

# 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

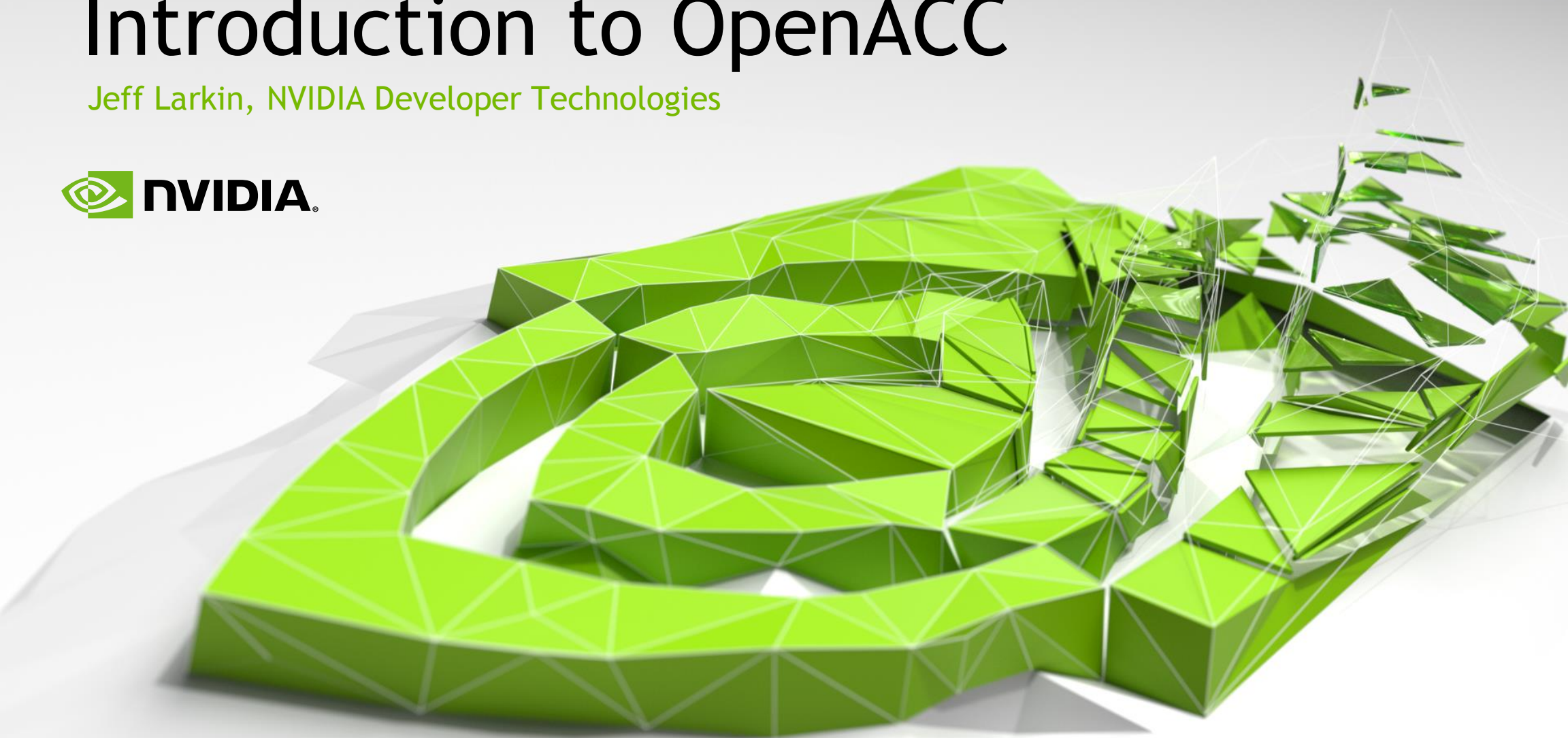
Nov 24: Office Hours

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

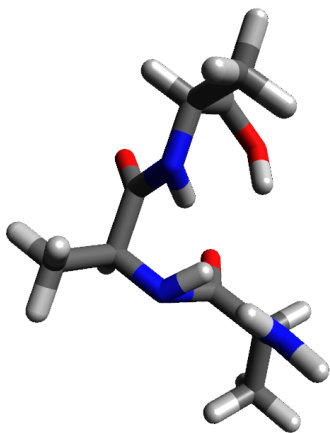
8000+

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.”

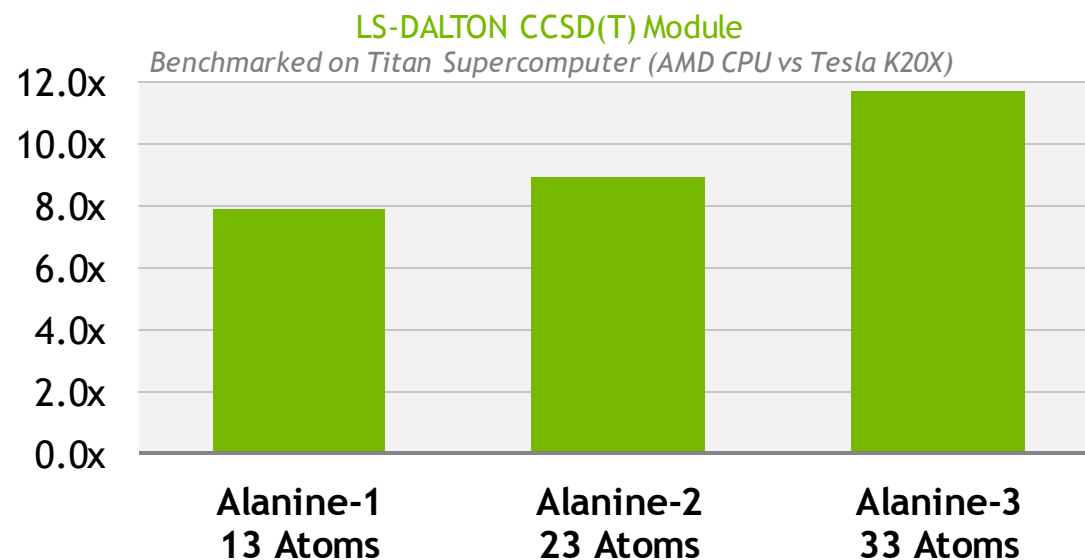
Janus Juul Eriksen, PhD Fellow  
qLEAP Center for Theoretical Chemistry, Aarhus University



## Minimal Effort

Lines of Code Modified	# of Weeks Required	# of Codes to Maintain
<b>&lt;100 Lines</b>	<b>1 Week</b>	<b>1 Source</b>

## Big Performance





# OpenACC Directives

Manage Data Movement → `#pragma acc data copyin(a,b) copyout(c)`  
{  
...  
Initiate Parallel Execution → `#pragma acc parallel`  
{  
Optimize Loop Mappings → `#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

