esiwace

CENTRE OF EXCELLENCE IN SIMULATION OF WEATHER AND CLIMATE IN EUROPE

ESiWACE3 - Excellence in Simulation of Weather and Climate in Europe, Phase 3

GPU Optimization with Kernel Tuner

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EuroHPC Joint Undertaking

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Background:

- 2017-now Research Software Engineer at the Netherlands eScience Center
  - Radio astronomy, climate modeling, biology, NLP, high-energy physics, medical imaging
- 2019 visiting scholar at Nanyang Technological University in Singapore
  - Real-time tracking of social insects
- 2015-2016 scientific programmer at ASTRON, the Netherlands Institute for Radio Astronomy
  - Designing and developing a real-time GPU pipeline for the Westerbork radio telescope
- 2012-2017 PhD at VU Amsterdam
  - "Accelerating Radio Astronomy with Auto-Tuning”
- 2011-2012 researcher at VU Amsterdam
  - Working on GPUs for radio astronomy

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- Research Software Engineer (RSE)
- Research interests in HPC include:
  - GPU programming, parallel algorithms, distributed systems, and scalable programming models.
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  - 2022-now, Research Software Engineer at Netherlands eScience Center
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  - 2012-2015, MSc Computer science at VU University Amsterdam

Outline for the day

10:00	–	10:15	Welcome
10:15	–	10:45	Introduction to auto-tuning and Kernel Tuner
10:45	–	11:30	Integrating Kernel Tuner with your code and user-defined metrics
11:30	–	11:45	Break
11:45	–	12:15	GPU optimizations and the search space
12:15	–	12:45	Performance portable applications and search strategies
12:45	–	13:00	Q&A

Administrative announcements

- We will have **four sessions** in which we start with introducing some new concepts and follow with a hands-on exercise
- The **hands-on exercises** include example kernels, but you are also welcome to experiment with your own code
- We will use **JupyterHub** hosted by the VSC for the hands-on, so you **don't** need to have a GPU or install anything locally
- You can download the slides here:
  - https://github.com/KernelTuner/kernel_tuner_tutorial/tree/master/slides/2024_VSC_ESiWACE3

Learning objectives

- Familiarize with the concept of auto-tuning
- Get to know the fundamentals of Kernel Tuner
- Tune the CUDA block dimensions
- Specify user-defined metrics and verify the output of tuned kernels
- Explore the interplay between code optimizations and auto-tuning
- Speed up tuning with search-space restrictions and optimization algorithms
- Integrate the tuning results into your application

Introduction to Auto-Tuning and Kernel Tuner

Auto-tuning GPU applications

To maximize GPU code performance, you need to find the **best combination** of:

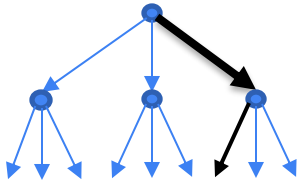
- Different mappings of the problem to threads and thread blocks
- Different data layouts in different memories (shared, constant, …)
- Different ways of exploiting special hardware features
- Thread block dimensions
- Work per thread in each dimension
- Loop unrolling factors
- Overlapping computation and communication
- …

Problem:

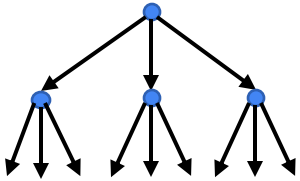
- Creates a very large **design space**

Manual optimization versus auto-tuning

- Optimizing code manually, you iteratively perform:
  - Modify the code
  - Run a few benchmarks
  - Revert or accept the change

