



DEEP
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PRACE Workshop: Deep Learning and GPU programming workshop

15 – 18 June 2020

VSB TECHNICAL
UNIVERSITY
OF OSTRAVA

IT4INNOVATIONS
NATIONAL SUPERCOMPUTING
CENTER



MODULE TWO: PROFILING

Dr. Volker Weinberg | LRZ | 16.06.2020

MODULE OVERVIEW

Topics to be covered

- Compiling and profiling sequential code
- Explanation of multicore programming
- Compiling and profiling multicore code

COMPILING SEQUENTIAL CODE

PGI COMPILER BASICS

pgcc, pgc++ and pgfortran

- The command to compile C code is 'pgcc'
- The command to compile C++ code is 'pgc++'
- The command to compile Fortran code is 'pgfortran'
- The -fast flag instructs the compiler to optimize the code to the best of its abilities

```
$ pgcc -fast main.c  
$ pgc++ -fast main.cpp  
$ pgfortran -fast main.F90
```

PGI COMPILER BASICS

-Minfo flag

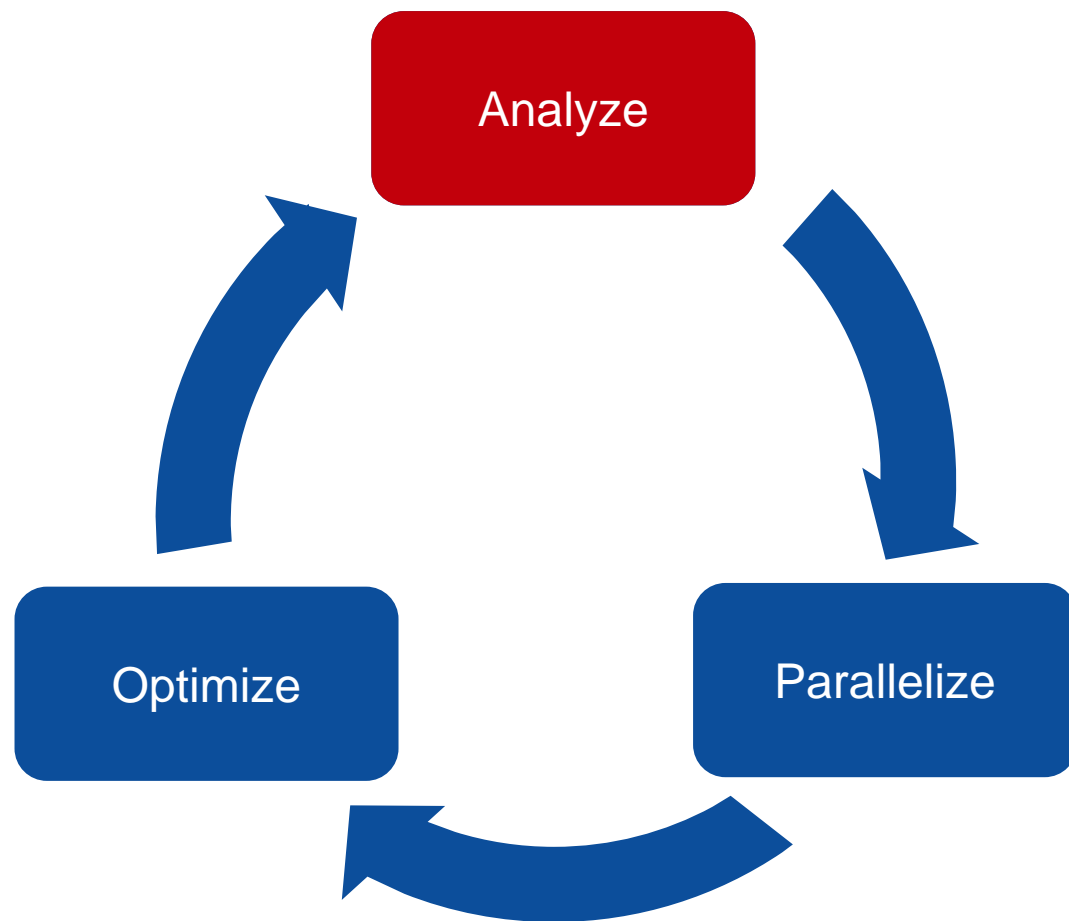
- The Minfo flag will instruct the compiler to print feedback about the compiled code
- -Minfo=accel will give us information about what parts of the code were accelerated via OpenACC
- -Minfo=opt will give information about all code optimizations
- -Minfo=all will give all code feedback, whether positive or negative

```
$ pgcc -fast -Minfo=all main.c  
$ pgc++ -fast -Minfo=all main.cpp  
$ pgfortran -fast -Minfo=all main.f90
```

PROFILING SEQUENTIAL CODE

OPENACC DEVELOPMENT CYCLE

- **Analyze** your code to determine most likely places needing parallelization or optimization.
- **Parallelize** your code by starting with the most time consuming parts, check for correctness and then analyze it again.
- **Optimize** your code to improve observed speed-up from parallelization.



PROFILING SEQUENTIAL CODE

Step 1: Run Your Code

Record the time it takes for your sequential program to run.

Note the final results to verify correctness later.

Always run a problem that is representative of your real jobs.

Terminal Window

```
$ pgcc -fast jacobi.c laplace2d.c
$ ./a.out
  0, 0.250000
 100, 0.002397
 200, 0.001204
 300, 0.000804
 400, 0.000603
 500, 0.000483
 600, 0.000403
 700, 0.000345
 800, 0.000302
 900, 0.000269
total: 39.432648 s
```

PROFILING SEQUENTIAL CODE

Step 2: Profile Your Code

Obtain detailed information about how the code ran.

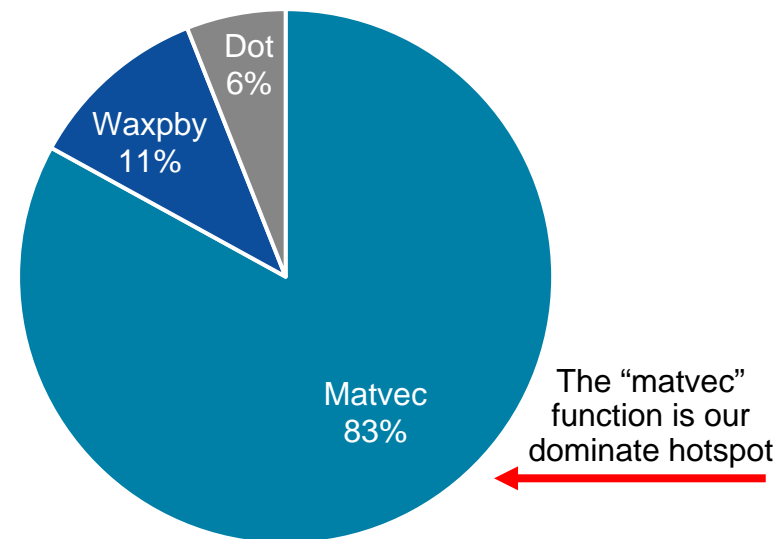
This can include information such as:

- Total runtime
- Runtime of individual routines
- Hardware counters

Identify the portions of code that took the longest to run. We want to focus on these “hotspots” when parallelizing.