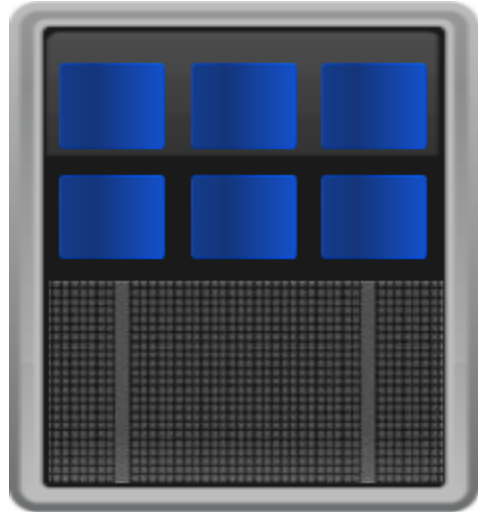
# Accelerated Computing Fundamentals

# Accelerated Computing

*10x Performance & 5x Energy Efficiency for HPC*

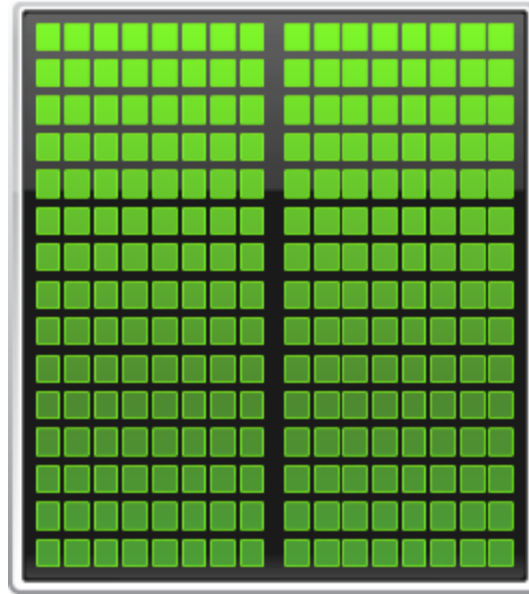
**CPU**

Optimized for  
Serial Tasks

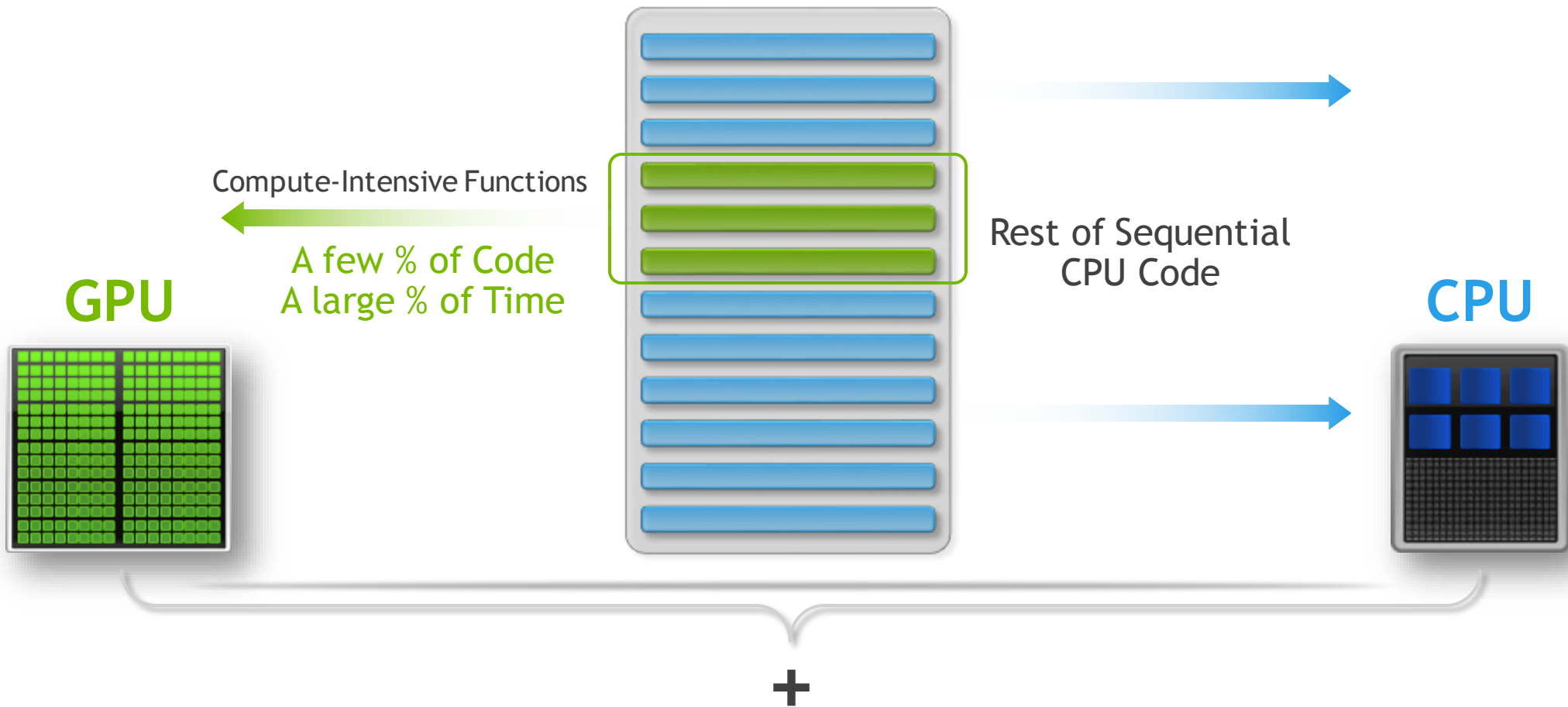


**GPU Accelerator**

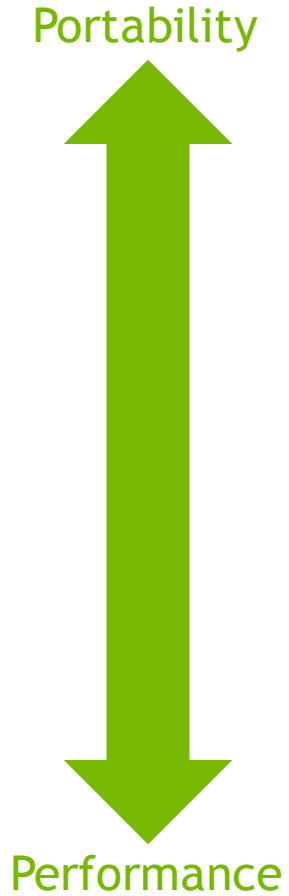
Optimized for  
Parallel Tasks



# What is Heterogeneous Programming?



# Portability & Performance



## 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

# Code for Portability & Performance

## Libraries

- Implement as much as possible using portable libraries

## Directives

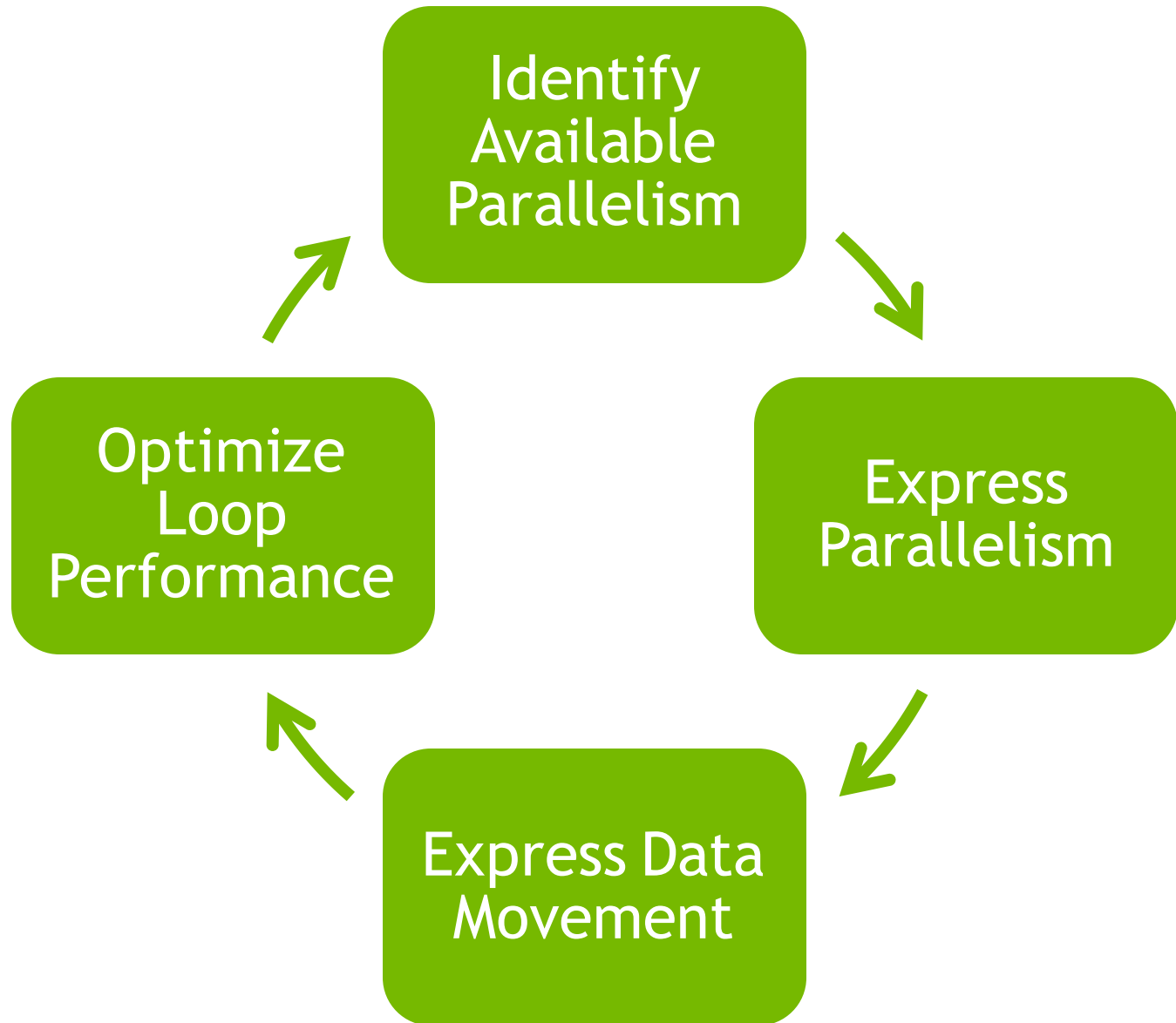
- Use directives for rapid and portable development