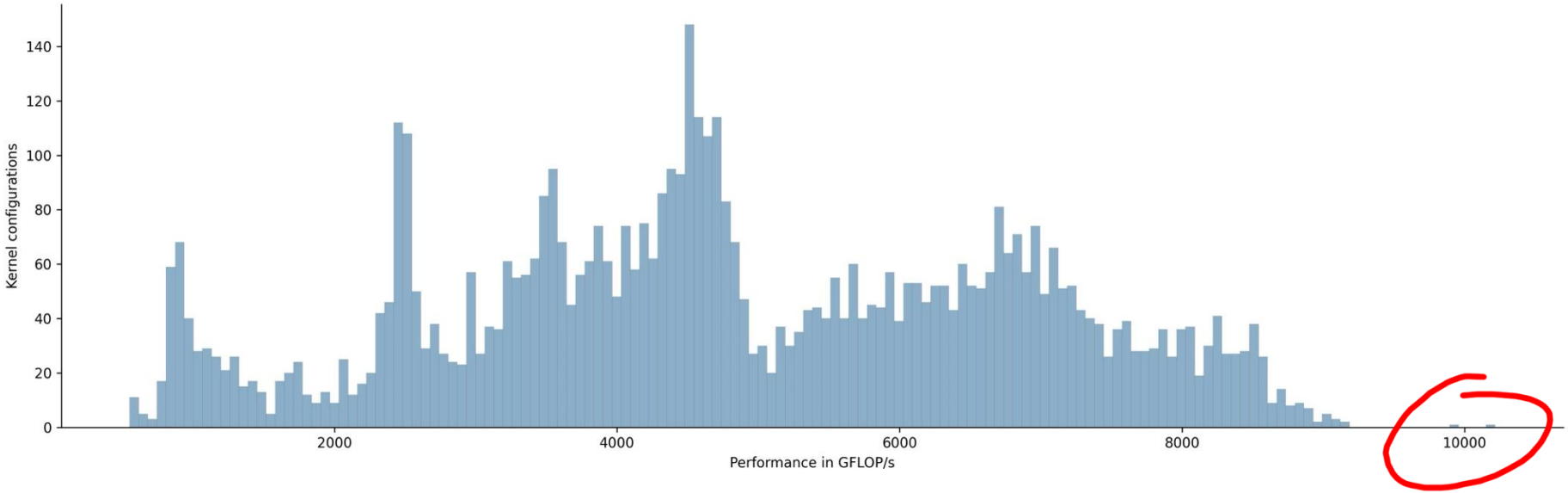


- With auto-tuning you:
  - Write a templated version of your code or a code generator
  - Benchmark the performance of all code variants

