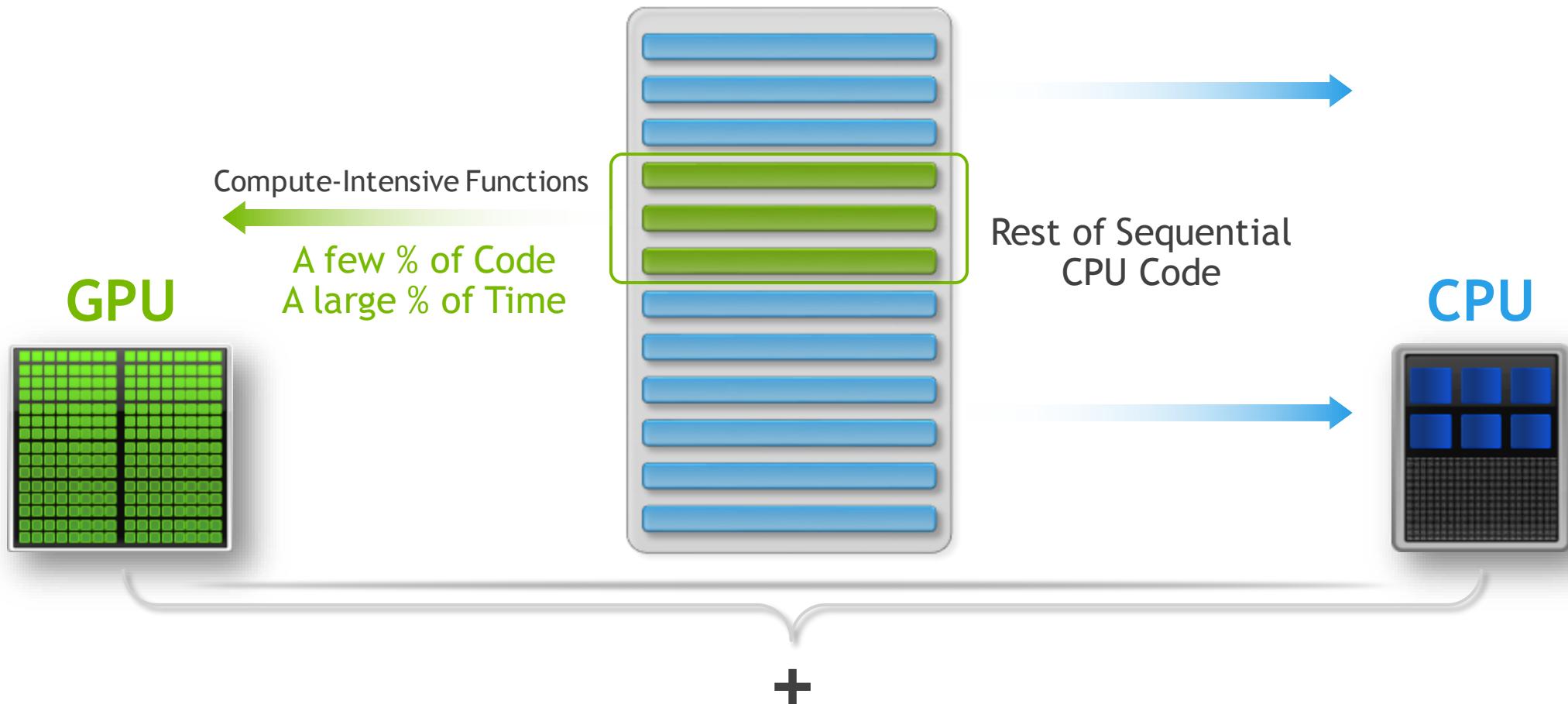


GPU Accelerator

Optimized for
Parallel Tasks



What is Heterogeneous Programming?



Portability & Performance

Portability



Accelerated Libraries

High performance with little or no code change

Limited by what libraries are available

Compiler Directives

High Level: Based on existing languages; simple, familiar, portable

High Level: Performance may not be optimal

Parallel Language Extensions

Greater flexibility and control for maximum performance

Often less portable and more time consuming to implement

Performance

Code for Portability & Performance

Libraries

- Implement as much as possible using portable libraries

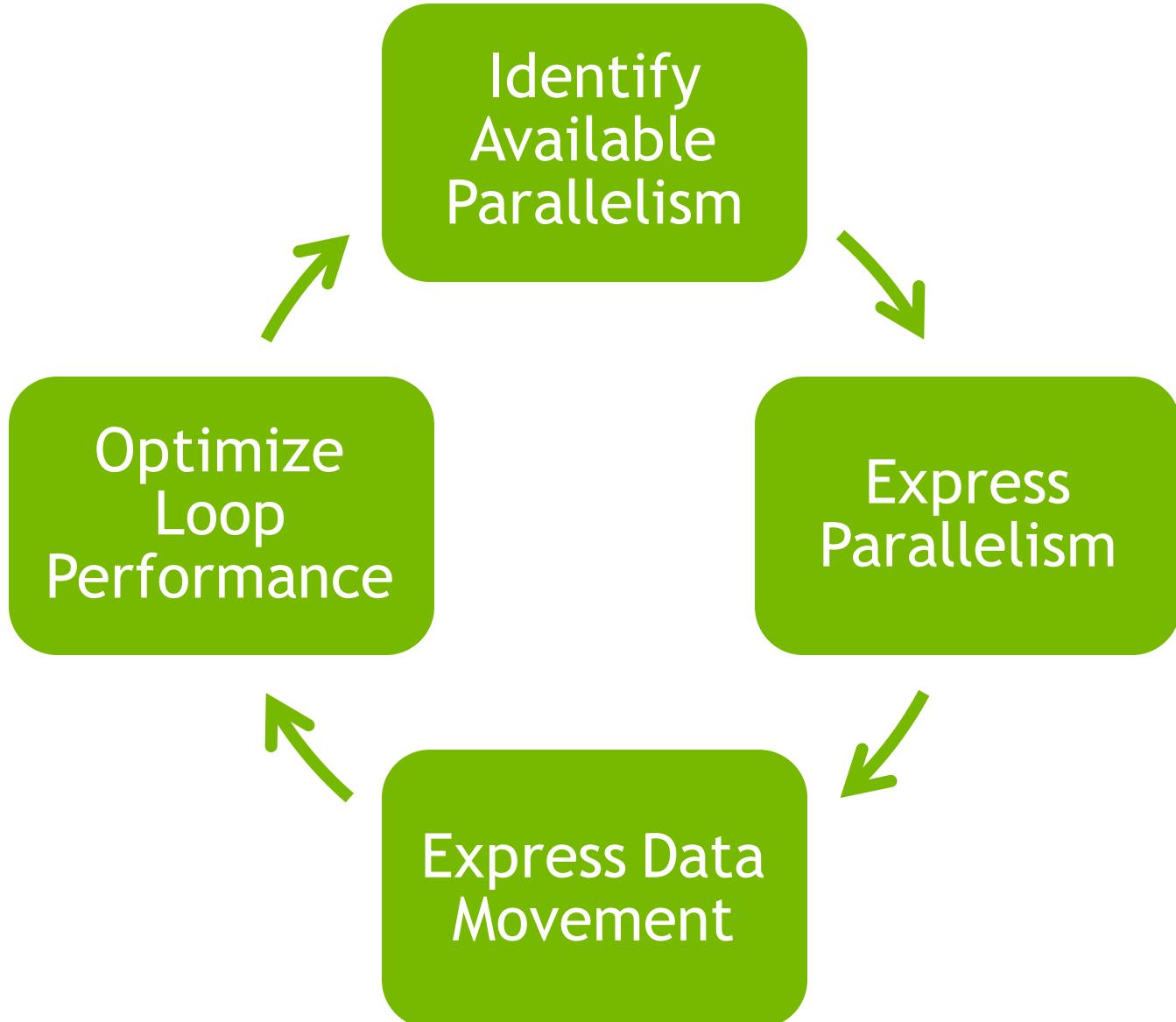
Directives

- Use directives for rapid and portable development

Languages

- Use lower level languages for important kernels

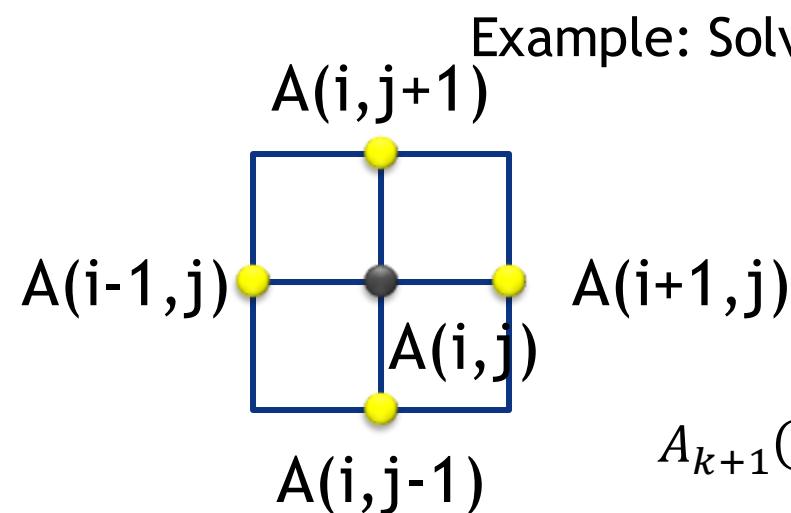
OpenACC Programming Cycle



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



$$A_{k+1}(i, j) = \frac{A_k(i - 1, j) + A_k(i + 1, j) + A_k(i, j - 1) + A_k(i, j + 1)}{4}$$