Sample Code: Conjugate Gradient

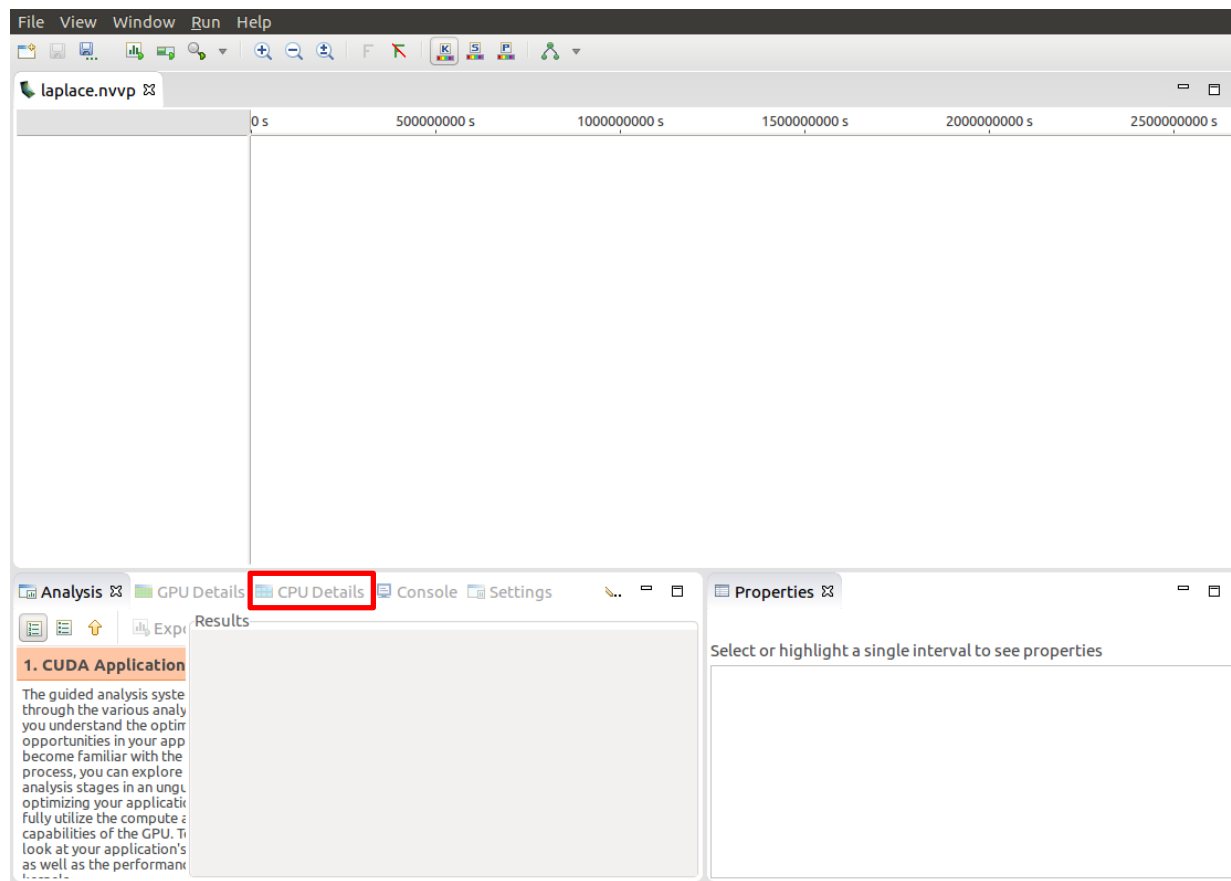
Total Runtime: 22.38 seconds



PROFILING SEQUENTIAL CODE

First sight when using PGPROF

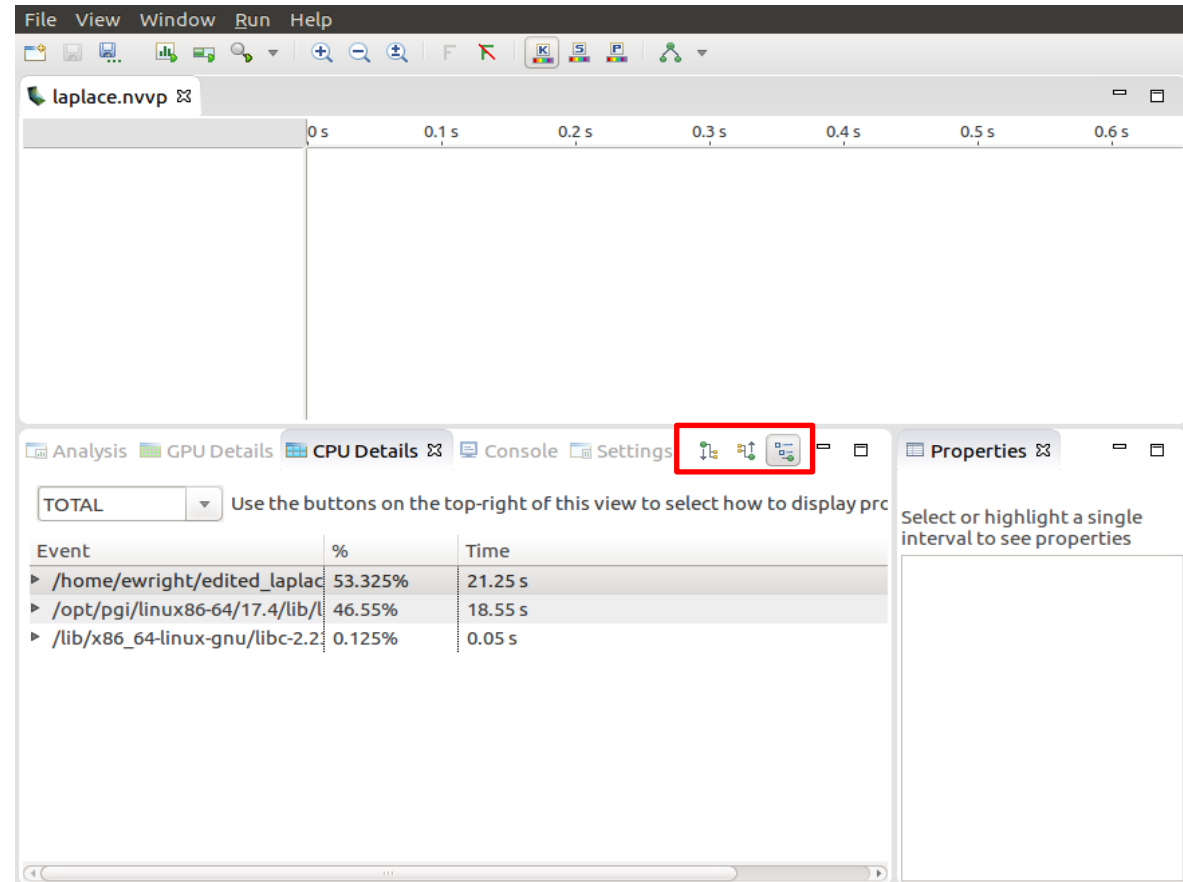
- Profiling a simple, sequential code
- Our sequential program will run on the CPU
- To view information about how our code ran, we should select the “CPU Details” tab



PROFILING SEQUENTIAL CODE

CPU Details

- Within the “CPU Details” tab, we can see the various parts of our code, and how long they took to run
- We can reorganize this info using the three options in the top-right portion of the tab
- We will expand this information, and see more details about our code



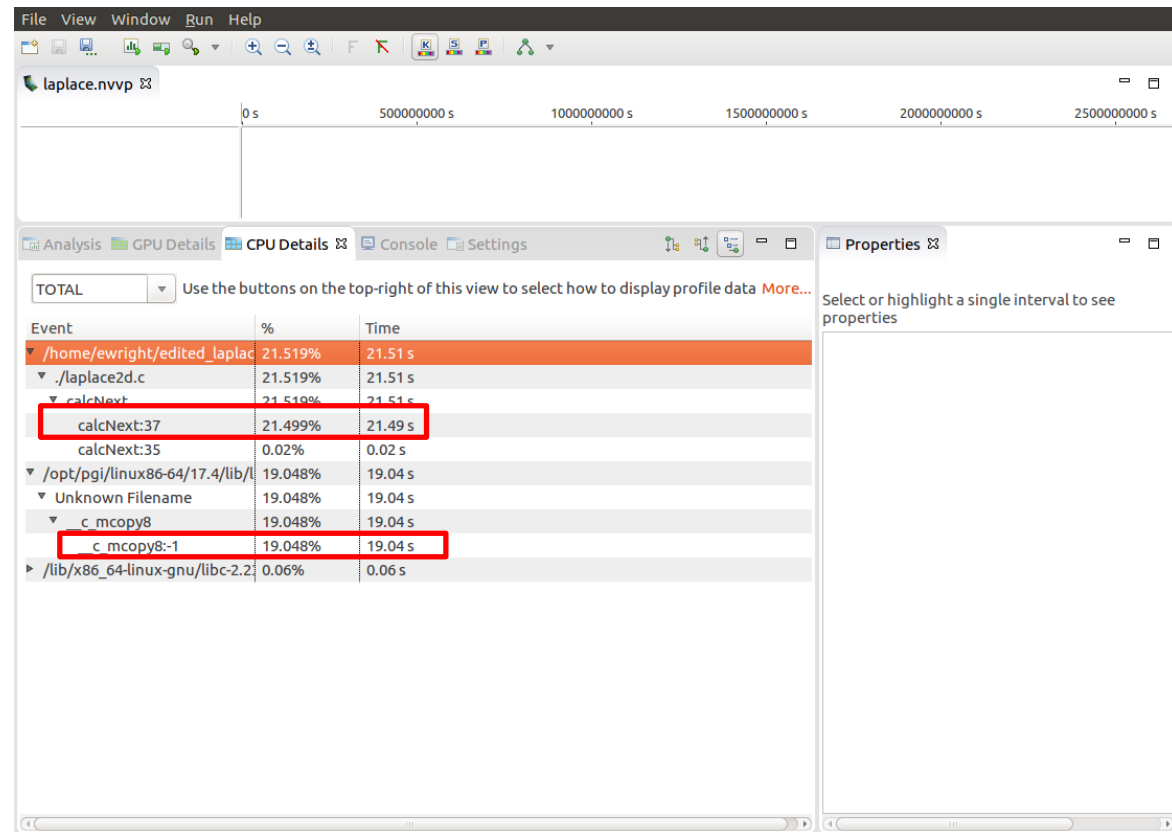
The screenshot shows the OpenACC CPU Details window. At the top, there is a timeline from 0 s to 0.6 s. Below the timeline is a table with columns for Event, %, and Time. The table contains three rows of data. A red box highlights the top-right corner of the CPU Details tab, which contains three icons for reorganizing the data: a bar chart, a list, and a pie chart. To the right of the table is a Properties panel with the text "Select or highlight a single interval to see properties".

| Event | % | Time |
|--|---------|---------|
| ▶ /home/ewright/edited_laplace.nvvp | 53.325% | 21.25 s |
| ▶ /opt/pgi/linux86-64/17.4/lib/libc.so.2 | 46.55% | 18.55 s |
| ▶ /lib/x86_64-linux-gnu/libc-2.23 | 0.125% | 0.05 s |

PROFILING SEQUENTIAL CODE

CPU Details

- We can see that there are two places that our code is spending most of its time
- 21.49 seconds in the “calcNext” function
- 19.04 seconds in a memcpy function
- The `c_memcpy8` that we see is actually a compiler optimization that is being applied to our “swap” function