## Languages

- Use lower level languages for important kernels



# OpenACC Programming Cycle

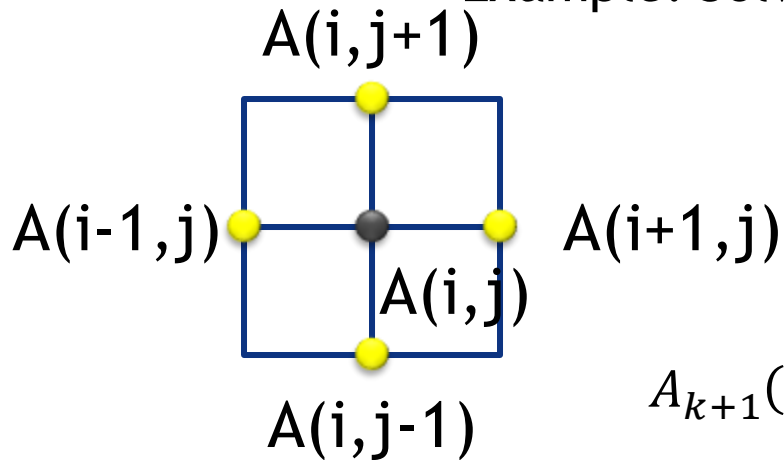


# Example: Jacobi Iteration

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

Common, useful algorithm

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



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

# 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



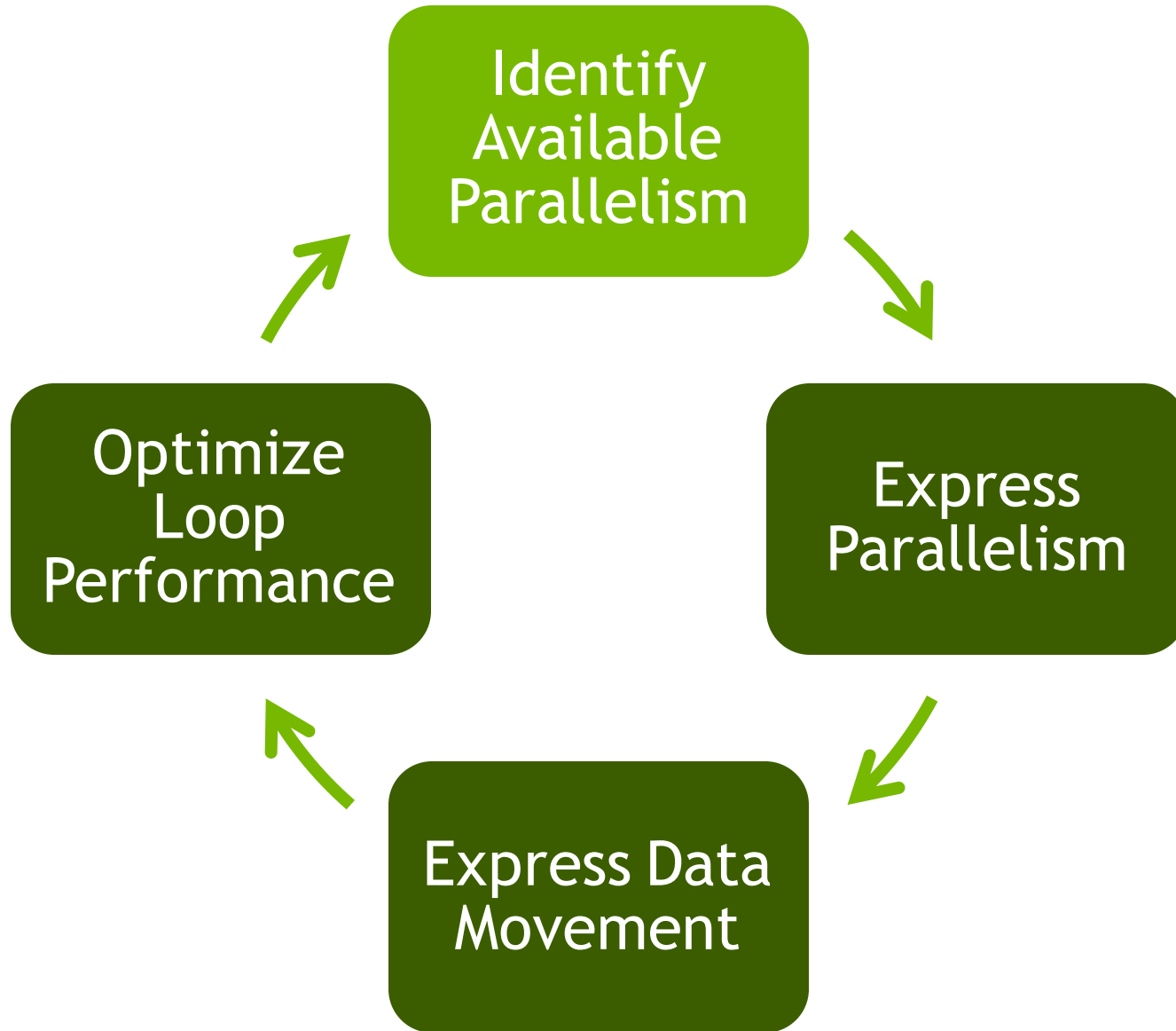
Calculate new value from neighbors



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.