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++;  
}
```

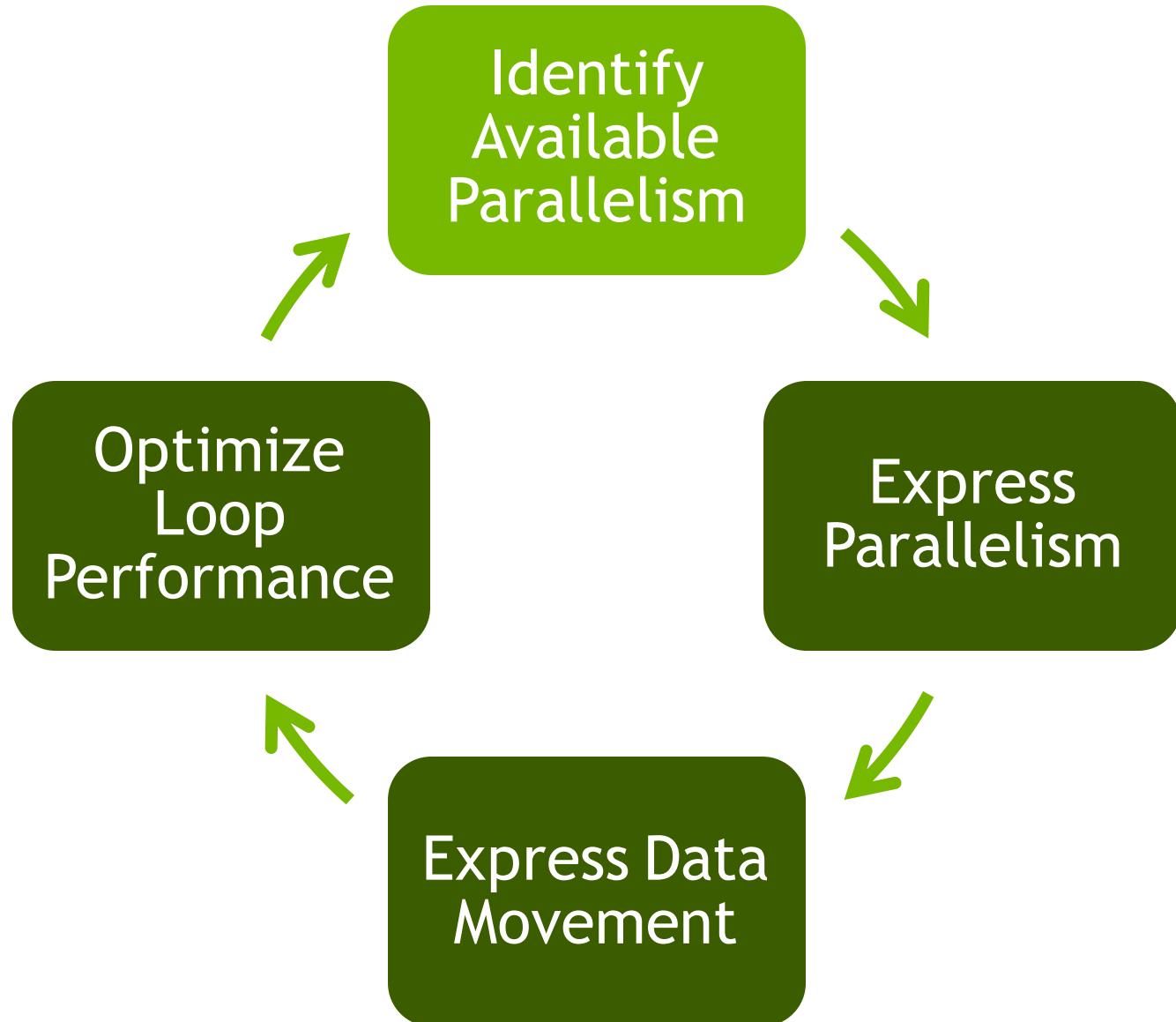
Iterate until converged

Iterate across matrix elements

Calculate new value from neighbors

Compute max error for convergence

Swap input/output arrays



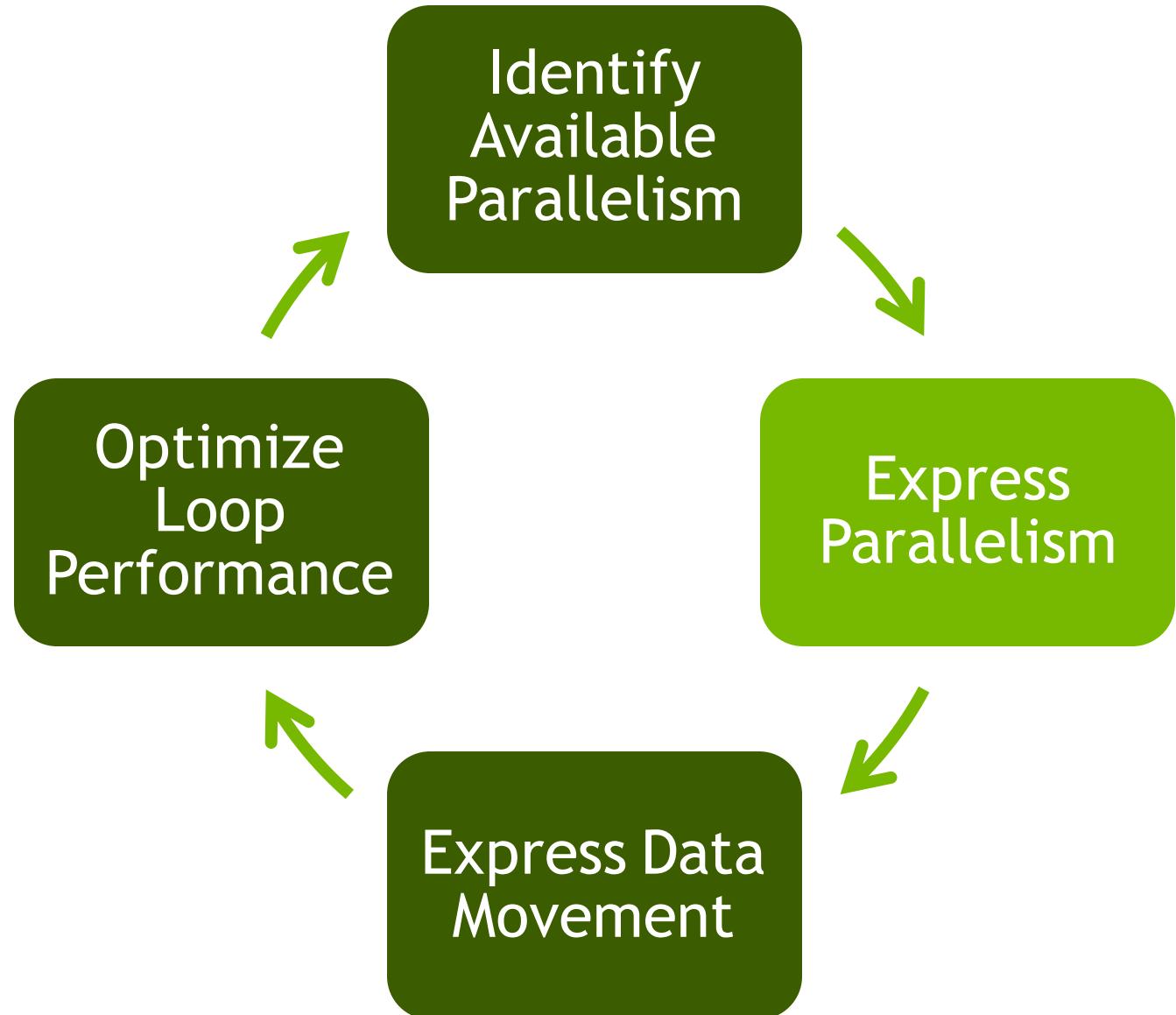
Identify Parallelism

```
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

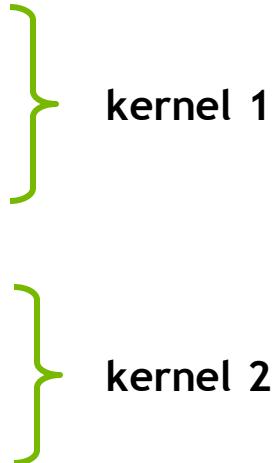


OpenACC kernels Directive

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];
    }
}
```



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++;
}
```