PROFILING SEQUENTIAL CODE

PGPROF

- We are also able to select the different elements in the CPU Details by double-clicking to open the associated source code
- Here we have selected the “calcNext:37” element, which opened up our code to show the exact line (line 37) that is associated with that element

The screenshot displays a code editor window titled 'laplace2d.c' with the following code:

```
30 #define OFFSET(x, y, m) (((x)*(m)) + (y))
31
32 double calcNext(double *restrict A, double *restrict Anew, int m, int n)
33 {
34     double error = 0.0;
35     for( int j = 1; j < n-1; j++)
36     {
37         for( int i = 1; i < m-1; i++ )
38         {
39             Anew[OFFSET(j, i, m)] = 0.25 * ( A[OFFSET(j, i+1, m)] + A[OFFSET(j, i-1, m)]
40             + A[OFFSET(j-1, i, m)] + A[OFFSET(j+1, i, m)]);
41             error = fmax( error, fabs(Anew[OFFSET(j, i, m)] - A[OFFSET(j, i, m)]));
42         }
43     }
44     return error;
45 }
46
47
48 void swap(double *restrict A, double *restrict Anew, int m, int n)
49 {
50     for( int j = 1; j < n-1; j++)
51     {
52         for( int i = 1; i < m-1; i++ )
53     {
```

The CPU Details window shows the following table:

| Event | % | Time |
|--|---------|---------|
| ▼ /home/ewright/edited_laplace2d.c | 21.519% | 21.51 s |
| ▼ ./laplace2d.c | 21.519% | 21.51 s |
| ▼ calcNext | 21.519% | 21.51 s |
| calcNext:37 | 21.499% | 21.49 s |
| calcNext:35 | 0.02% | 0.02 s |
| ▶ /opt/pgi/linux86-64/17.4/lib/libc.so.2 | 19.048% | 19.04 s |
| ▶ /lib/x86_64-linux-gnu/libc-2.27.so | 0.06% | 0.06 s |

PROFILING SEQUENTIAL CODE

Step 2: Profile Your Code

Obtain detailed information about how the code ran.

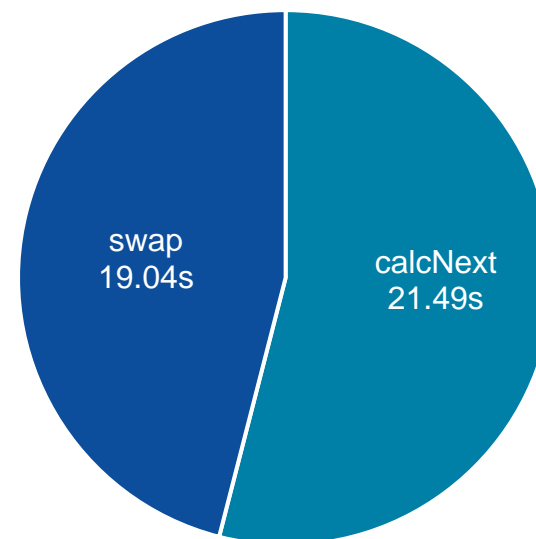
This can include information such as:

- Total runtime
- Runtime of individual routines
- Hardware counters

Identify the portions of code that took the longest to run. We want to focus on these “hotspots” when parallelizing.

Lab Code: Laplace Heat Transfer

Total Runtime: 39.43 seconds



PROFILING SEQUENTIAL CODE

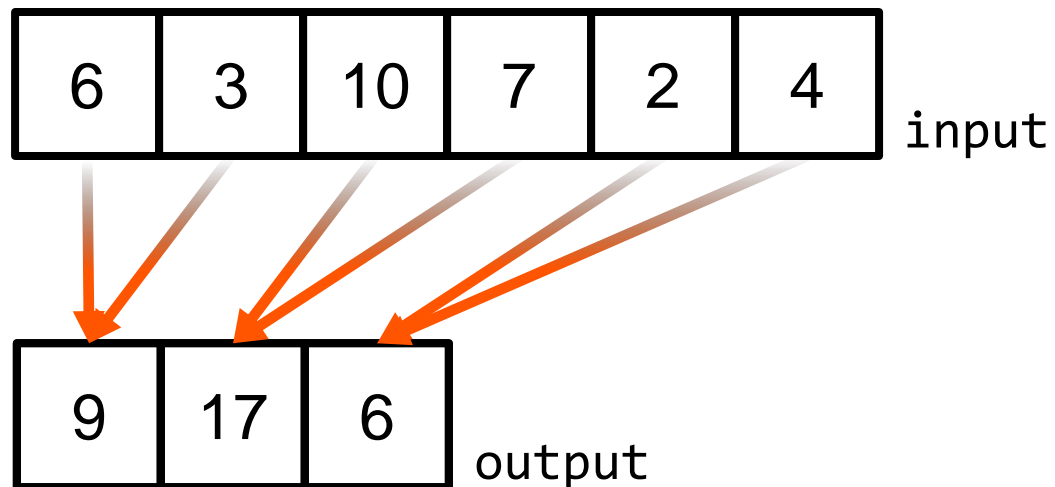
Step 3: Identify Parallelism

Observe the loops contained within the identified hotspots

Are these loops parallelizable?
Can the loop iterations execute independently of each other?
Are the loops multi-dimensional, and does that make them very large?

Loops that are good to parallelize tend to have a lot of iterations to map to parallel hardware.

```
void pairing(int *input, int *output, int N){  
    for(int i = 0; i < N; i++){  
        output[i] = input[i*2] + input[i*2+1];  
    }  
}
```



PLEASE START LAB NOW!

TRAINING SETUP

- To get started, follow these steps:
- Create an NVIDIA Developer account at <http://courses.nvidia.com/join> Select "Log in with my NVIDIA Account" and then "Create Account" (done yesterday)
- Visit <http://courses.nvidia.com/dli-event> and enter the event code

PRACE_OACC_AMBASSADOR_JU20

TRAINING SETUP

The screenshot shows the NVIDIA course interface. At the top, the URL is <https://courses.nvidia.com/courses/course-v1%3ADLI%2BC-AC-03%2BV1/course/>. The user is logged in as 'Volker_Weinberg_Test'. The course title is 'Fundamentals of Accelerated Computing with OpenACC'. A search bar and a 'Resume Course' button are visible. Below the course title, there is a 'Click here to get started' button with a 'Resume Course' link next to it. An orange arrow points to this button. To the right, there are sections for 'Course Tools' (Bookmarks), 'Important Course Dates' (Today is Jun 15, 2020 17:20 CEST), and 'Course Handouts' (No Course Handouts).

Fundamentals of Accelerated Computing with OpenACC

[Bookmark this page](#)



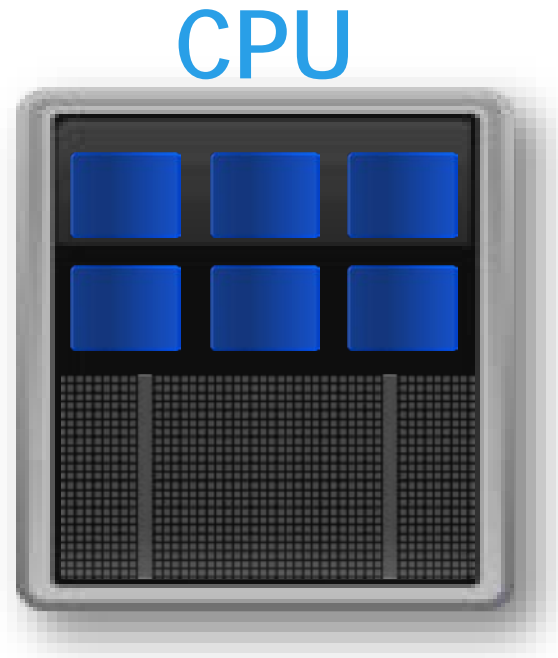
Please wait 5 - 10 minutes while your interactive GPU enabled environment loads. When the "Launch" button appears, click it to get started.

PROFILING MULTICORE CODE

PROFILING MULTICORE CODE

What is multicore?