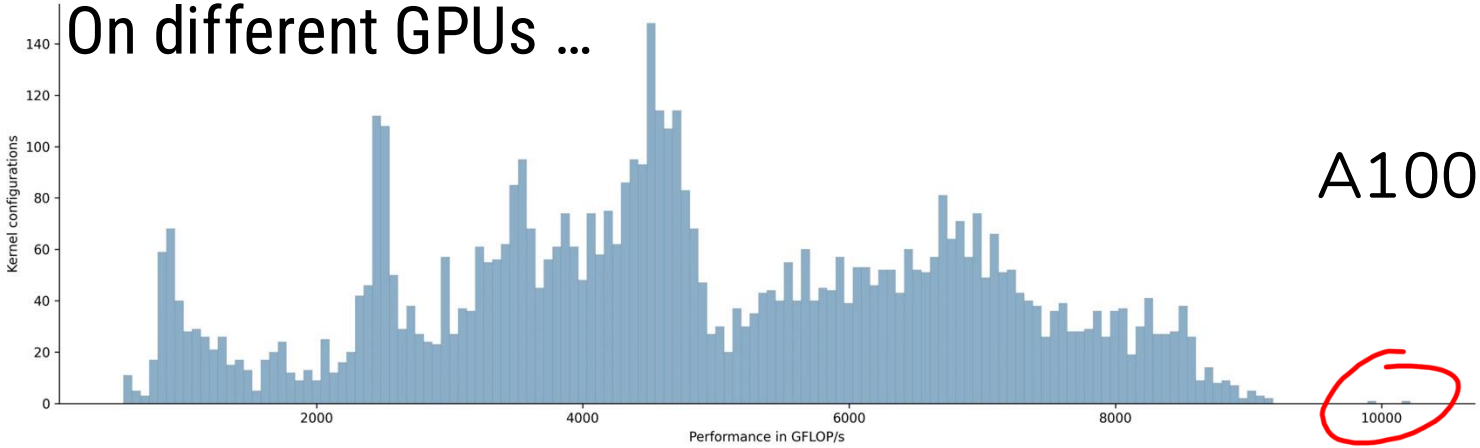


Large search space of kernel configurations

Auto-tuning a Convolution kernel on Nvidia A100



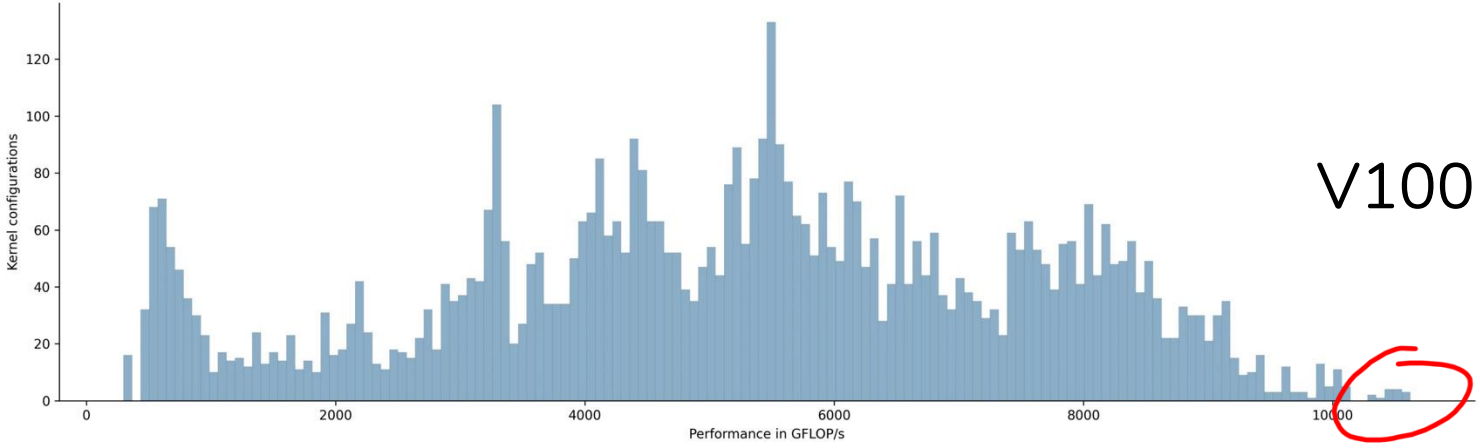
On different GPUs …



A100

top 5% on A100

8,16,2,2,1,0
8,32,2,1,1,0



V100

top 5% on V100

4,32,5,1,1,0
4,32,5,1,1,1
32,4,1,4,0,0
32,4,1,4,0,1
32,4,1,4,1,0
32,4,1,4,1,1
64,2,1,4,0,0
64,2,1,4,1,0
64,4,1,4,0,0
64,4,1,4,0,1
64,4,1,4,1,0
64,4,1,4,1,1
128,2,1,8,0,0
128,2,1,8,1,0