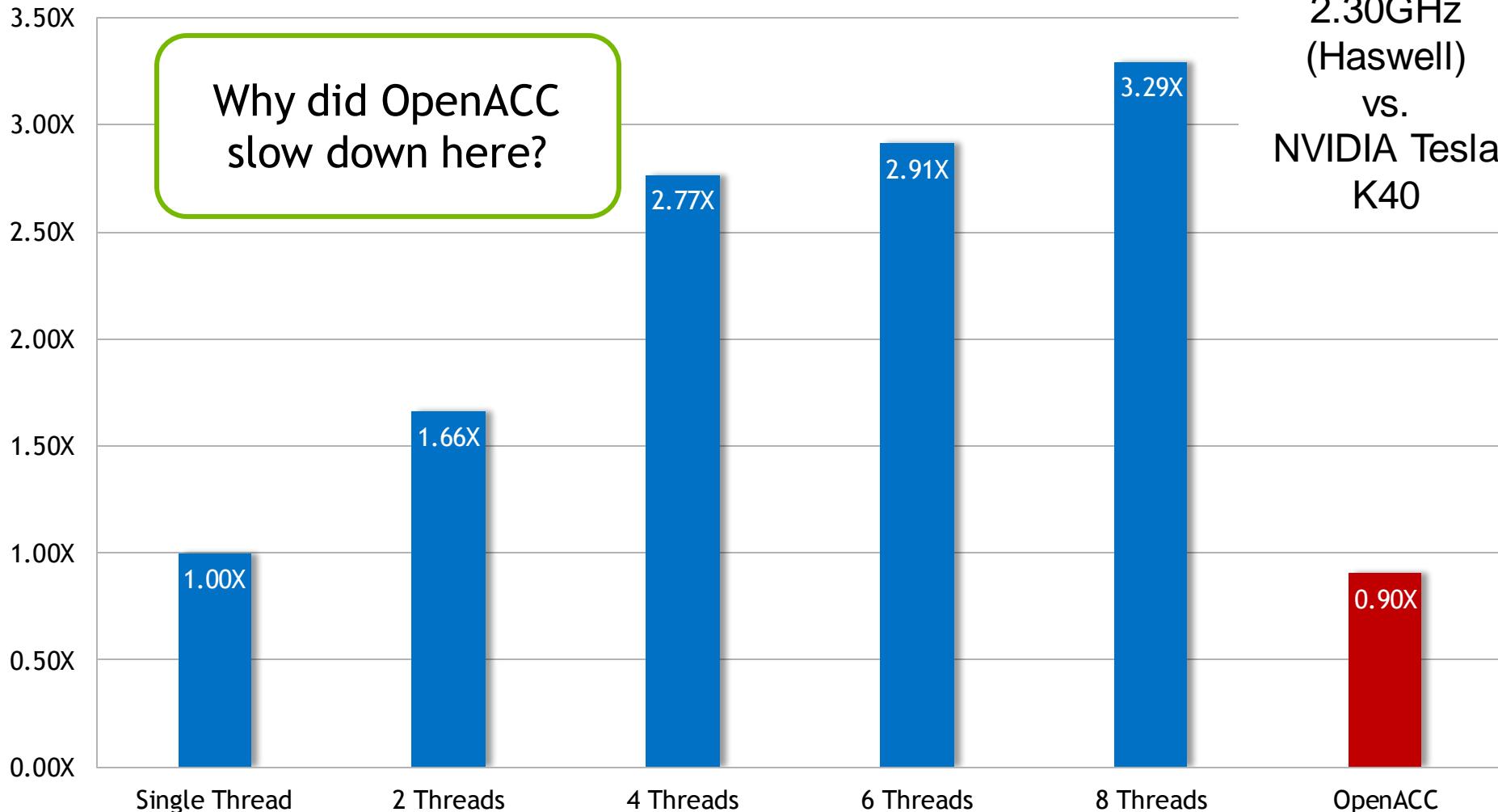
Look for parallelism
within this region.