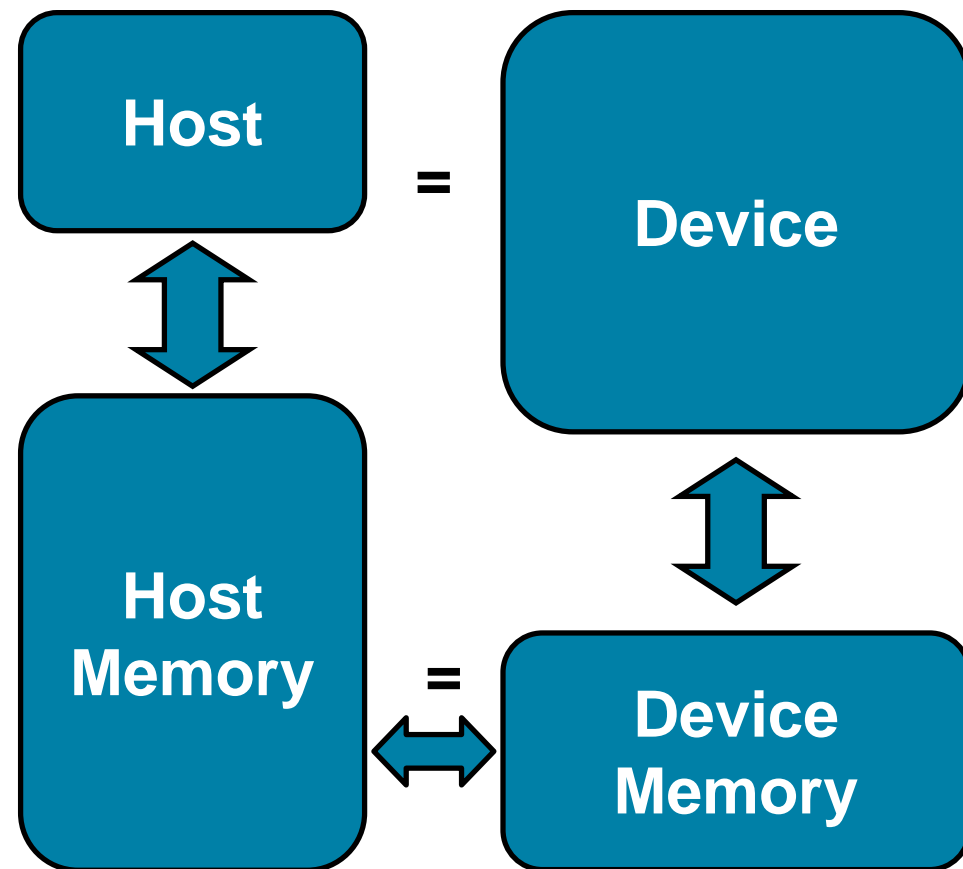
- *Multicore* refers to using a CPU with multiple computational cores as our parallel device
- These cores can run independently of each other, but have shared access to memory
- Loop iterations can be spread across CPU threads and can utilize SIMD/vector instructions (SSE, AVX, etc.)
- Parallelizing on a multicore CPU is a good starting place, since data management is unnecessary



PROFILING MULTICORE CODE

Using a multicore CPU with OpenACC

- OpenACC's generic model involves a combination of a host and a device
- Host generally means a CPU, and the device is some parallel hardware
- When running with a multicore CPU as our device, typically this means that our host/device will be the same
- This also means that their memories will be the same



PROFILING MULTICORE CODE

Compiling code for a specific parallel hardware

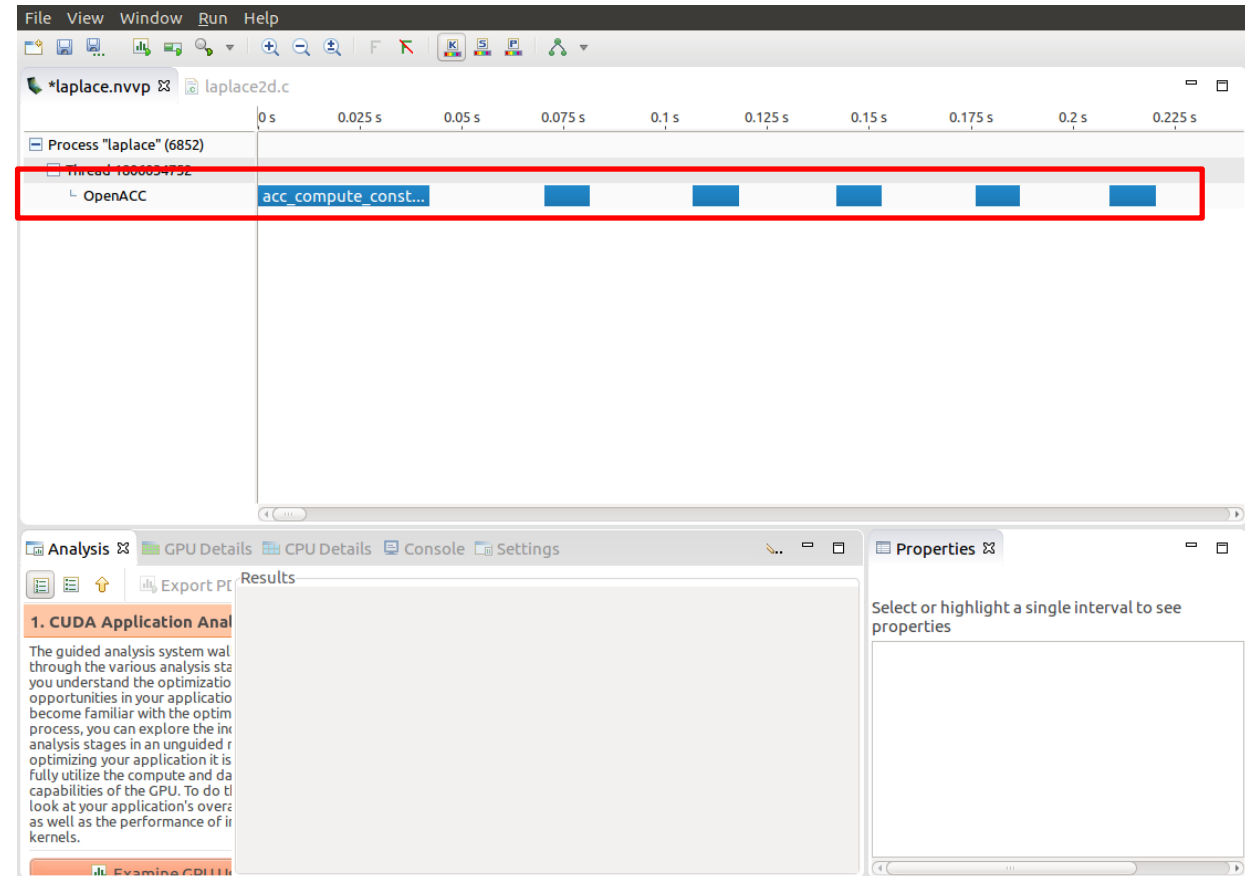
- The '-ta' flag will allow us to compile our code for a specific, target parallel hardware
- 'ta' stands for "Target Accelerator," an accelerator being another way to refer to a parallel hardware
- Our OpenACC code can be compiled for many different kinds of parallel hardware without having to change the code

```
$ pgcc -fast -Minfo=accel -ta=multicore laplace2d.c  
calcNext:  
    35, Generating Multicore code  
    36, #pragma acc loop gang
```


PROFILING MULTICORE CODE

PGPROF

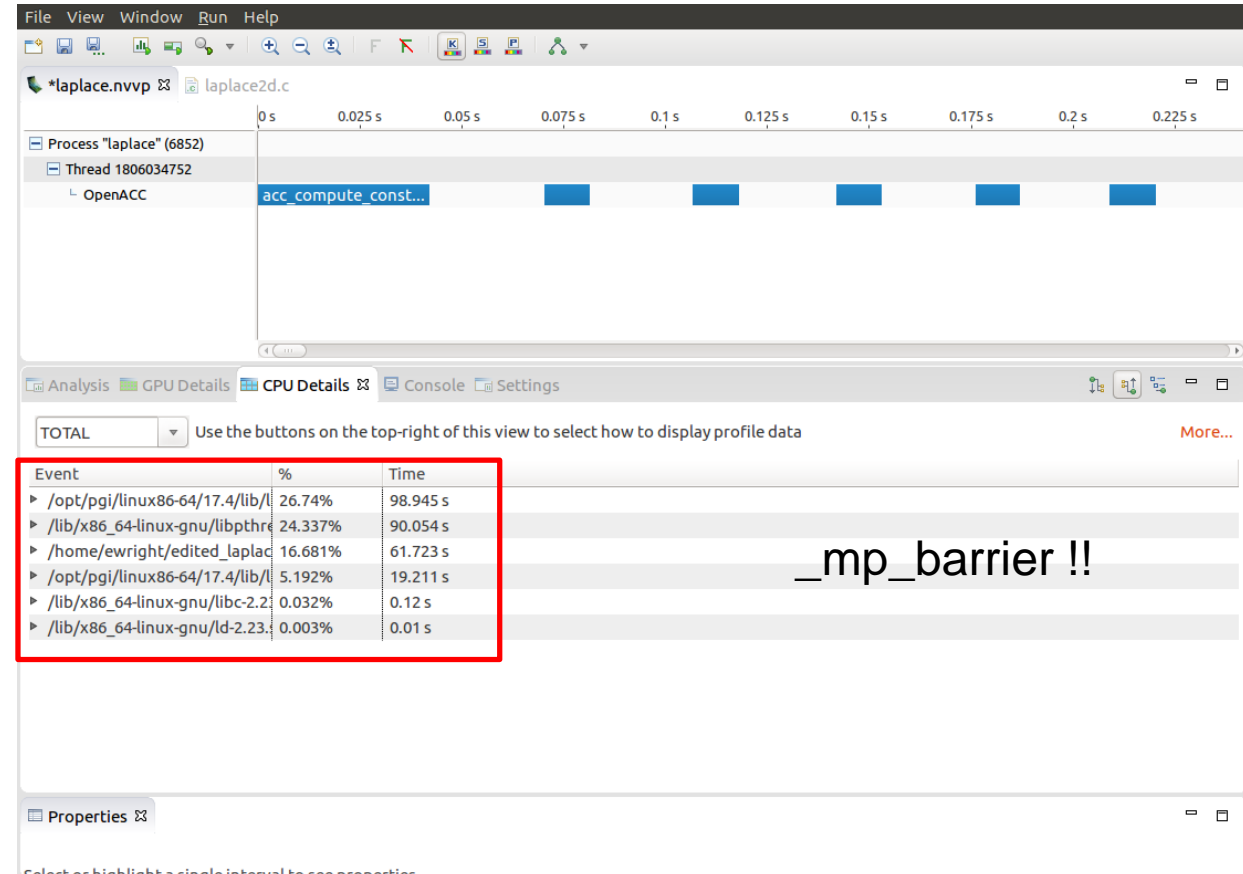
- The first difference we see in this multicore profile is that there is now a “timeline”
- This timeline will show when our parallel hardware is being used, and how it is being used
- Each of the blue bars represent a portion of our program that was run on the multicore CPU