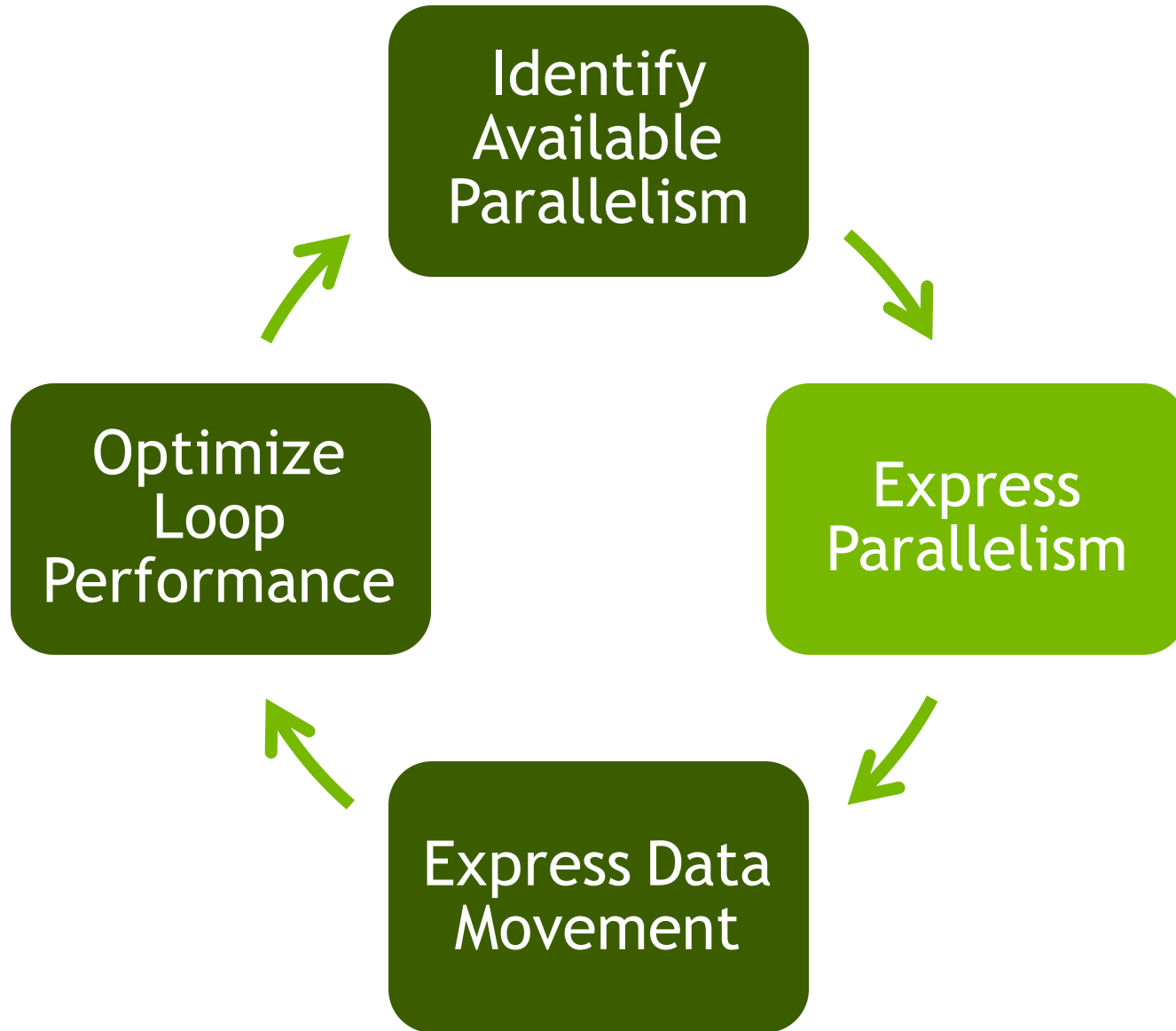


Independent loop  
iterations



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];
}
}
```

} 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.

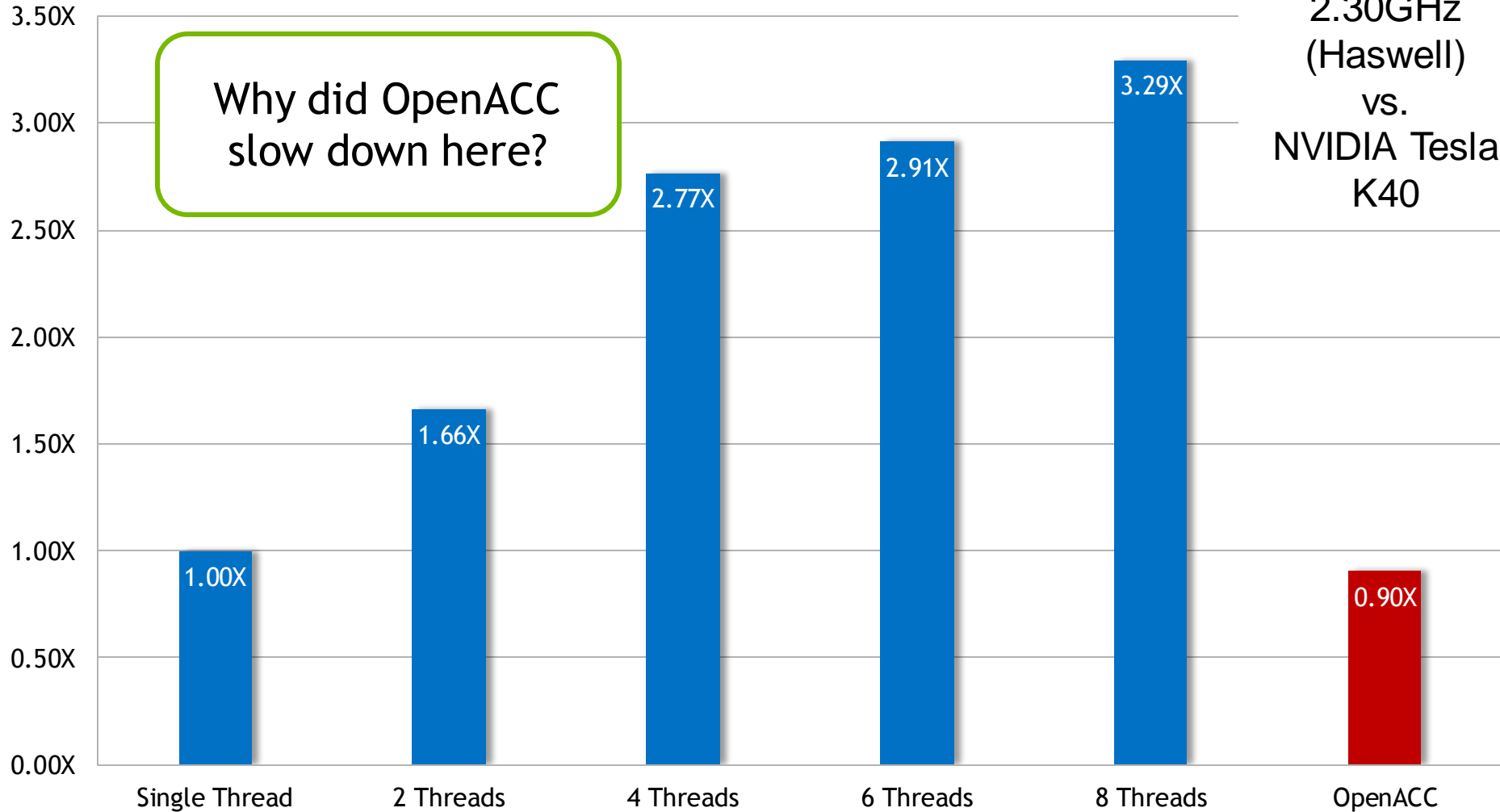
# Building the code

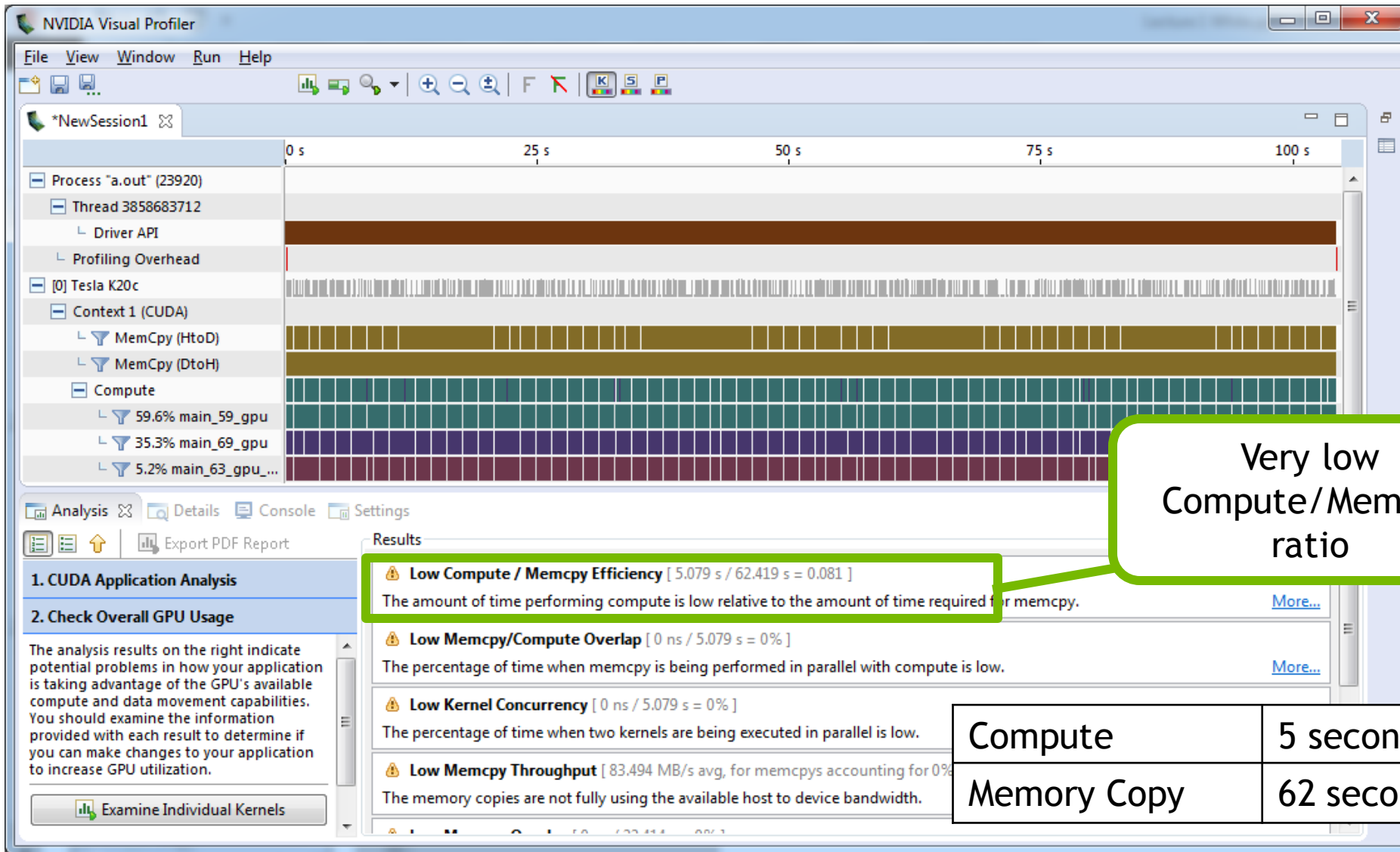
```
$ pgcc -fast -ta=tesla -Minfo=all laplace2d.c
main:
  40, Loop not fused: function call before adjacent loop
      Generated vector sse code for the loop
  51, Loop not vectorized/parallelized: potential early exits
  55, Generating copyout(Anew[1:4094][1:4094])
      Generating copyin(A[:,:])
 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