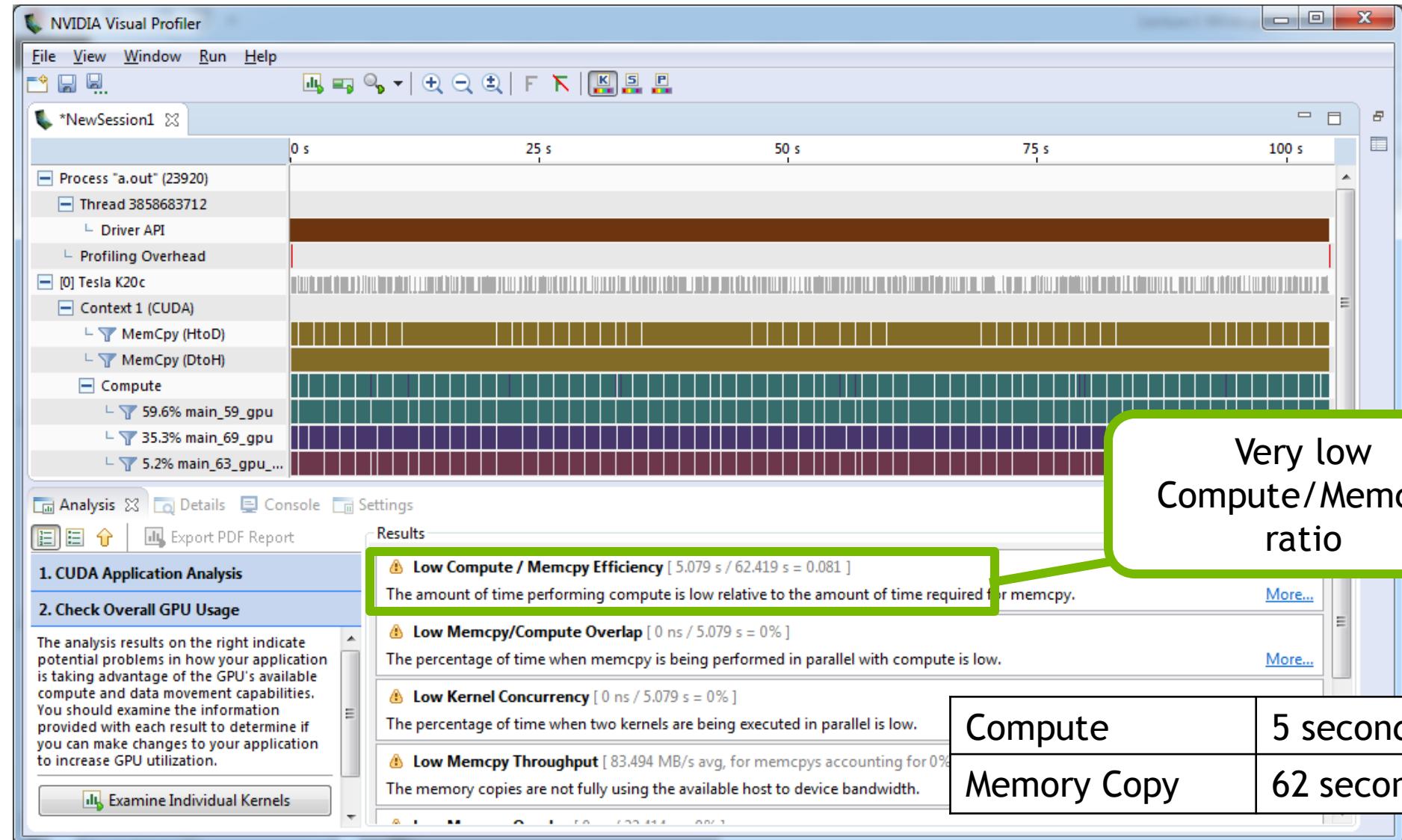
Building the code

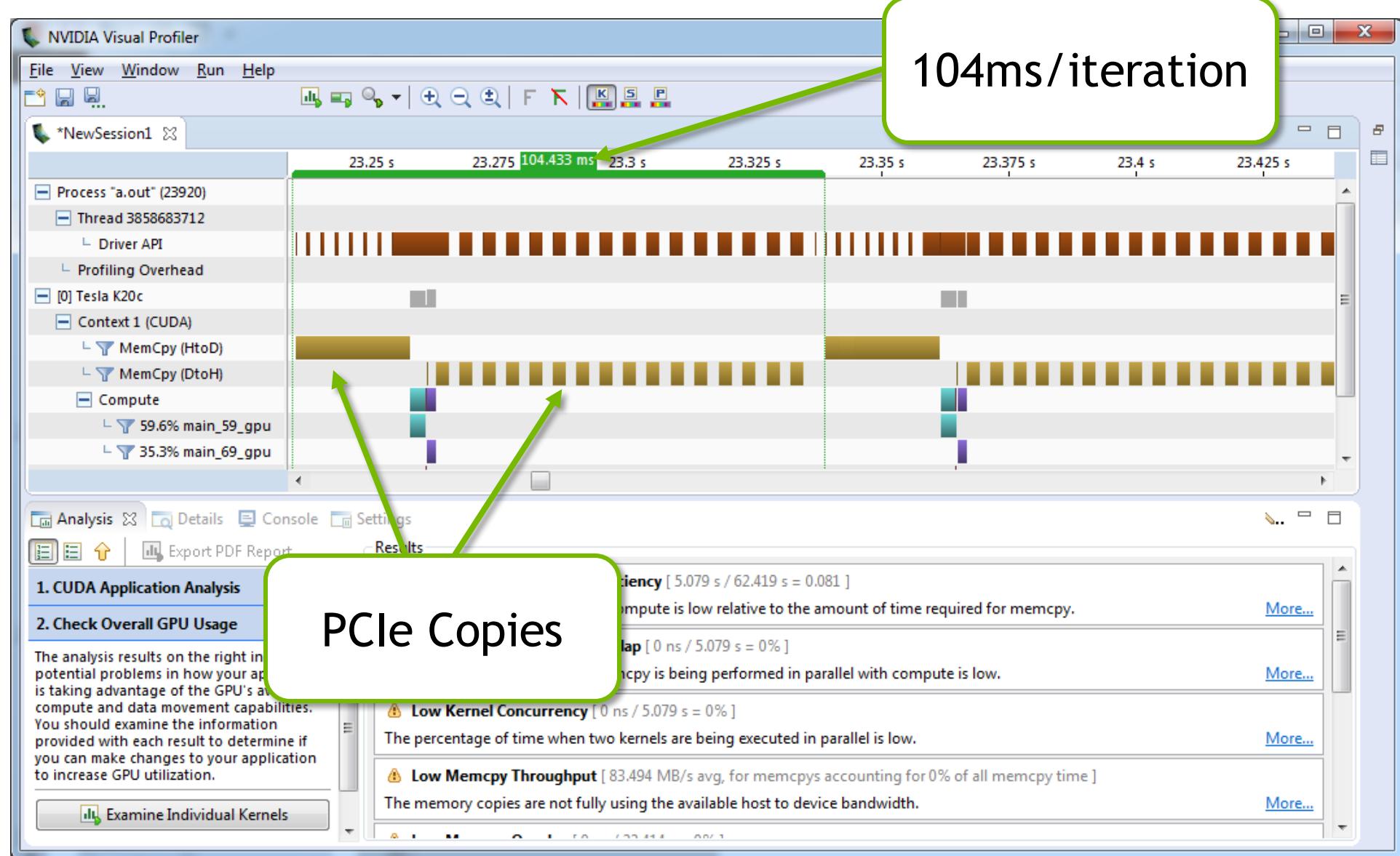
```
$ pgcc -fast -ta=tesla -Minfo=all laplace2d.c
main:
  40, Loop not fused: function call before adjacent loop
      Generated vector sse code for the loop
  51, Loop not vectorized/parallelized: potential early exits
  55, Generating copyout(Anew[1:4094][1:4094])
      Generating copyin(A[:,:])
      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 */
```

Intel Xeon E5-
2698 v3 @
2.30GHz
(Haswell)
vs.
NVIDIA Tesla
K40

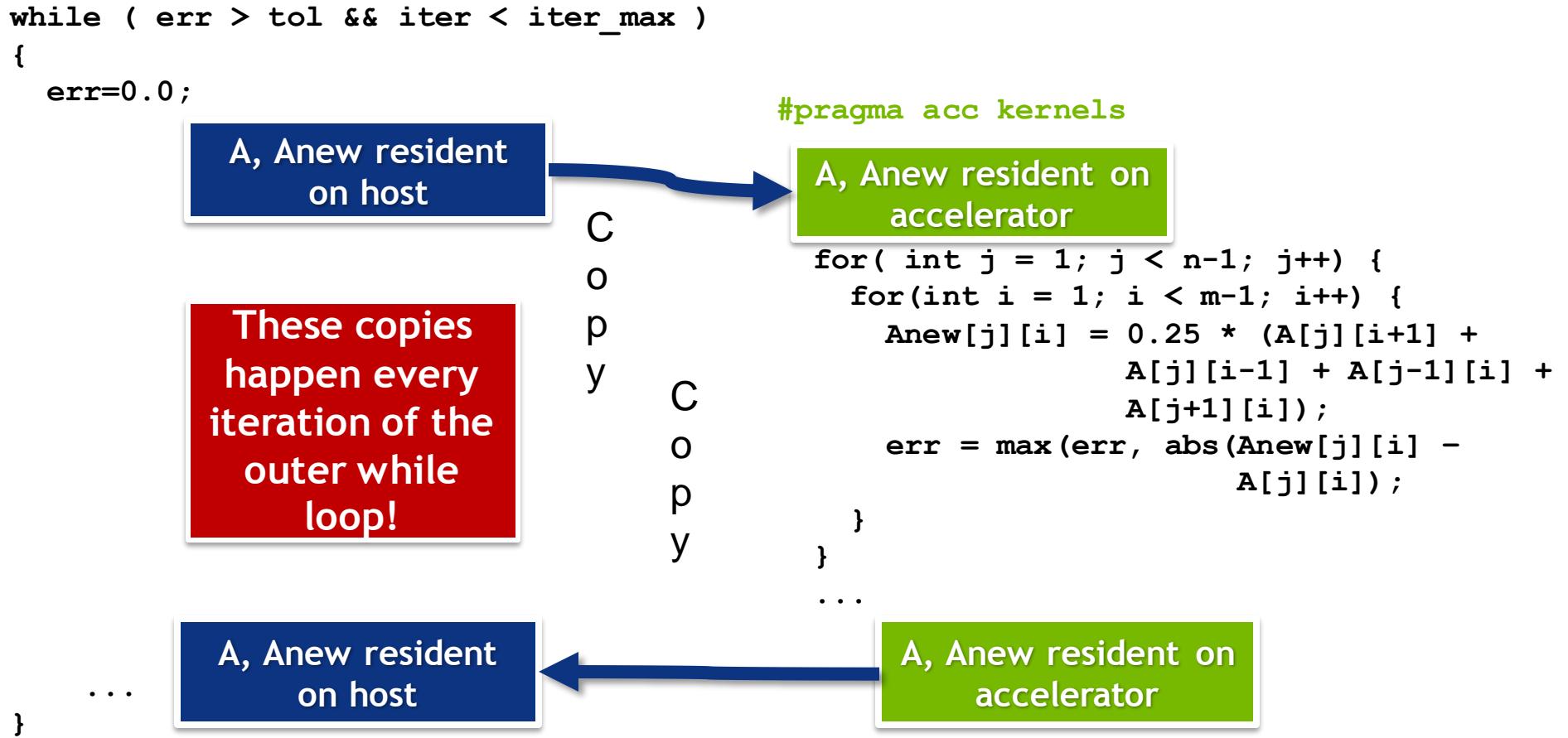
Speed-up (Higher is Better)