PROFILING MULTICORE CODE

CPU Details

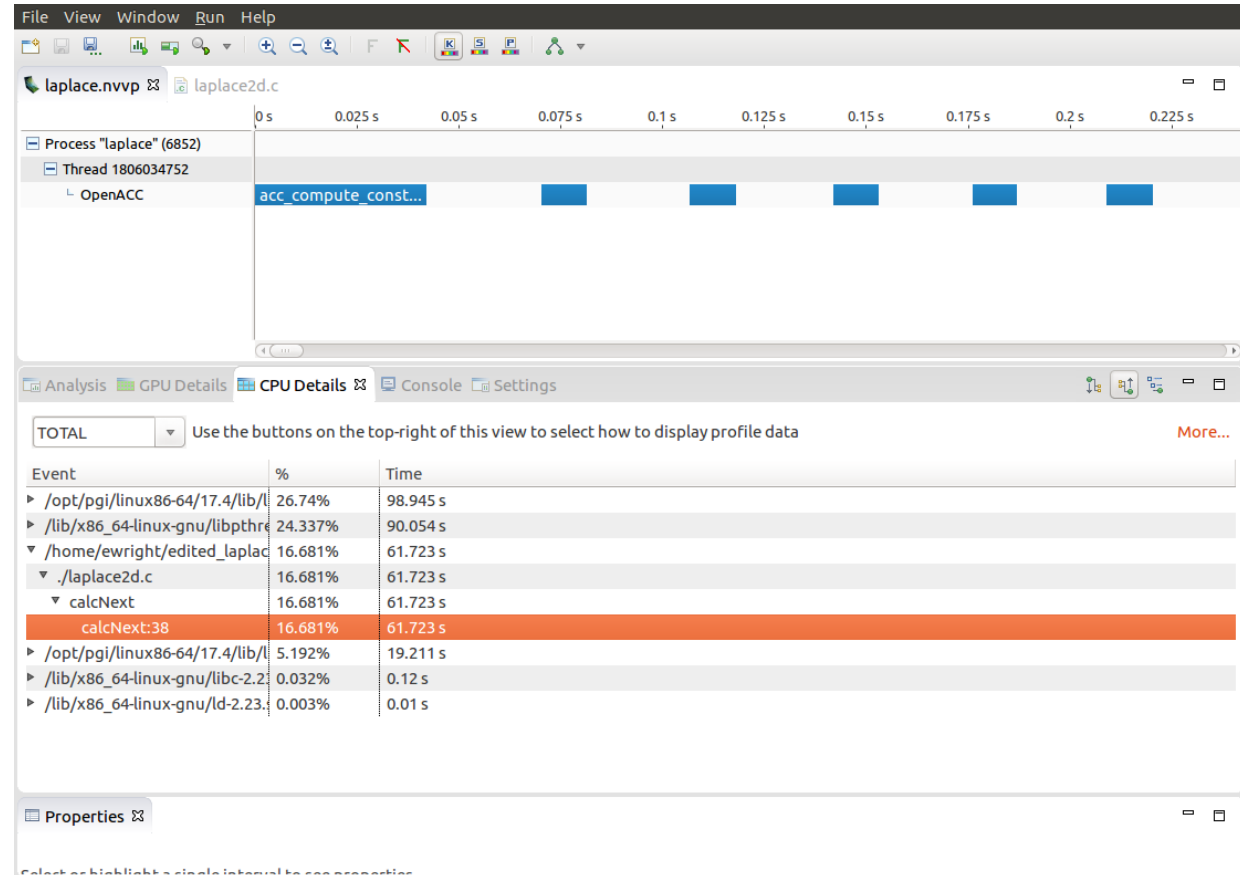
- Looking at our CPU Details, we can see that there is a lot more happening compared to our sequential program
- For the most part, these extra details revolve around the need for the CPU cores to communicate with each other



PROFILING MULTICORE CODE

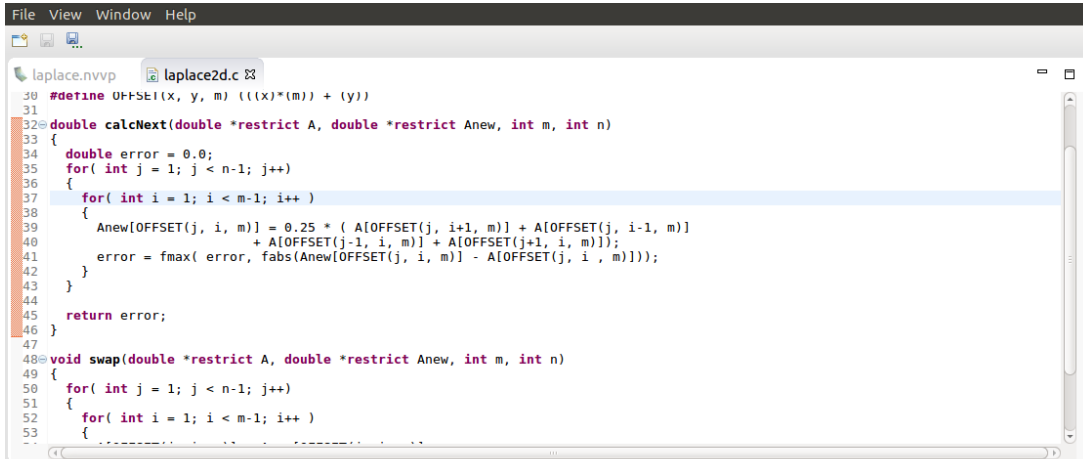
PGPROF

- Just like earlier, we see our “calcNext” function
- We also see that PGPROF is reporting this function to take 61.72 seconds to run
- Looking at the program now, it looks like it performs much worse than the sequential version



PROFILING MULTICORE CODE

PGPROF



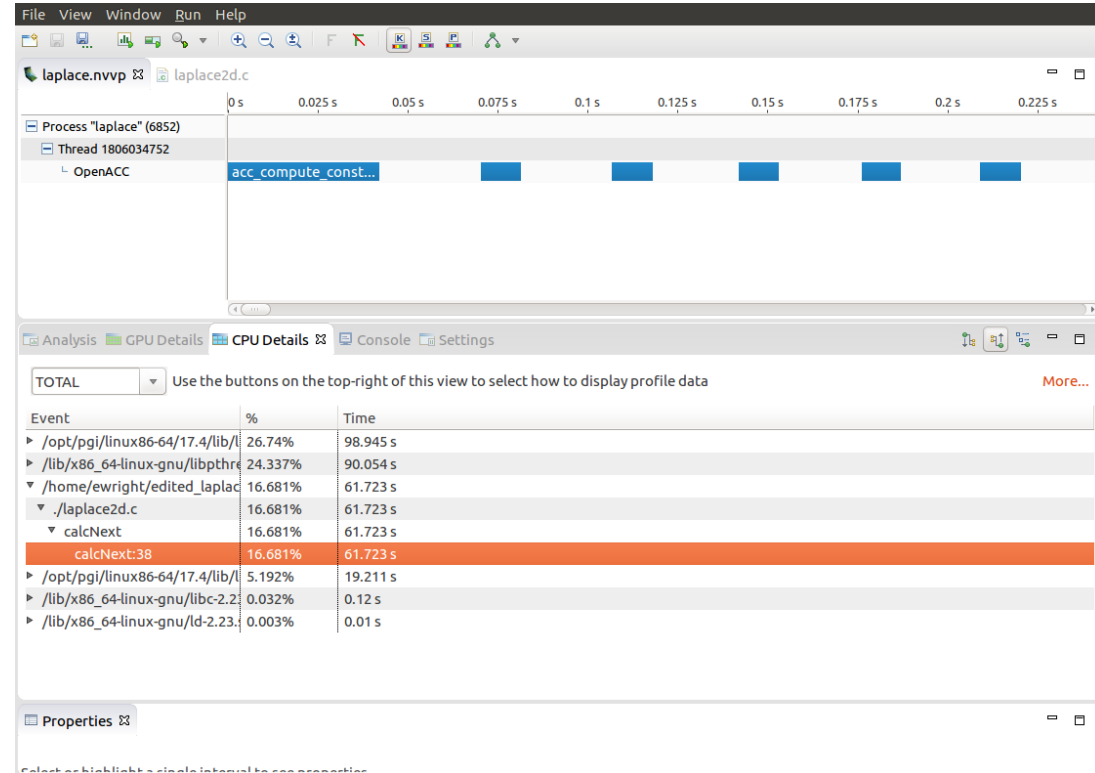
```
laplace.nvvp laplace2d.c
30 #define OFFSET(x, y, m) (((x)*(m)) + (y))
31
32 double calcNext(double *restrict A, double *restrict Anew, int m, int n)
33 {
34     double error = 0.0;
35     for( int j = 1; j < n-1; j++)
36     {
37         for( int i = 1; i < m-1; i++)
38         {
39             Anew[OFFSET(j, i, m)] = 0.25 * ( A[OFFSET(j, i+1, m)] + A[OFFSET(j, i-1, m)]
40             + A[OFFSET(j-1, i, m)] + A[OFFSET(j+1, i, m)]);
41             error = fmax( error, fabs(Anew[OFFSET(j, i, m)] - A[OFFSET(j, i, m)]));
42         }
43     }
44     return error;
45 }
46
47 void swap(double *restrict A, double *restrict Anew, int m, int n)
48 {
49     for( int j = 1; j < n-1; j++)
50     {
51         for( int i = 1; i < m-1; i++)
52         {
53             ...
54         }
55     }
56 }
```

Analysis GPU Details CPU Details Console Settings Properties

TOTAL Use the buttons on the top-right of this view to select how to display profile data More...

| Event | % | Time |
|------------------------------------|---------|---------|
| ▼ /home/ewright/edited_laplace2d.c | 21.519% | 21.51 s |
| ▼ ./laplace2d.c | 21.519% | 21.51 s |
| ▼ calcNext | 21.519% | 21.51 s |
| calcNext:37 | 21.499% | 21.49 s |
| calcNext:35 | 0.02% | 0.02 s |
| ▶ /opt/pgi/linux86-64/17.4/lib/ | 19.048% | 19.04 s |
| ▶ /lib/x86_64-linux-gnu/libc-2.2 | 0.06% | 0.06 s |

Select or highlight a single interval to see properties



laplace.nvvp laplace2d.c

0 s 0.025 s 0.05 s 0.075 s 0.1 s 0.125 s 0.15 s 0.175 s 0.2 s 0.225 s

Process "laplace" (6852)

Thread 1806034752

OpenACC acc_compute_const...