Kernel Tuner

A tool for automatic performance tuning of GPU kernels

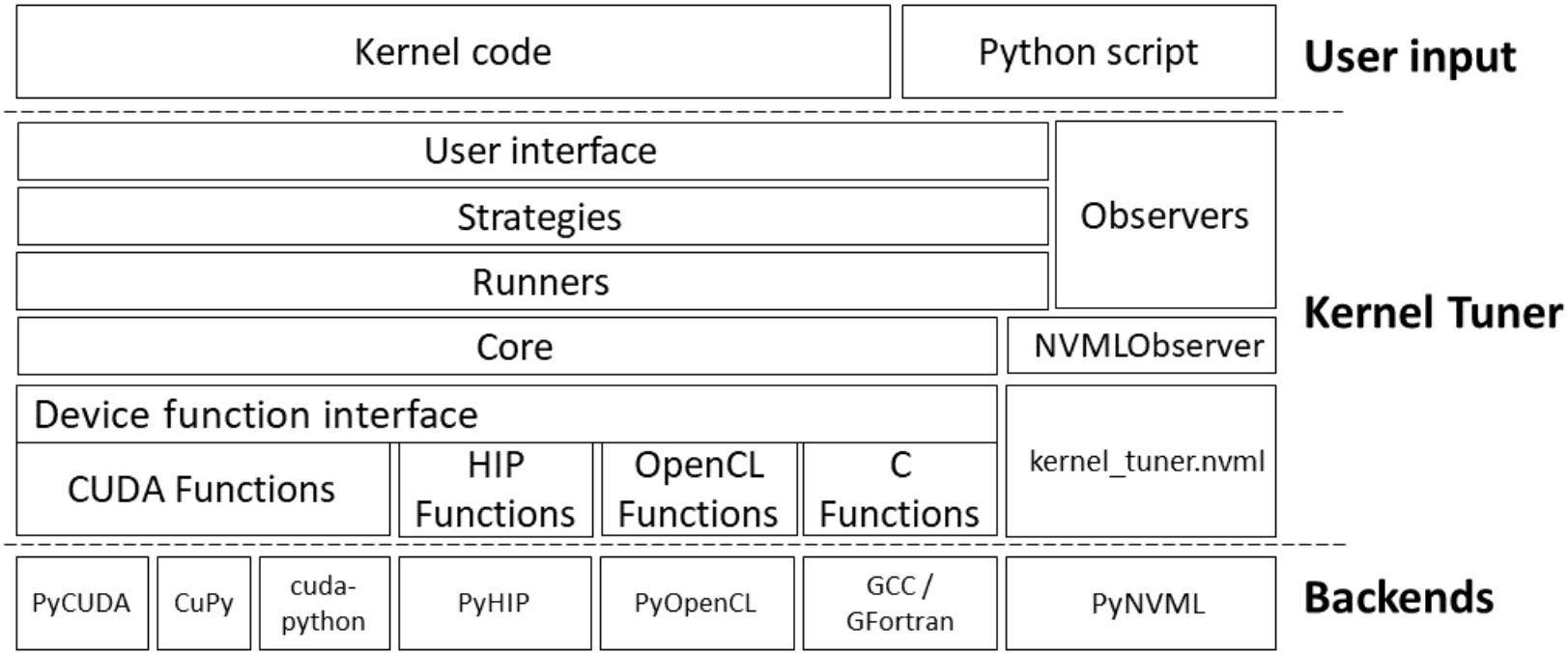
- Developed open source (Apache 2.0)
- Funded by several national (NL) and European projects
- Used by 10+ eScience center projects, and 10+ other universities & organizations
- Supports:
  - CUDA, HIP, OpenCL, C, Fortran, OpenACC
  - 20+ search optimization algorithms
  - Energy measurement of GPU kernels
  - Many different use cases

netherlands eScience center · CWI · ASTRON · Universiteit Leiden The Netherlands

https://github.com/KernelTuner/kernel_tuner

- Kernel Tuner is:
  - **Empirical**
    - optimization methods may use models internally
  - **Compile-time**
    - or preferably even development-time
  - **Software-based**
  - Easy to **integrate** into existing applications
  - Capable of tuning **discrete** parameters in kernel code

Kernel Tuner architecture



Minimal example

```
import numpy
from kernel_tuner import tune_kernel

kernel_string = """
__global__ void vector_add(float *c, float *a, float *b, int n) {
    int i = blockIdx.x * block_size_x + threadIdx.x;
    if (i<n) {
        c[i] = a[i] + b[i];
    }
}"""

n = numpy.int32(1e7)
a = numpy.random.randn(n).astype(numpy.float32)
b = numpy.random.randn(n).astype(numpy.float32)
c = numpy.zeros_like(b)
args = [c, a, b, n]
tune_params = {"block_size_x": [32, 64, 128, 256, 512]}

tune_kernel("vector_add", kernel_string, n, args, tune_params)
```

What Kernel Tuner does

- Creates the search space:
  - Computed as the **Cartesian product** of all values of all tunable parameters
- For each selected configuration:
  - Insert preprocessor definitions for each tuning parameter
  - Compile the kernel created for this instance
  - Benchmark the kernel
  - Store the averaged execution time
- Return the full data set

Installation on your system

- Prerequisites:
  - Python 3.9 or newer
  - CUDA or OpenCL device with necessary drivers and compilers installed
  - PyCUDA, PyOpenCL, or CuPy installed
- To install Kernel Tuner:
  - pip install kernel_tuner
- For more information:
  - https://kerneltuner.github.io/kernel_tuner/stable/install.html
- **Note**: this is not required for the hands-on exercises