Excessive Data Transfers

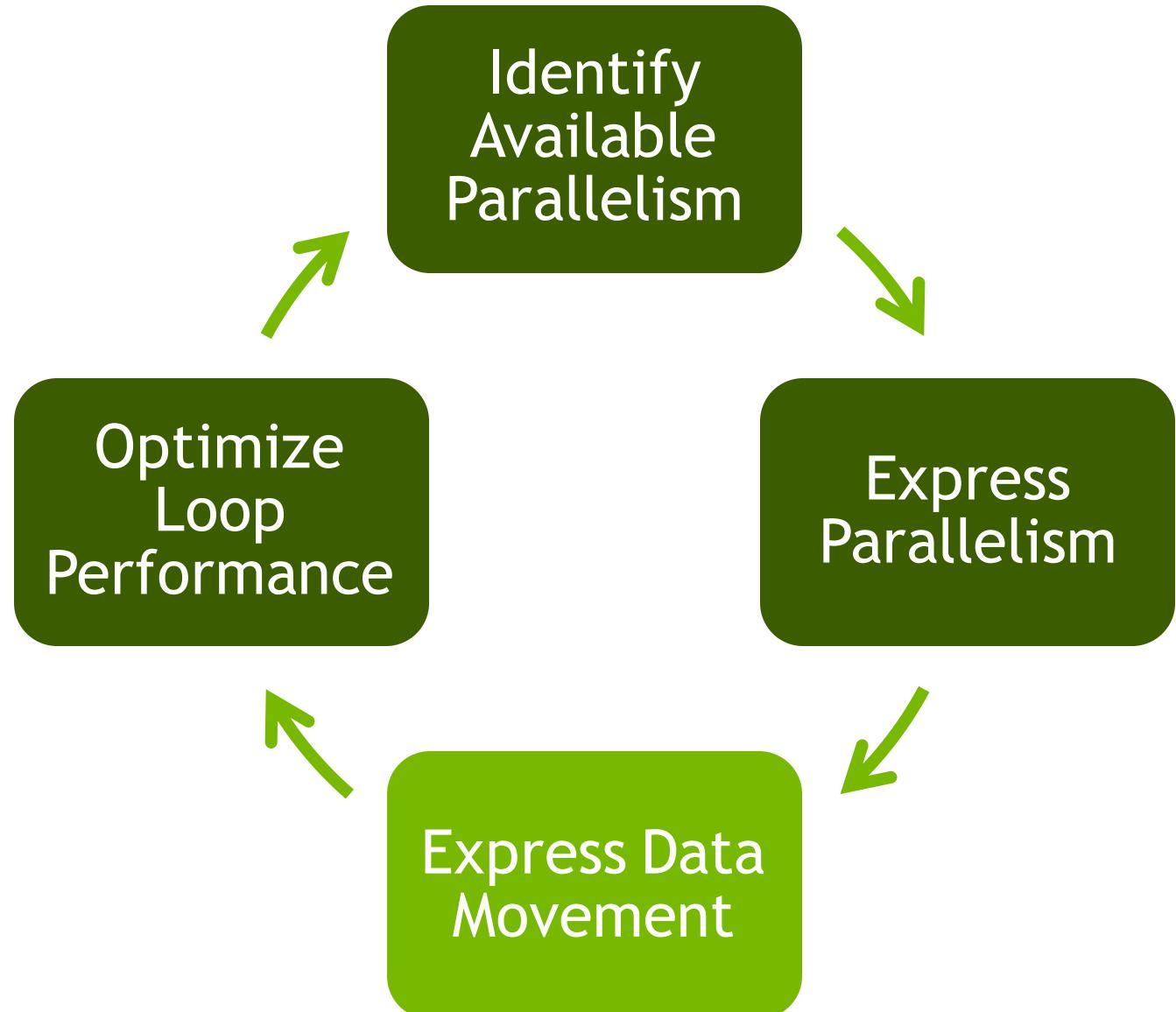


Identifying Data Locality

```
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?



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
...
}
```



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

Data Clauses

<code>copy (list)</code>	Allocates memory on GPU and copies data from host to GPU when entering region and copies data to the host when exiting region.
<code>copyin (list)</code>	Allocates memory on GPU and copies data from host to GPU when entering region.
<code>copyout (list)</code>	Allocates memory on GPU and copies data to the host when exiting region.
<code>create (list)</code>	Allocates memory on GPU but does not copy.