Analysis GPU Details CPU Details Console Settings

TOTAL Use the buttons on the top-right of this view to select how to display profile data More...

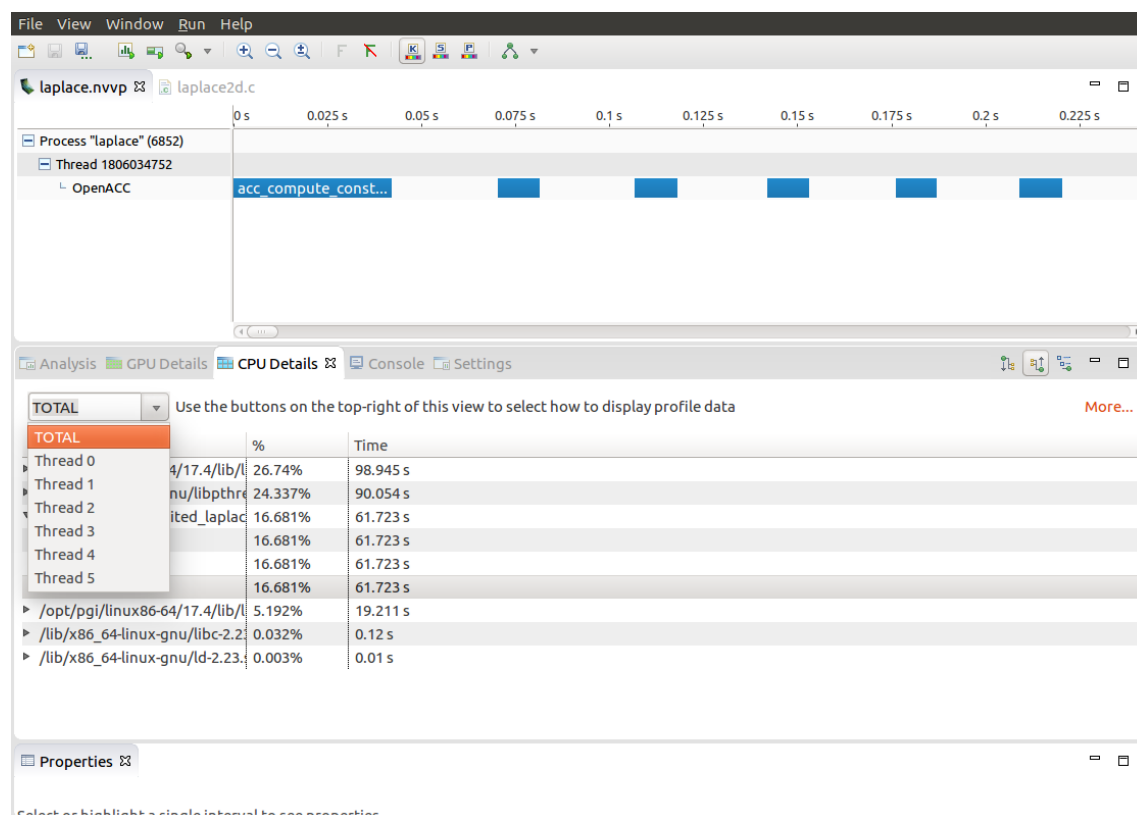
| Event | % | Time |
|------------------------------------|---------|----------|
| ▶ /opt/pgi/linux86-64/17.4/lib/ | 26.74% | 98.945 s |
| ▶ /lib/x86_64-linux-gnu/libpthread | 24.337% | 90.054 s |
| ▼ /home/ewright/edited_laplace2d.c | 16.681% | 61.723 s |
| ▼ ./laplace2d.c | 16.681% | 61.723 s |
| ▼ calcNext | 16.681% | 61.723 s |
| calcNext:38 | 16.681% | 61.723 s |
| ▶ /opt/pgi/linux86-64/17.4/lib/ | 5.192% | 19.211 s |
| ▶ /lib/x86_64-linux-gnu/libc-2.2 | 0.032% | 0.12 s |
| ▶ /lib/x86_64-linux-gnu/ld-2.23 | 0.003% | 0.01 s |

Properties

PROFILING MULTICORE CODE

View of all computational threads

- The program is actually performing better than the sequential version
- We are only looking at the “TOTAL” view, which means that PGPROF is combining information from all of our CPU cores



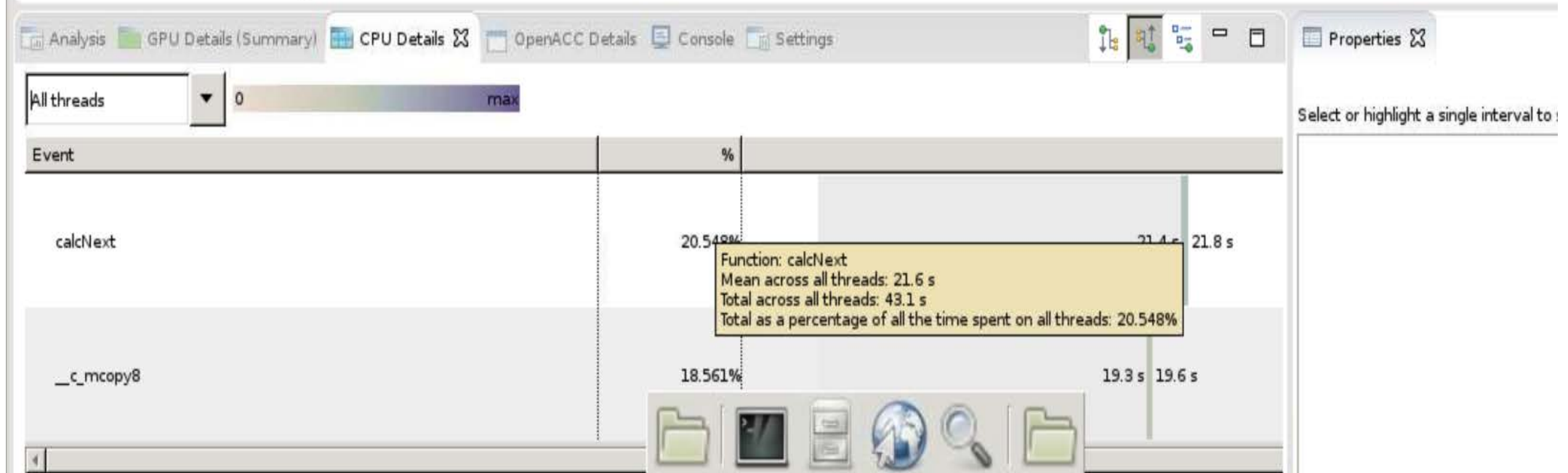
PROFILING MULTICORE CODE

View of all computational threads

- The new PGPROF 18.4 installed on VNC changed the dropdown box labeled TOTAL into “All threads” and displays min, max and mean values graphically.
- When moving the mouse on the % value, one can see
 - Mean across all threads
 - Total across all threads
 - Total as a percentage of all the time spent on all threads.