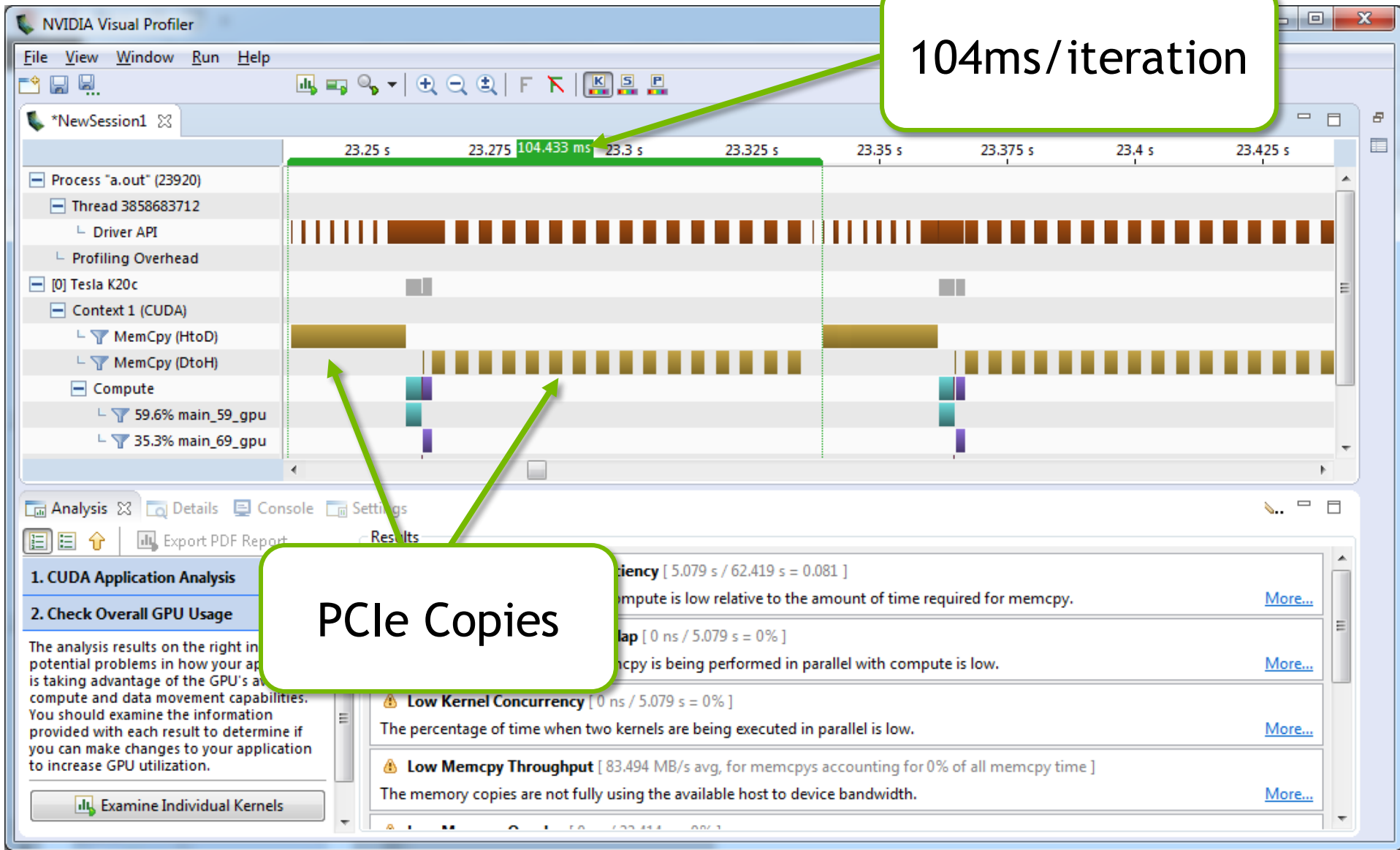
Intel Xeon E5-2698 v3 @ 2.30GHz (Haswell)  
vs.  
NVIDIA Tesla K40

Why did OpenACC slow down here?









# Excessive Data Transfers

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

A, Anew resident  
on host

These copies  
happen every  
iteration of the  
outer while  
loop!

A, Anew resident  
on host

`#pragma acc kernels`

A, Anew resident on  
accelerator

```
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]));  
  }  
}
```

...