<code>present (list)</code>	Data is already present on GPU from another containing data region.
<code>deviceptr(list)</code>	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++;
}
```

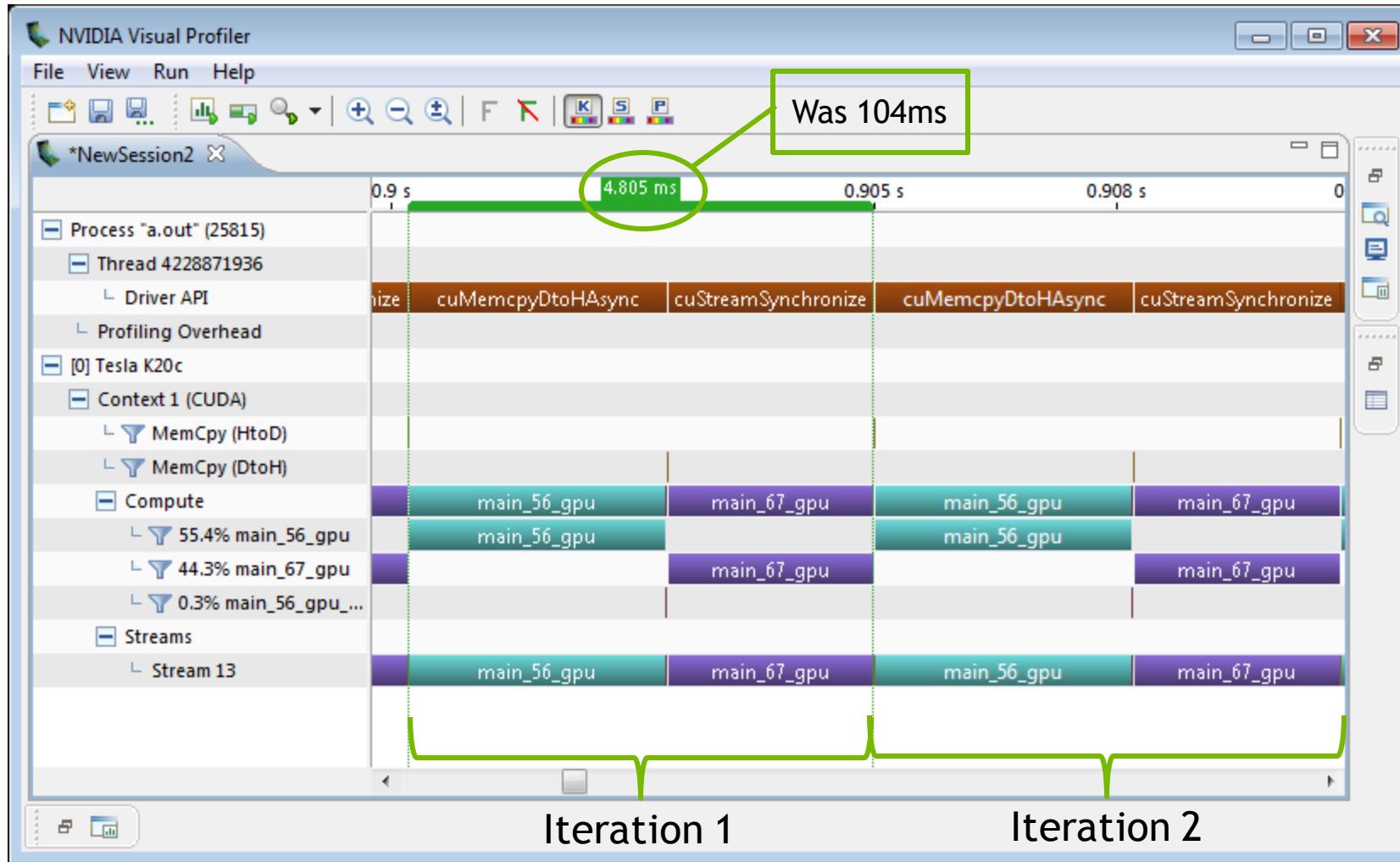
Copy A to/from the accelerator only when needed.

Create Anew as a device temporary.

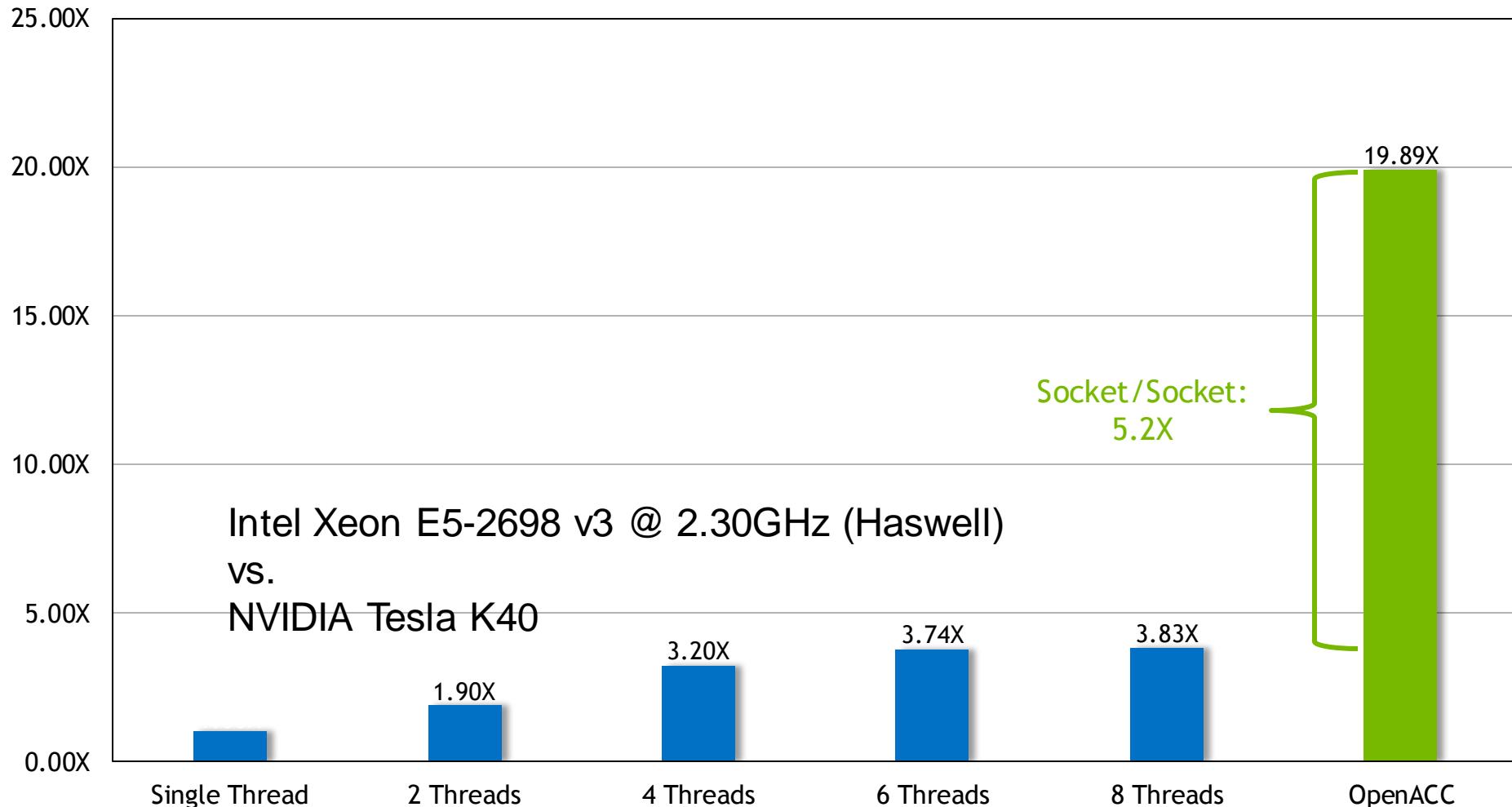
Rebuilding the code

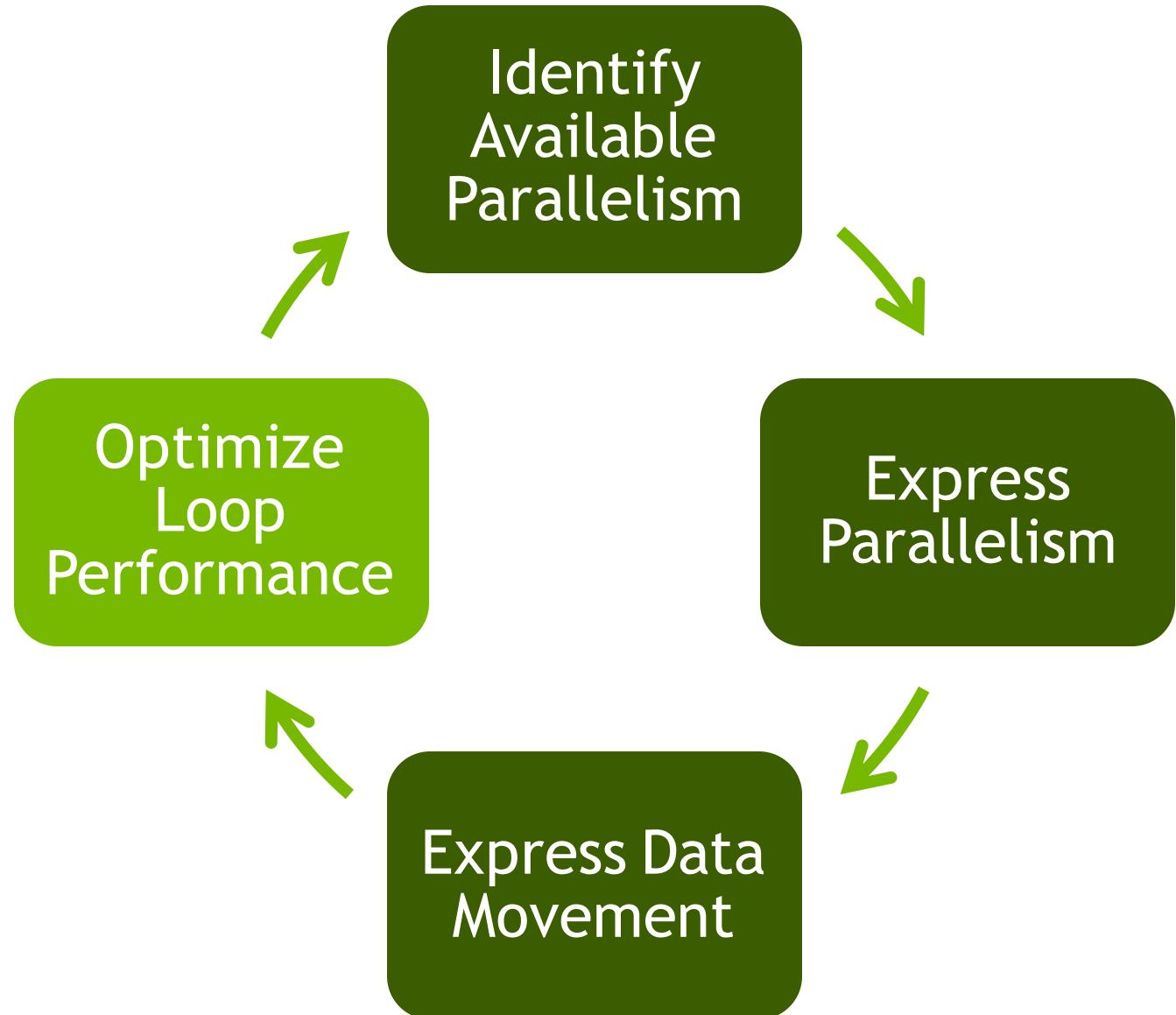
```
$ pgcc -fast -acc -ta=tesla -Minfo=all laplace2d.c
main:
  40, Loop not fused: function call before adjacent loop
      Generated vector sse code for the loop
  51, Generating copy(A[:, :])
      Generating create(Anew[:, :])
      Loop not vectorized/parallelized: potential early exits
  56, Accelerator 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)