First hands-on

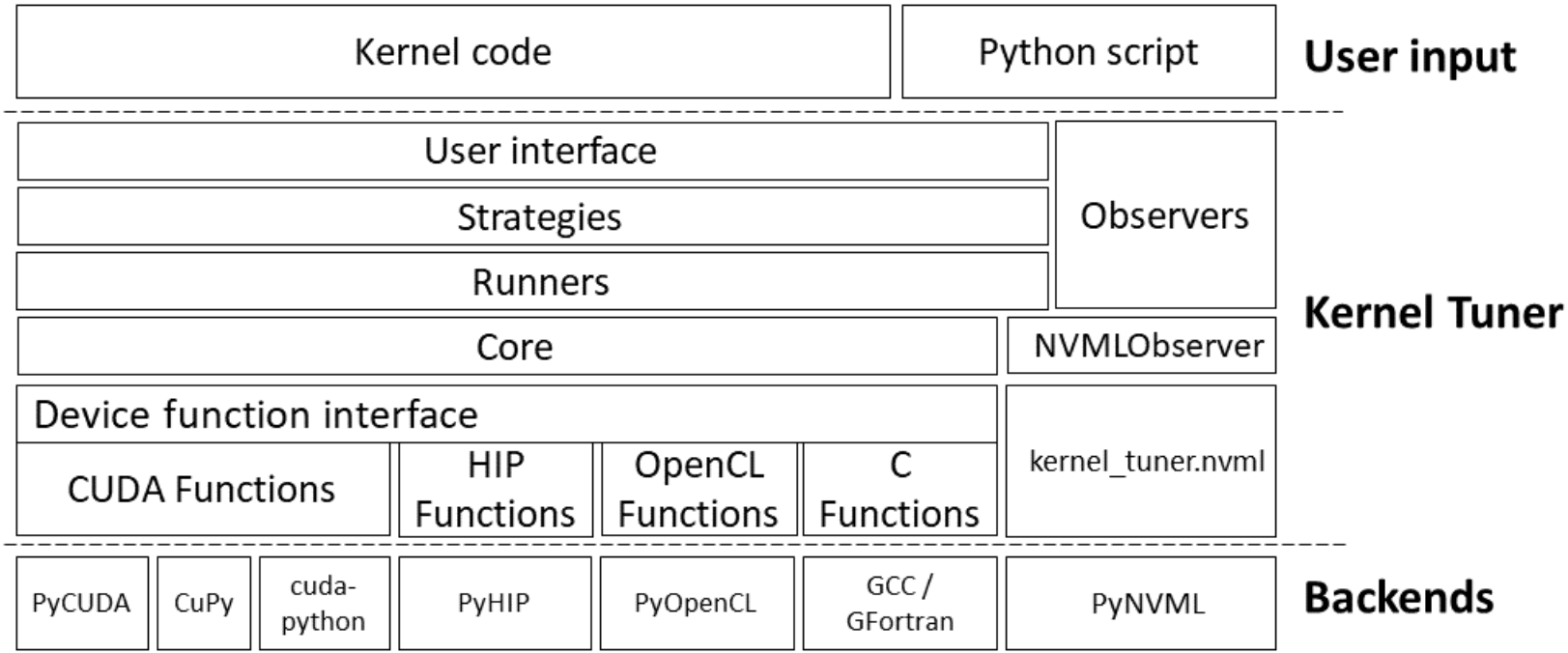
First hands-on

- The first hands-on notebook is:
  - https://github.com/KernelTuner/kernel_tuner_tutorial/blob/master/hands-on/esiwace3/00_Kernel_Tuner_Introduction.ipynb

- The goal of this hands-on is to familiarize with how to use Kernel Tuner
- Please follow the instructions in the Notebook
- Feel free to ask questions to instructors and mentors