A, Anew resident on  
accelerator

...  
}

C  
o  
p  
y  
C  
o  
p  
y

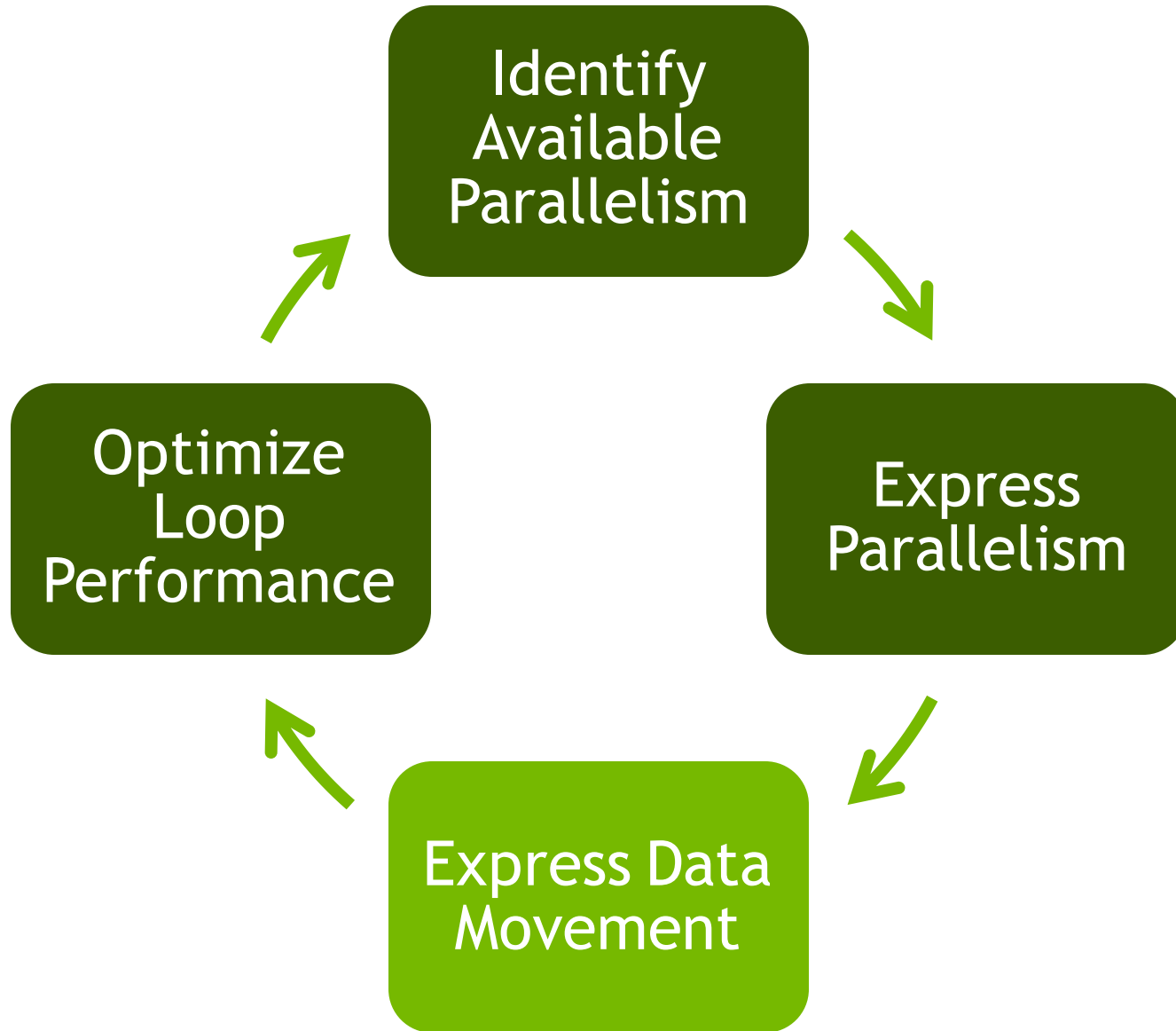


# Identifying Data Locality

```
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  
...  
}
```



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++;
}
```



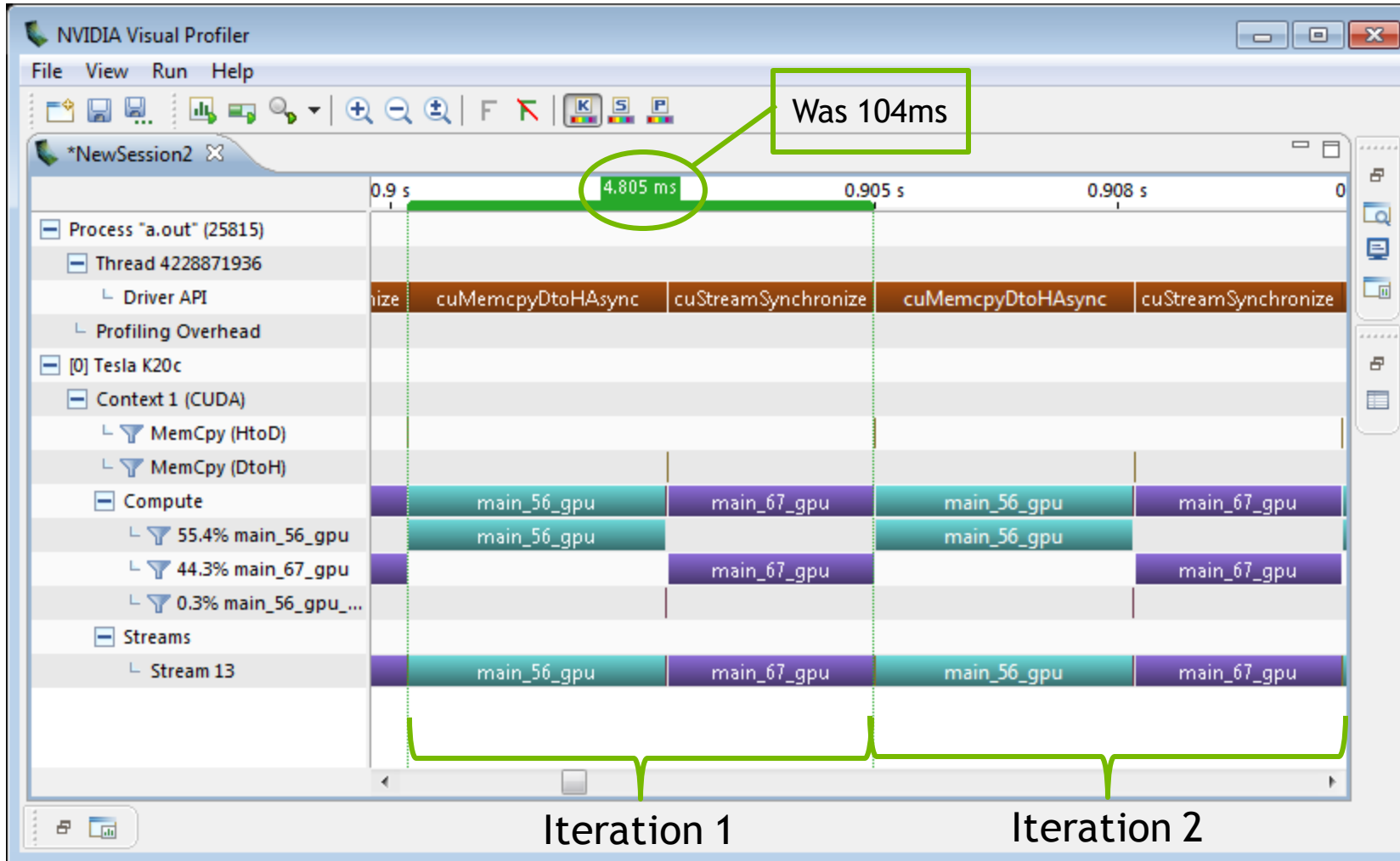
Copy A to/from the accelerator only when needed.

Create Anew as a device temporary.

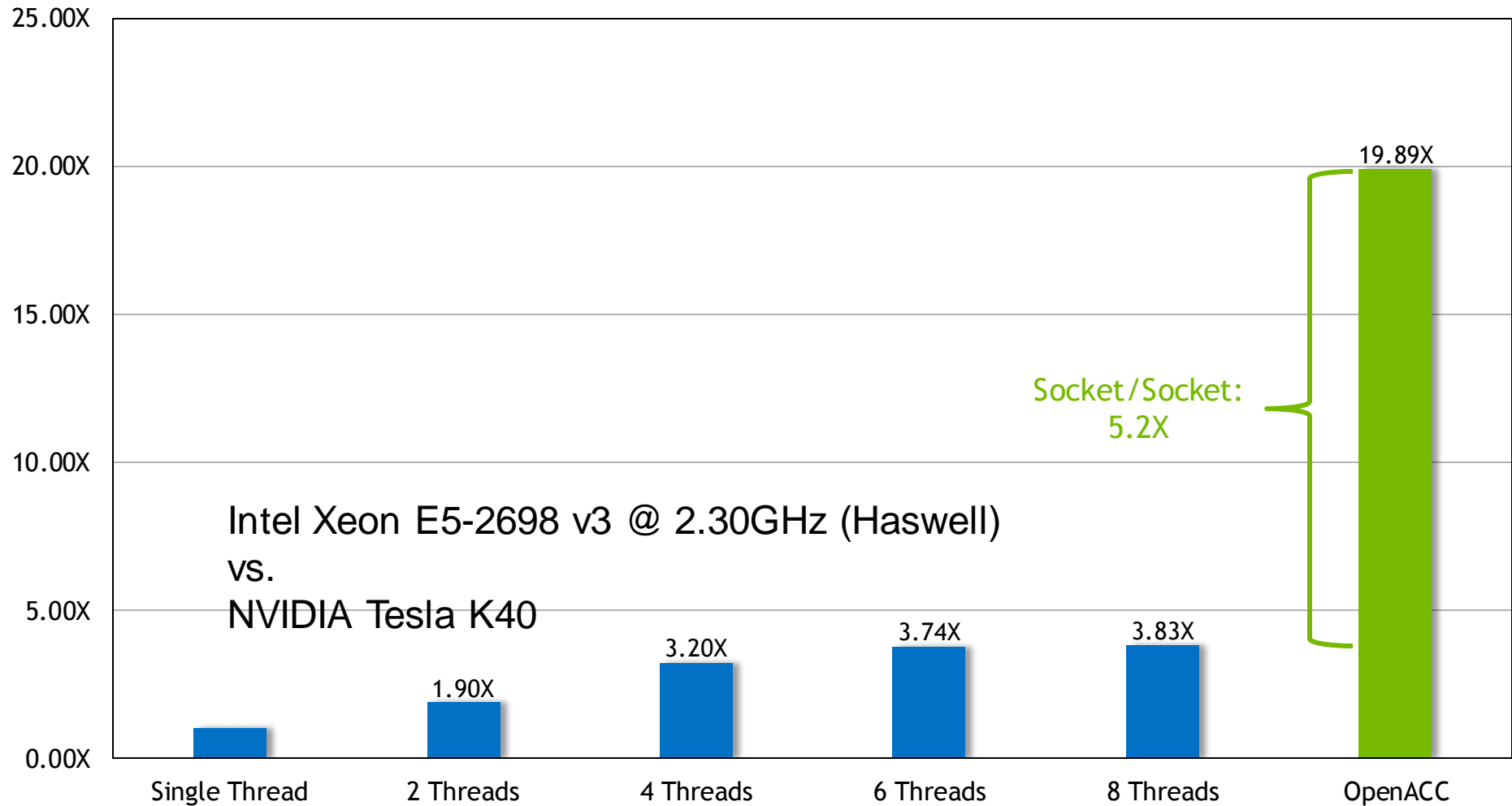