PROFILING MULTICORE CODE

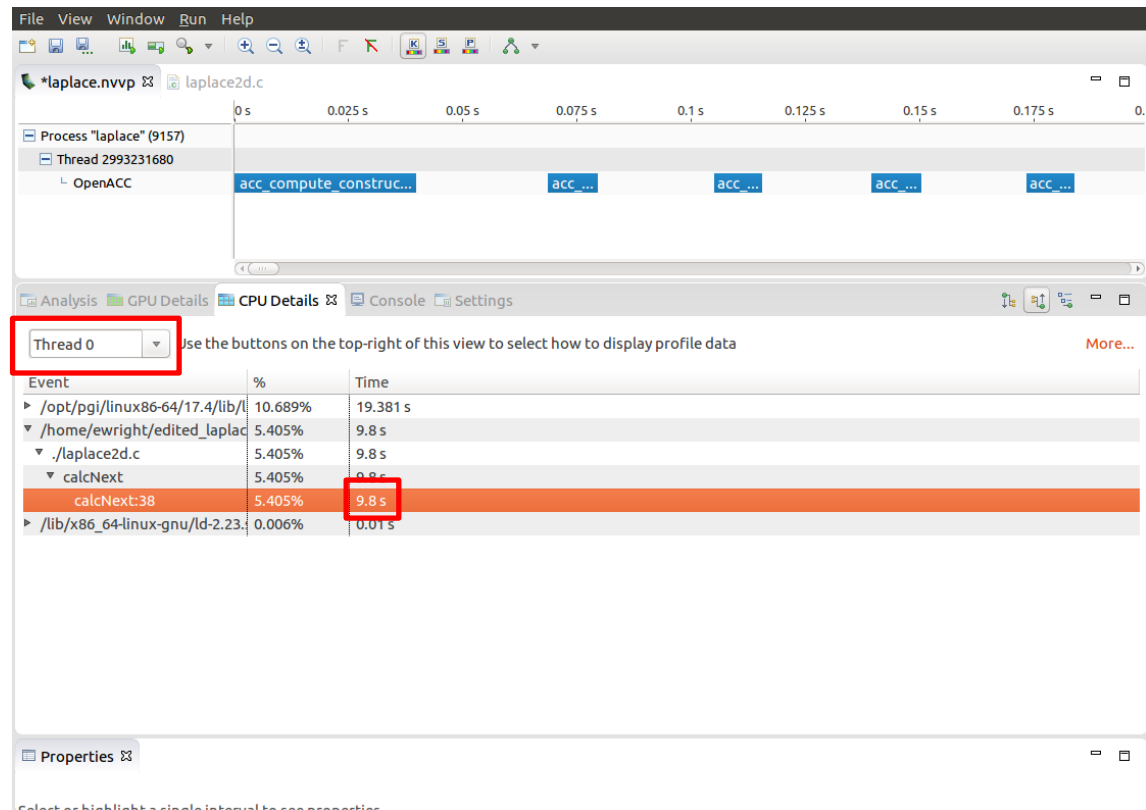
View of all computational threads



PROFILING MULTICORE CODE

Observing a single thread

- Now we have selected to view a specific thread (for us, a thread would be a single CPU core)
- We can see that this single thread only spent 9.8 seconds running calcNext
- Each thread will take a similar amount of time and execute simultaneously, resulting in a faster run



LAPLACE HEAT TRANSFER

Introduction to lab code - visual

We will observe a simple simulation of heat distributing across a metal plate.

We will apply a consistent heat to the top of the plate.

Then, we will simulate the heat distributing across the plate.

Very Hot

Room Temp



LAPLACE HEAT TRANSFER

Introduction to lab code - technical

The lab simulates a very basic 2-dimensional heat transfer problem. We have two 2-dimensional arrays, **A** and **Anew**.

The arrays represent a 2-dimensional, metal plate. Each element in the array is a **double** value that represents temperature.

We will simulate the distribution of heat until a **minimum change value** is achieved, or until we exceed a **maximum number of iterations**.

A

| | | | |
|-----|-----|-----|-----|
| 0.0 | 0.0 | 0.0 | 0.0 |
| 0.0 | 0.0 | 0.0 | 0.0 |
| 0.0 | 0.0 | 0.0 | 0.0 |
| 0.0 | 0.0 | 0.0 | 0.0 |

Anew

| | | | |
|-----|-----|-----|-----|
| 0.0 | 0.0 | 0.0 | 0.0 |
| 0.0 | 0.0 | 0.0 | 0.0 |
| 0.0 | 0.0 | 0.0 | 0.0 |
| 0.0 | 0.0 | 0.0 | 0.0 |

LAPLACE HEAT TRANSFER

Introduction to lab code - technical

We initialize the top row to be a temperature of 1.0

The **calcNext** function will iterate through all of the inner elements of array A, and update the corresponding elements in Anew

We will take the average of the neighboring cells, and record it in **Anew**.

The **swap** function will copy the contents of Anew to A

A

| | | | |
|-----|-----|-----|-----|
| 0.0 | 0.0 | 0.0 | 0.0 |
| 0.0 | 0.0 | 0.0 | 0.0 |
| 0.0 | 0.0 | 0.0 | 0.0 |
| 0.0 | 0.0 | 0.0 | 0.0 |



Anew

| | | | |
|-----|------|------|-----|
| 0.0 | 0.0 | 0.0 | 0.0 |
| 0.0 | 0.25 | 0.25 | 0.0 |
| 0.0 | 0.0 | 0.0 | 0.0 |
| 0.0 | 0.0 | 0.0 | 0.0 |

LAPLACE HEAT TRANSFER

Introduction to lab code

A

| | | | |
|-----|------|------|-----|
| 1.0 | 1.0 | 1.0 | 1.0 |
| 0.0 | 0.25 | 0.25 | 0.0 |
| 0.0 | 0.0 | 0.0 | 0.0 |
| 0.0 | 0.0 | 0.0 | 0.0 |



Anew

| | | | |
|-----|------|------|-----|
| 1.0 | 1.0 | 1.0 | 1.0 |
| 0.0 | 0.25 | 0.25 | 0.0 |
| 0.0 | 0.0 | 0.0 | 0.0 |
| 0.0 | 0.0 | 0.0 | 0.0 |

The **swap** function will copy the contents of Anew to A

KEY CONCEPTS

In this module we discussed...

- Compiling sequential and parallel code
- CPU profiling for sequential and parallel execution
- Specifics of our Laplace Heat Transfer lab code

LAB GOALS

In this lab you will do the following...

- Build and run the example code using the PGI compiler
- Use PGProf to understand where the program spends its time

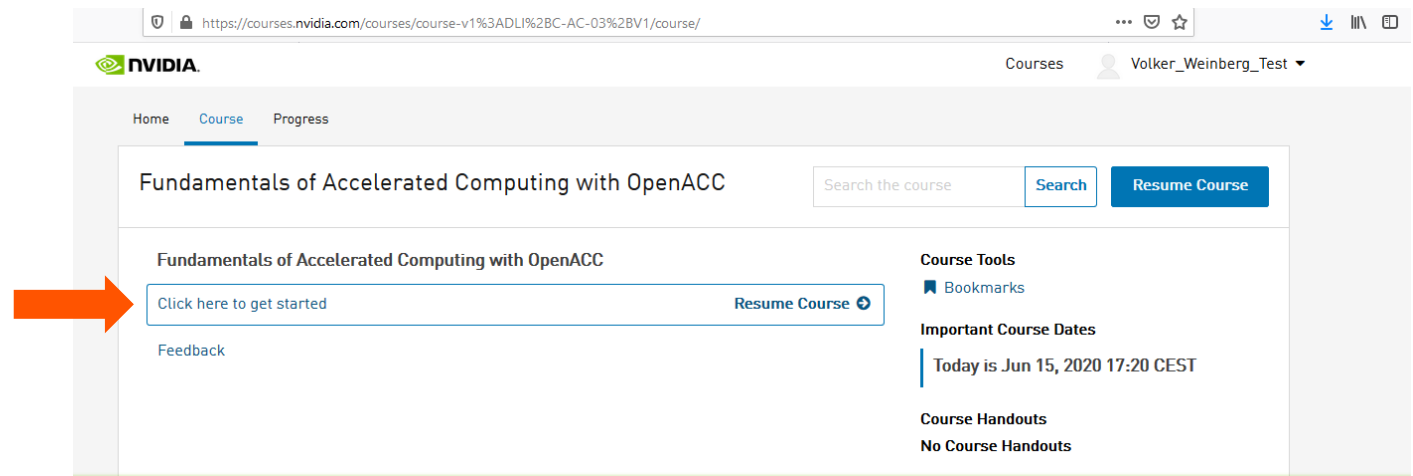
THANK YOU

TRAINING SETUP

- To get started, follow these steps:
- Create an NVIDIA Developer account at <http://courses.nvidia.com/join> Select "Log in with my NVIDIA Account" and then "Create Account" (done yesterday)
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PRACE_OACC_AMBASSADOR_JU20

TRAINING SETUP



The screenshot shows the NVIDIA course interface. At the top, the URL is <https://courses.nvidia.com/courses/course-v1%3ADLI%2BC-AC-03%2BV1/course/>. The user is logged in as 'Volker_Weinberg_Test'. The course title is 'Fundamentals of Accelerated Computing with OpenACC'. A search bar and a 'Resume Course' button are visible. Below the course title, there is a 'Click here to get started' button with a 'Resume Course' link next to it. An orange arrow points to this button. To the right, there are sections for 'Course Tools' (Bookmarks), 'Important Course Dates' (Today is Jun 15, 2020 17:20 CEST), and 'Course Handouts' (No Course Handouts).

Fundamentals of Accelerated Computing with OpenACC

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Please wait 5 - 10 minutes while your interactive GPU enabled environment loads. When the "Launch" button appears, click it to get started.

TRAINING SETUP

Fundamentals of Accelerated Computing with OpenACC

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1 : 56 : 47

REMAINING TIME



LAUNCH TASK



STOP TASK

Please wait 5 - 10 minutes while your interactive GPU enabled environment loads. When the "Launch" button appears, click it to get started.