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

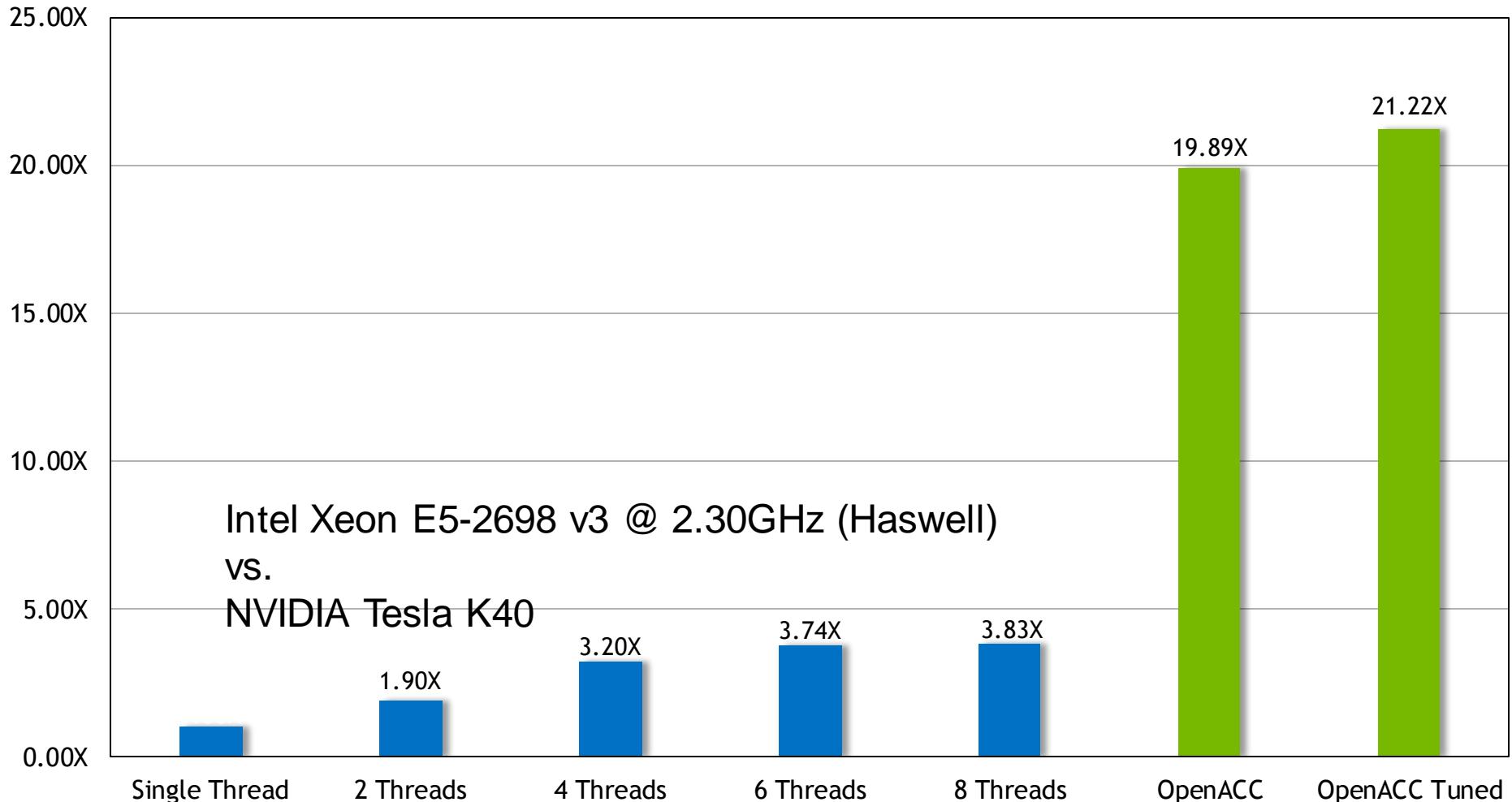
```
#pragma acc data copy(A) create(Anew)
while ( err > tol && iter < iter_max ) {
    err=0.0;
#pragma acc kernels
{
#pragma acc loop device_type(nvidia) tile(32,4)
    for( int j = 1; j < n-1; j++) {
        for(int i = 1; i < m-1; i++) {

            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)



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

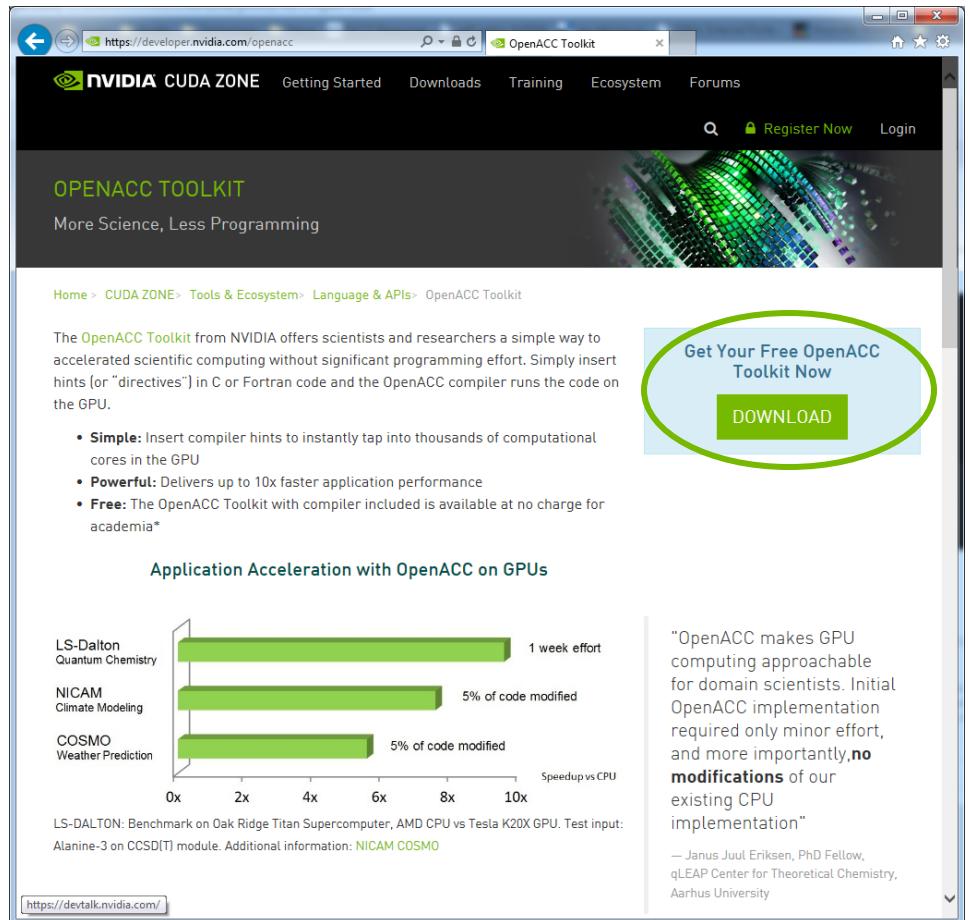


Documentation

Quick start guide, Best practices, Forums

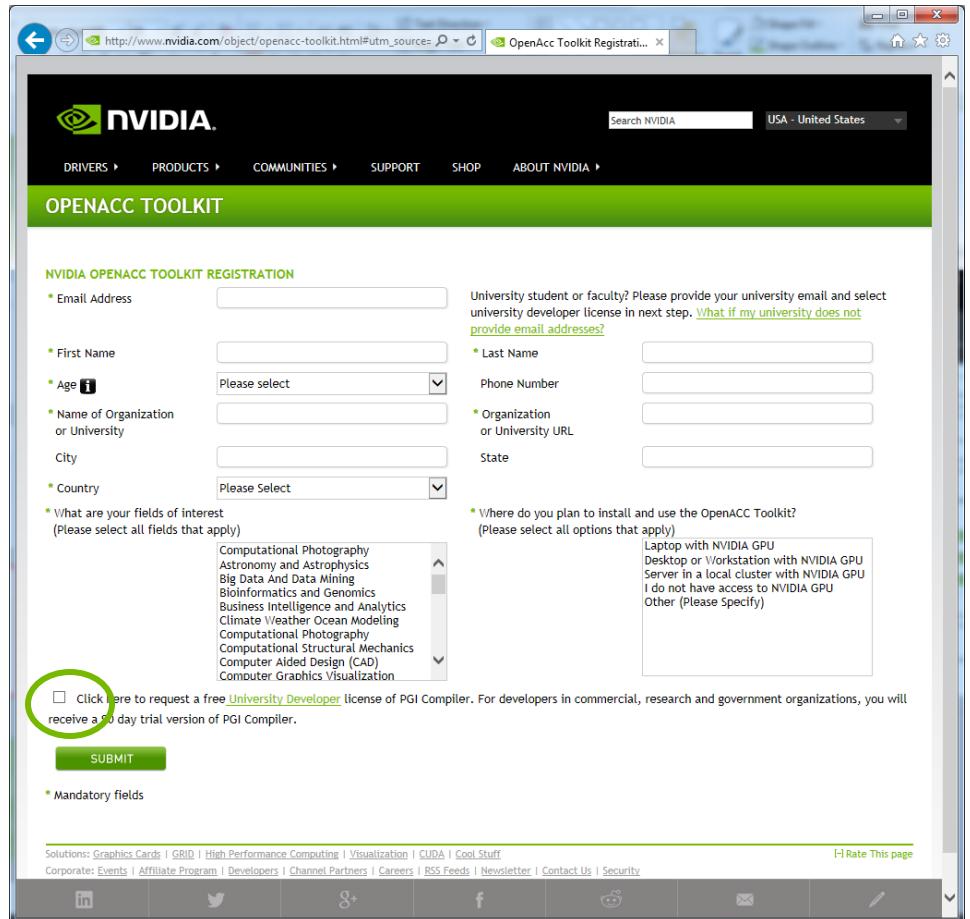
Download the OpenACC Toolkit

- ▶ Go to
<https://developer.nvidia.com/openacc>



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.



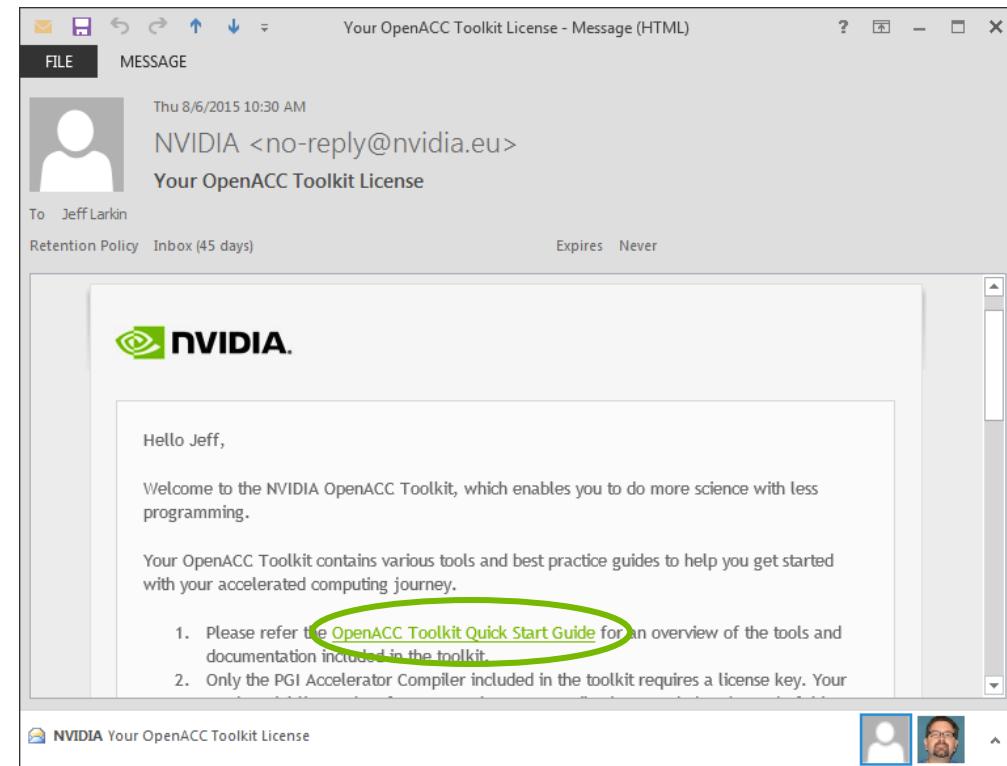
The screenshot shows the NVIDIA OpenACC Toolkit registration form. At the top, there's a navigation bar with links for DRIVERS, PRODUCTS, COMMUNITIES, SUPPORT, SHOP, and ABOUT NVIDIA. Below that is a green header bar with the text "OPENACC TOOLKIT". The main form area has several input fields:

- Email Address
- First Name
- Age (dropdown menu: Please select)
- Name of Organization or University URL
- City
- Country (dropdown menu: Please Select)
- Fields of Interest (checkboxes): Computational Photography, Astronomy and Astrophysics, Big Data And Data Mining, Bioinformatics and Genomics, Business Intelligence and Analytics, Climate /Weather Ocean Modeling, Computational Photography, Computational Structural Mechanics, Computer Aided Design (CAD), Computer Graphics Visualization
- Where do you plan to install and use the OpenACC Toolkit? (checkboxes): Laptop with NVIDIA GPU, Desktop or Workstation with NVIDIA GPU, Server in a local cluster with NVIDIA GPU, I do not have access to NVIDIA GPU, Other (Please Specify)

A green circle highlights the checkbox for requesting a PGI Compiler trial license, which is described as "Click here to request a free University Developer license of PGI Compiler. For developers in commercial, research and government organizations, you will receive a 30 day trial version of PGI Compiler." At the bottom, there's a "SUBMIT" button and a note about mandatory fields.

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



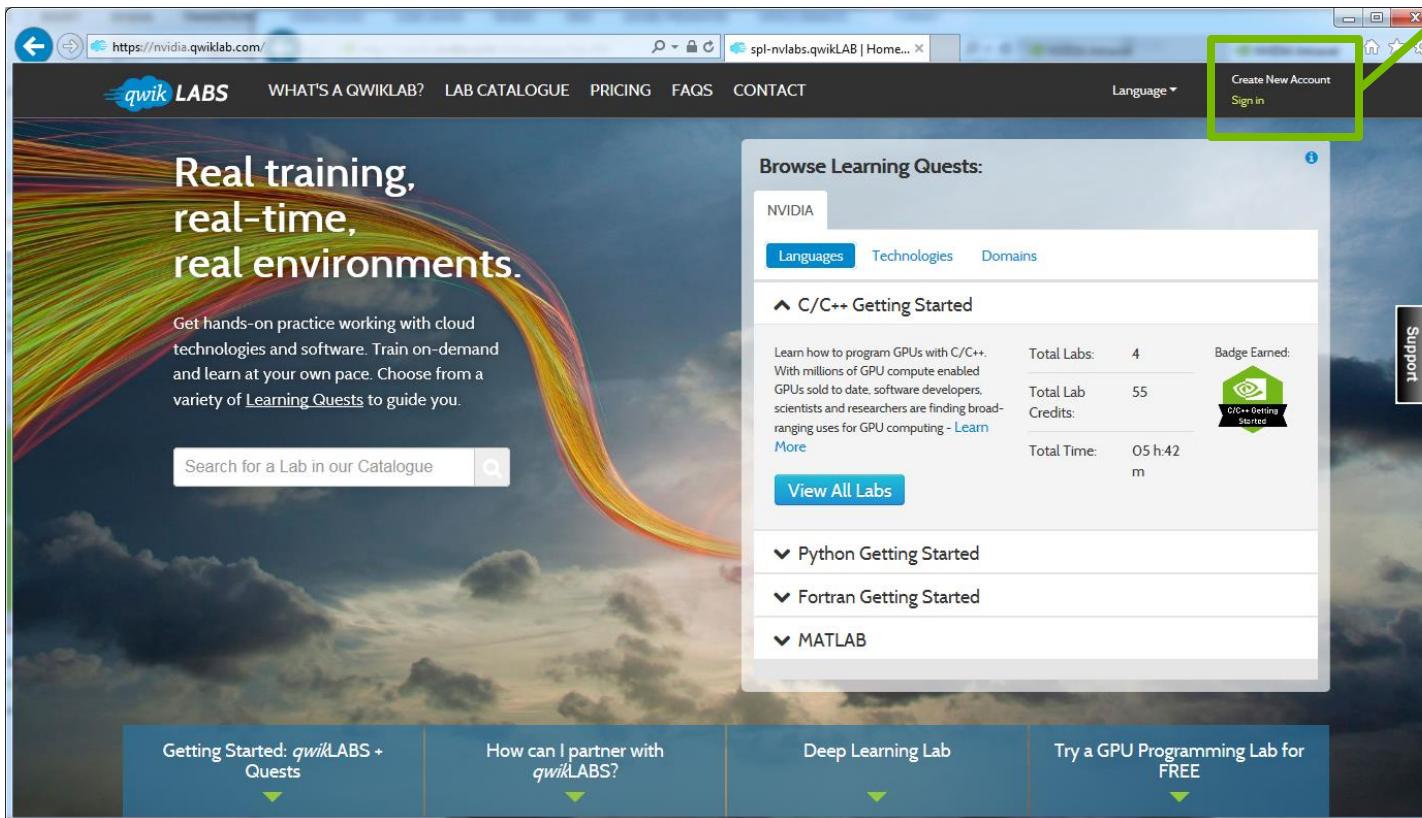
Windows/Mac Developers

- 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.

Using QwikLabs

Getting access

Go to nvidia.qwiklab.com, log-in or create an account



The screenshot shows the QwikLABS homepage with a banner featuring a colorful, swirling cloud pattern. The main content area displays 'Browse Learning Quests' for NVIDIA, specifically the 'C/C++ Getting Started' quest. The quest details include:

- Total Labs: 4
- Total Lab Credits: 55
- Total Time: 05 h.42 m

Badges earned: C/C++ Getting Started

Other quest options listed are Python Getting Started, Fortran Getting Started, and MATLAB.

At the top right of the page, there is a 'Create New Account' and 'Sign in' button, which is highlighted with a green rectangular box. A green arrow points from this box to a callout box on the right side of the slide.

Sign In or Create a New Account

Homework

Complete “2X in 4 Steps” Qwiklab

- ▶ C: <http://bit.ly/nvoacclab1c>