# Rebuilding the code

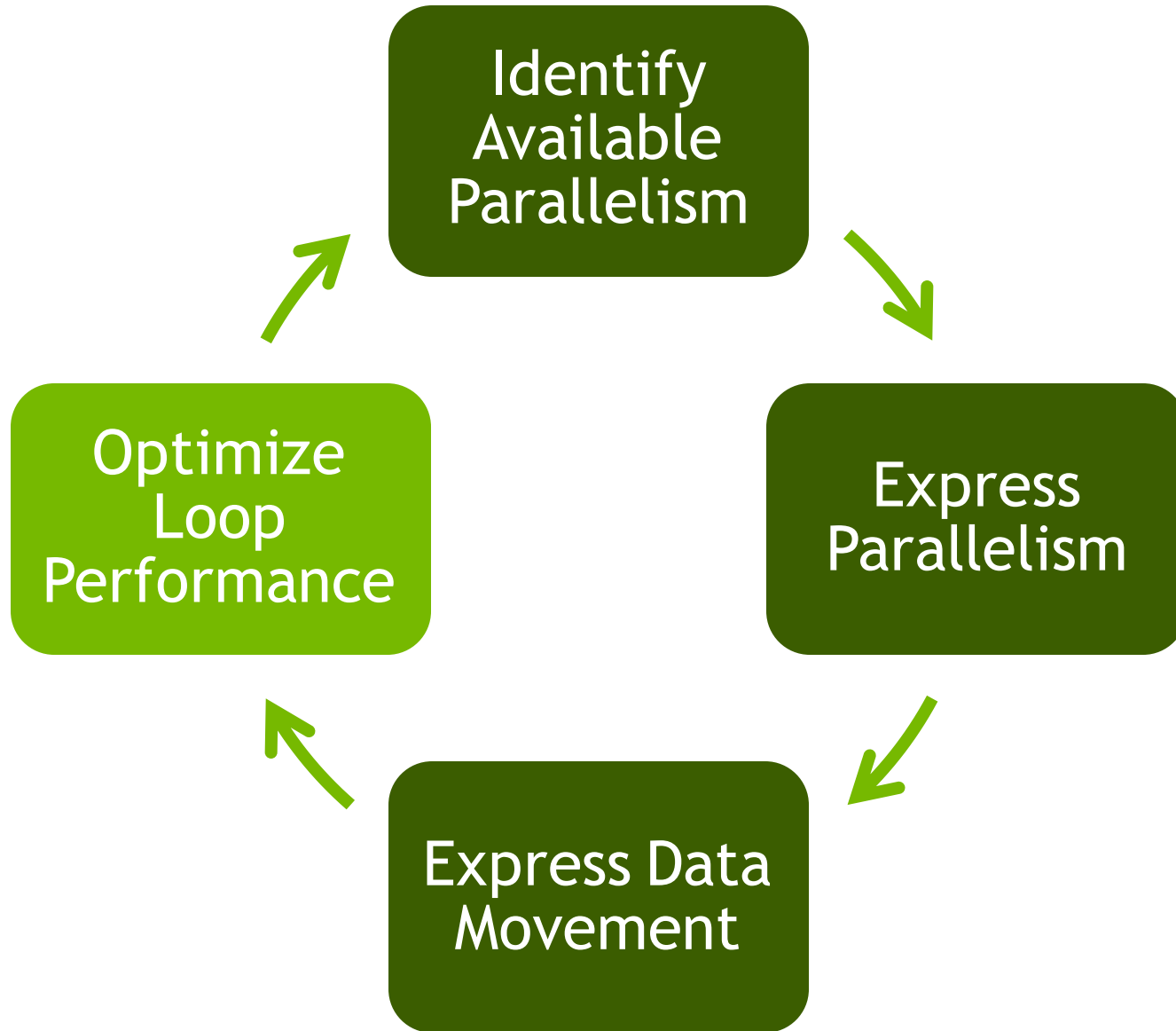
```
$ pgcc -fast -acc -ta=tesla -Minfo=all laplace2d.c
main:
  40, Loop not fused: function call before adjacent loop
      Generated vector sse code for the loop
  51, Generating copy(A[:][:])
      Generating create(Anew[:][:])
      Loop not vectorized/parallelized: potential early exits
  56, Accelerator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