TRAINING SETUP


ec2-18-224-153-130.us-east-2.compute.amazonaws.com/tree

jupyter Quit

Files Running Clusters

Select items to perform actions on them. Upload New ▾ ↻

| <input type="checkbox"/> 0 ▾ | / | Name ▾ | Last Modified | File size |
|------------------------------|---------------|------------------|---------------|-----------|
| <input type="checkbox"/> | folder | module2 | 2 months ago | |
| <input type="checkbox"/> | folder | module3 | 2 months ago | |
| <input type="checkbox"/> | folder | module4 | 2 months ago | |
| <input type="checkbox"/> | folder | module5 | 2 months ago | |
| <input type="checkbox"/> | folder | module6 | 2 months ago | |
| <input type="checkbox"/> | notebook icon | START HERE.ipynb | 2 months ago | 1.36 kB |



TRAINING SETUP

Welcome to the OpenACC labs

Please select the appropriate lab below.



- [Module 2](#) - Application Profiling with PGProf Lab - This lab introduces students to application profiling using the PGProf profiler.
- [Module 3](#) - OpenACC Directives Basics - This lab introduces OpenACC directives.
- [Module 4](#) - GPU Programming with OpenACC - This lab introduces GPU programming with OpenACC.
- [Module 5](#) - Data Management with OpenACC - This lab introduces OpenACC data management directives.
- [Module 6](#) - OpenACC Loop Optimizations - This lab introduces students to loop optimizations in OpenACC.

Application Profiling with PGProf Lab

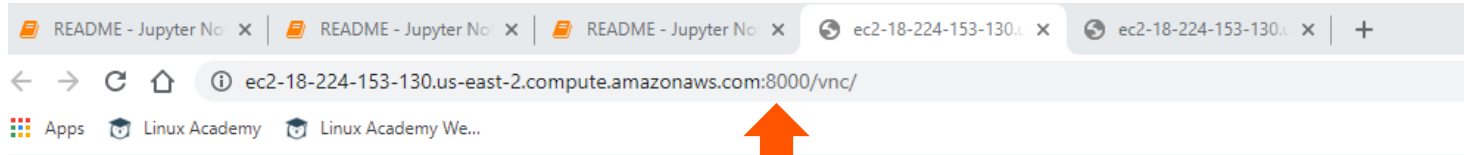
This lab is meant to accompany Module 2 of the OpenACC.org teaching materials. The purpose of this lab is to introduce students to application profiling using the PGProf profiler. Lab instructions and source code is available for C/C++ and Fortran.

Please see the following files to begin the lab:



- [C/C++](#)
- [Fortran](#)

VNC USAGE



**Remove :8000 and
use /vnc**



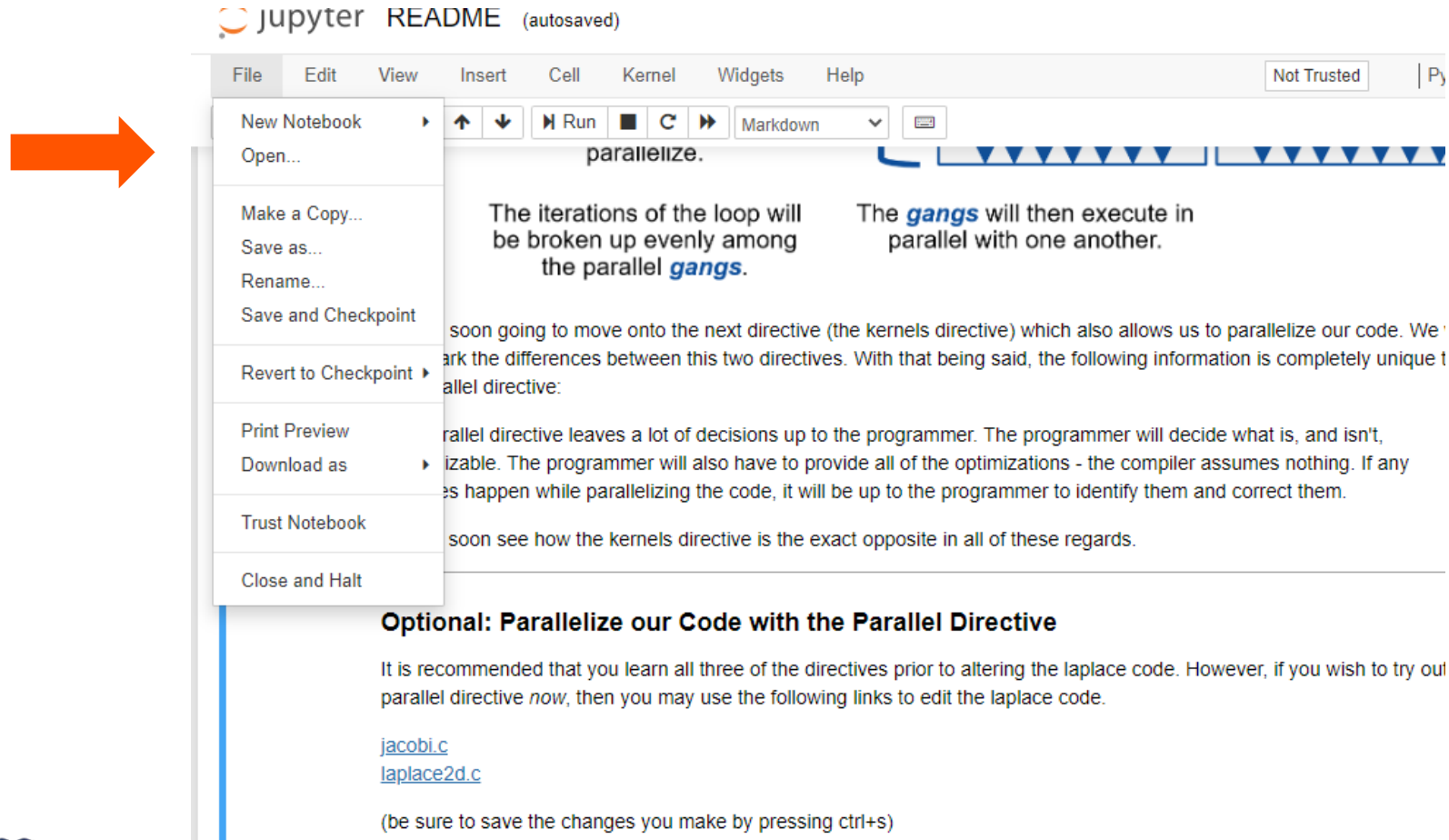
Diese Seite funktioniert nicht

`ec2-18-224-153-130.us-east-2.compute.amazonaws.com` hat keine Daten gesendet.

ERR_EMPTY_RESPONSE

Neu laden

HOW TO EDIT FILES IN MOD2 (METHOD 1)



jupyter README (autosaved)

File Edit View Insert Cell Kernel Widgets Help Not Trusted | Py

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parallelize.

The iterations of the loop will be broken up evenly among the parallel **gangs**.

The **gangs** will then execute in parallel with one another.

soon going to move onto the next directive (the kernels directive) which also allows us to parallelize our code. We mark the differences between this two directives. With that being said, the following information is completely unique to parallel directive:

parallel directive leaves a lot of decisions up to the programmer. The programmer will decide what is, and isn't, parallelizable. The programmer will also have to provide all of the optimizations - the compiler assumes nothing. If any issues happen while parallelizing the code, it will be up to the programmer to identify them and correct them.

soon see how the kernels directive is the exact opposite in all of these regards.

Optional: Parallelize our Code with the Parallel Directive

It is recommended that you learn all three of the directives prior to altering the laplace code. However, if you wish to try out parallel directive *now*, then you may use the following links to edit the laplace code.

[jacobi.c](#)

[laplace2d.c](#)

(be sure to save the changes you make by pressing ctrl+s)

HOW TO EDIT FILES IN MOD2 (METHOD 1)

Files Running Clusters

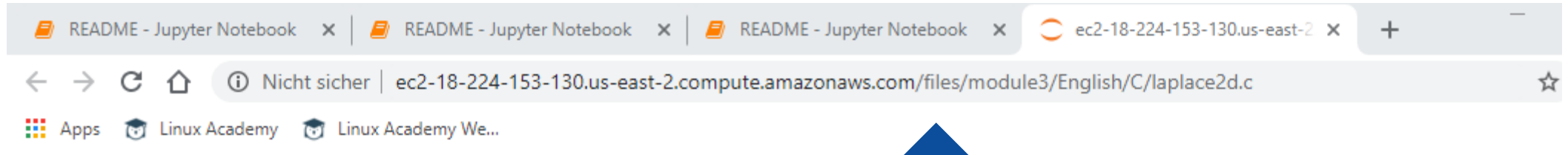
Select items to perform actions on them. Upload New ▾ ↻

0 ▾ / module3 / English / C Name ▾ Last Modified File size

| | | | |
|---------------------------------------|---------|-----------------------|---------|
| <input type="checkbox"/> .. | | vor ein paar Sekunden | |
| <input type="checkbox"/> solutions | | vor 2 Monaten | |
| <input type="checkbox"/> README.ipynb | Running | vor 12 Minuten | 27.6 kB |
| <input type="checkbox"/> jacobi.c | | vor 2 Monaten | 1.55 kB |
| <input type="checkbox"/> jacobi.o | | vor 14 Minuten | 4.4 kB |
| <input type="checkbox"/> laplace | | vor 14 Minuten | 14.9 kB |
| <input type="checkbox"/> laplace2d.c | | vor 2 Monaten | 1.79 kB |
| <input type="checkbox"/> laplace2d.h | | vor 2 Monaten | 1.85 kB |
| <input type="checkbox"/> laplace2d.o | | vor 14 Minuten | 5.6 kB |



HOW TO EDIT FILES IN MOD2 (METHOD 2)



```
/*  
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```

**Replace /files/ with
/edit/ !!!!**