- ▶ F90: <http://bit.ly/nvoacclab1f>
- ▶ This lab is browser-based and should take you roughly 1 hour.

The screenshot shows the NVIDIA Qwiklab website at https://nvidia.qwiklab.com/lab_catalogue. The page displays a catalog of labs, with the 'Labs (21)' tab selected. On the right, a detailed view of the 'OpenACC - 2X in 4 Steps in C/C++' lab is shown. The lab is categorized under 'OpenACC' and is marked as 'Beginner' level with '15 Credits'. It has a 5-star rating from 58 reviews. The description explains that the lab teaches how to accelerate C/C++ applications using OpenACC. The lab consists of four steps: 1. Characterize and profile.

Install the OpenACC Toolkit (Optional)

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

The screenshot shows a web browser window displaying the NVIDIA CUDA Zone website at <https://developer.nvidia.com/openacc>. The page is titled "OPENACC TOOLKIT" and features a sub-headline "More Science, Less Programming". A navigation bar at the top includes links for Getting Started, Downloads, Training, Ecosystem, and Forums. A search bar and user account links for "Register Now" and "Login" are also present. The main content area describes the OpenACC Toolkit as a simple way to accelerate scientific computing. It highlights three key features: Simple (insert compiler hints), Powerful (up to 10x faster performance), and Free (available at no charge for academia). A call-to-action button "GET YOUR FREE OPENACC TOOLKIT NOW" with a "DOWNLOAD" link is visible. Below this, a section titled "APPLICATION ACCELERATION WITH OPENACC ON GPUs" contains a chart comparing GPU vs CPU speedup for three applications: LS-Dalton, NICAM, and COSMO. The chart shows significant speedups (up to 10x) with minimal code modification (5% of code modified). A quote from Janus Juul Eriksen of Aarhus University emphasizes that OpenACC makes GPU computing approachable and requires only minor modifications to existing CPU implementations.

OPENACC TOOLKIT
More Science, Less Programming

Home > CUDA ZONE > Tools & Ecosystem > Language & APIs > OpenACC Toolkit

The OpenACC Toolkit from NVIDIA offers scientists and researchers a simple way to accelerated scientific computing without significant programming effort. Simply insert hints (or "directives") in C or Fortran code and the OpenACC compiler runs the code on the GPU.

- **Simple:** Insert compiler hints to instantly tap into thousands of computational cores in the GPU
- **Powerful:** Delivers up to 10x faster application performance
- **Free:** The OpenACC Toolkit with compiler included is available at no charge for academia*

Application Acceleration with OpenACC on GPUs

Application	Speedup vs CPU	Effort
LS-Dalton Quantum Chemistry	~10x	1 week effort
NICAM Climate Modeling	~8x	5% of code modified
COSMO Weather Prediction	~6x	5% of code modified

LS-DALTON: Benchmark on Oak Ridge Titan Supercomputer, AMD CPU vs Tesla K20X GPU. Test input: Alanine-3 on CCSD[T] module. Additional information: [NICAM](#) [COSMO](#)

"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

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/>

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

Recordings:

<https://developer.nvidia.com/openacc-course>