# 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]);

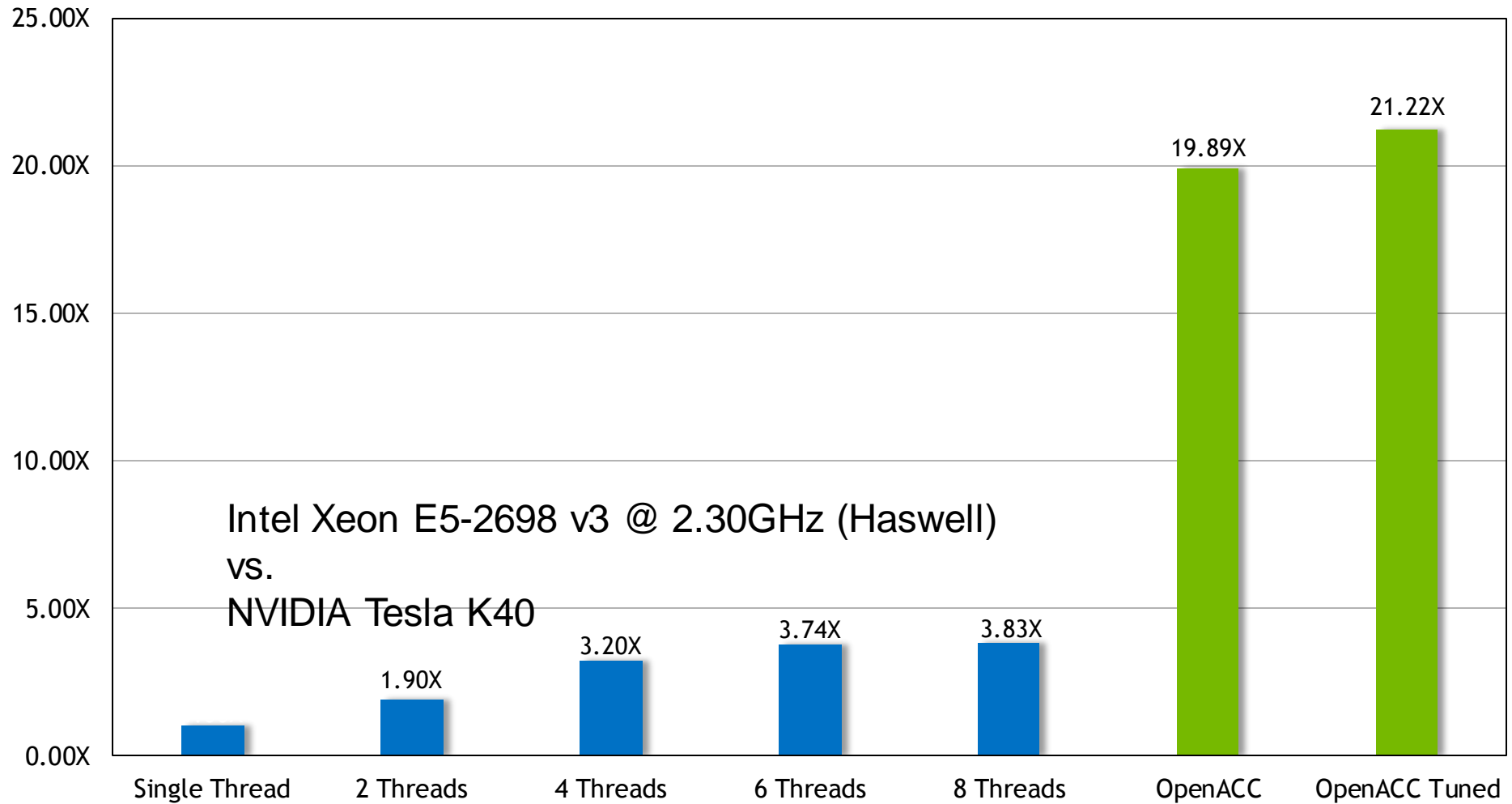
                err = max(err, abs(Anew[j][i] - A[j][i]));
            }
        }
    #pragma acc loop device_type(nvidia) tile(32,4)
        for( int j = 1; j < n-1; j++) {
            for( int i = 1; i < m-1; i++ ) {
                A[j][i] = Anew[j][i];
            }
        }
    }
    iter++;
}
```



“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>

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

**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	Effort / Code Modified	Speedup vs CPU
LS-Dalton Quantum Chemistry	1 week effort	~9x
NICAM Climate Modeling	5% of code modified	~8x
COSMO Weather Prediction	5% of code modified	~6x

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

<https://devtalk.nvidia.com/>

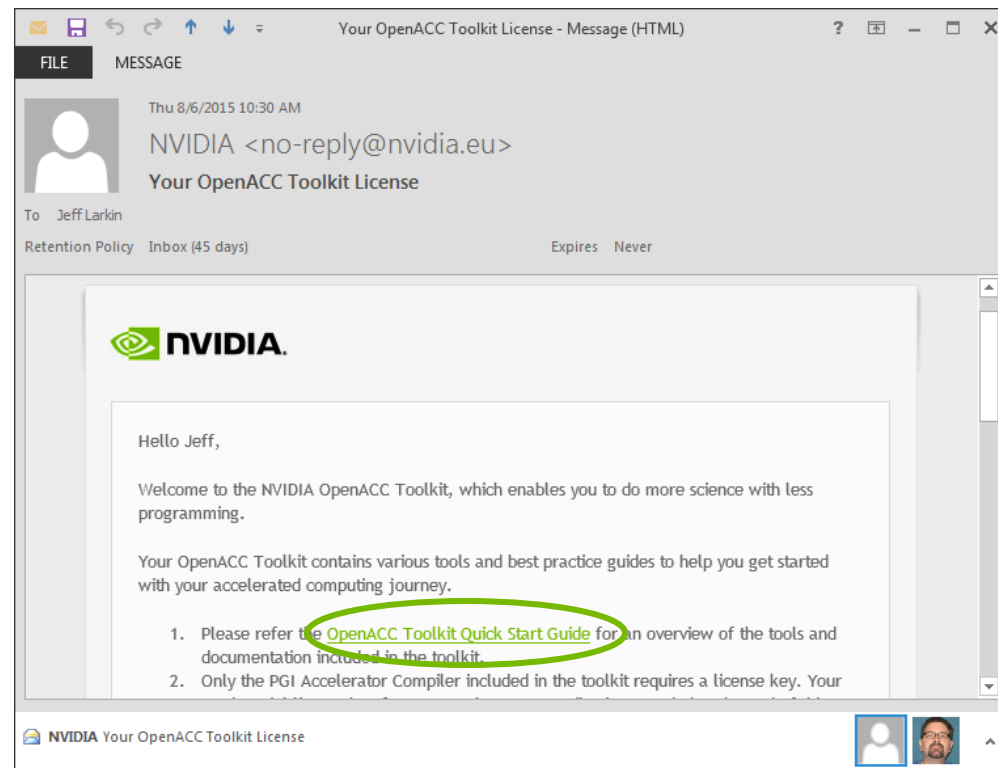
# Download the OpenACC Toolkit

- ▶ 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 page. The page has a green header with the NVIDIA logo and navigation links. The main content area is titled 'OPENACC TOOLKIT' and contains a registration form. The form includes fields for Email Address, First Name, Age, Name of Organization or University, City, Country, Last Name, Phone Number, Organization or University URL, and State. There is also a section for 'What are your fields of interest' with a list of options including 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), and Computer Graphics Visualization. A checkbox is circled in red, with the text: 'Click here to request a free University Developer license of PGI Compiler. For developers in commercial, research and government organizations, you will receive a 90 day trial version of PGI Compiler.' Below the checkbox is a green 'SUBMIT' button. At the bottom of the page, there are links for Solutions, Corporate, and Events, and a footer with social media icons and the NVIDIA logo.

# 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](https://nvidia.qwiklab.com), log-in or create an account

Sign In or Create a New Account

The screenshot shows the NVIDIA QwikLABS website. The header includes the QwikLABS logo, navigation links (WHAT'S A QWIKLAB?, LAB CATALOGUE, PRICING, FAQs, CONTACT), a language dropdown, and a user menu with 'Create New Account' and 'Sign In' options. The main content area features a large banner with the text 'Real training, real-time, real environments.' and a search bar. Below the banner is the 'Browse Learning Quests' section, which is currently filtered by 'NVIDIA'. The 'C/C++ Getting Started' quest is expanded, showing a table of statistics and a 'View All Labs' button. Other quest categories like 'Python Getting Started', 'Fortran Getting Started', and 'MATLAB' are listed below. The footer contains four navigation buttons: 'Getting Started: qwikLABS + Quests', 'How can I partner with qwikLABS?', 'Deep Learning Lab', and 'Try a GPU Programming Lab for FREE'.

Quest Name	Total Labs	Total Lab Credits	Total Time	Badge Earned
C/C++ Getting Started	4	55	05 h 42 m	C/C++ Getting Started

# 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 Qwiklabs Lab Catalogue interface. The browser address bar displays [https://nvidia.qwiklab.com/lab\\_catalogue](https://nvidia.qwiklab.com/lab_catalogue). The page header includes the Qwik Labs logo and navigation links: WHAT'S A QWIKLAB?, LAB CATALOGUE, PRICING, FAQs, CONTACT, Language, and Create New Account / Sign in. A search bar is located below the header.

The main content area features a table of labs. The selected lab, "OpenACC - 2X in 4 Steps in C/C++", is highlighted in green. The table columns are Title, Level, and Cost. The lab details on the right include a "Select" button, a price of 15 Credits, a duration of 01 h:30 m, an access time of 01 h:55 m, a setup time of 00 h:03 m, and a level of Beginner. The lab description states: "Learn how to accelerate your C/C++ application using OpenACC to harness the massively parallel power of NVIDIA GPUs. OpenACC is a directive based approach to computing where you provide compiler hints to accelerate your code, instead of writing the accelerator code yourself. In 90 minutes, you will experience a four-step process for accelerating applications using OpenACC." The available languages are listed as English.

Title	Level	Cost
Accelerating Applications with CUDA Python	Beginner	FREE
Accelerating Applications with GPU-Accelerated Libraries in Python	Beginner	FREE
GPU Memory Optimizations (C/C++)	Intermediate	15 Credits
<b>OpenACC - 2X in 4 Steps in C/C++</b>	Beginner	15 Credits
Using Thrust to Accelerate C++	Beginner	15 Credits
Accelerating Applications with CUDA C/C++	Beginner	15 Credits
Accelerating Applications with GPU-Accelerated Libraries in C/C++	Beginner	10 Credits
Convolution: 3 approaches	Intermediate	15 Credits

# Install the OpenACC Toolkit (Optional)

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

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

**NVIDIA CUDA ZONE** Getting Started Downloads Training Ecosystem Forums

Register Now Login

## 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\*

**Get Your Free OpenACC Toolkit Now**

**DOWNLOAD**

### Application Acceleration with OpenACC on GPUs

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

Speedup vs CPU

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

<https://devtalk.nvidia.com/>

# 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>