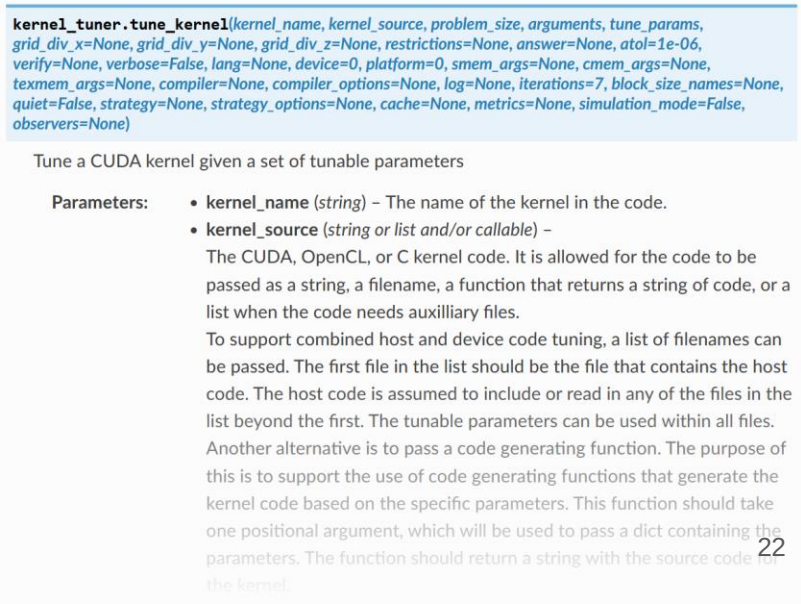
Integrating Kernel Tuner with your Code and User-Defined Metrics

Kernel Tuner architecture



Kernel Tuner compiles and benchmarks many kernel configurations

- We need to tell Kernel Tuner everything needed to **compile** and **run** our kernel, including source code and compiler options
  - This is easier if your kernel code can be compiled separately, so without including many other files
- Kernel Tuner is written in Python, so we need to load/create the input/output data in Python



kernel_tuner.tune_kernel(*kernel_name, kernel_source, problem_size, arguments, tune_params, grid_div_x=None, grid_div_y=None, grid_div_z=None, restrictions=None, answer=None, atol=1e-06, verify=None, verbose=False, lang=None, device=0, platform=0, smem_args=None, cmem_args=None, texmem_args=None, compiler=None, compiler_options=None, log=None, iterations=7, block_size_names=None, quiet=False, strategy=None, strategy_options=None, cache=None, metrics=None, simulation_mode=False, observers=None*)

Tune a CUDA kernel given a set of tunable parameters

Parameters:
- **kernel_name** (*string*) – The name of the kernel in the code.
- **kernel_source** (*string or list and/or callable*) –

The CUDA, OpenCL, or C kernel code. It is allowed for the code to be passed as a string, a filename, a function that returns a string of code, or a list when the code needs auxilliary files.

To support combined host and device code tuning, a list of filenames can be passed. The first file in the list should be the file that contains the host code. The host code is assumed to include or read in any of the files in the list beyond the first. The tunable parameters can be used within all files.

Another alternative is to pass a code generating function. The purpose of this is to support the use of code generating functions that generate the kernel code based on the specific parameters. This function should take one positional argument, which will be used to pass a dict containing the parameters. The function should return a string with the source code for the kernel.

Specifying Kernel source code

- The 2nd positional argument of `tune_kernel()` is `kernel_source`
- `kernel_source` can be a string with the **code**, a **filename**, or a **function**
  - The function option is useful for code generators or when using a templating engine such as jinja
- Kernel Tuner automatically detects the programming language and selects a backend
  - Defaults are PyCUDA for CUDA and PyOpenCL for OpenCL
  - To select a different backend use the lang option, e.g. `lang="CuPy"` to select the CuPy backend

Kernel compilation

- Kernel Tuner will compile the same kernel with different parameters inserted
- If your code includes many headers with all kinds of template expansions the compilation time may become prohibitive
- Recommendation: isolate device code from the rest of your application
  - Easy trick is to put kernel code in separate source files and include these in the host code where needed

Kernel arguments

Kernel Tuner allocates GPU memory and moves data in and out of the GPU for you

Kernel Tuner supports the following types for kernel arguments:

- NumPy scalars (`np.int32`, `np.float32`, …)
- NumPy ndarrays
- CuPy arrays
- Torch tensors

Kernel argument types

While NumPy arrays can be of mixed types to mimic more complex types, these can be difficult to reconstruct correctly in Python.

It may be difficult (although still possible) to use Kernel Tuner on kernels with custom types for **input** arrays instead of simple arrays of primitive types.

A general performance recommendation for GPU programming is to use **not use arrays of structs** whenever you can.

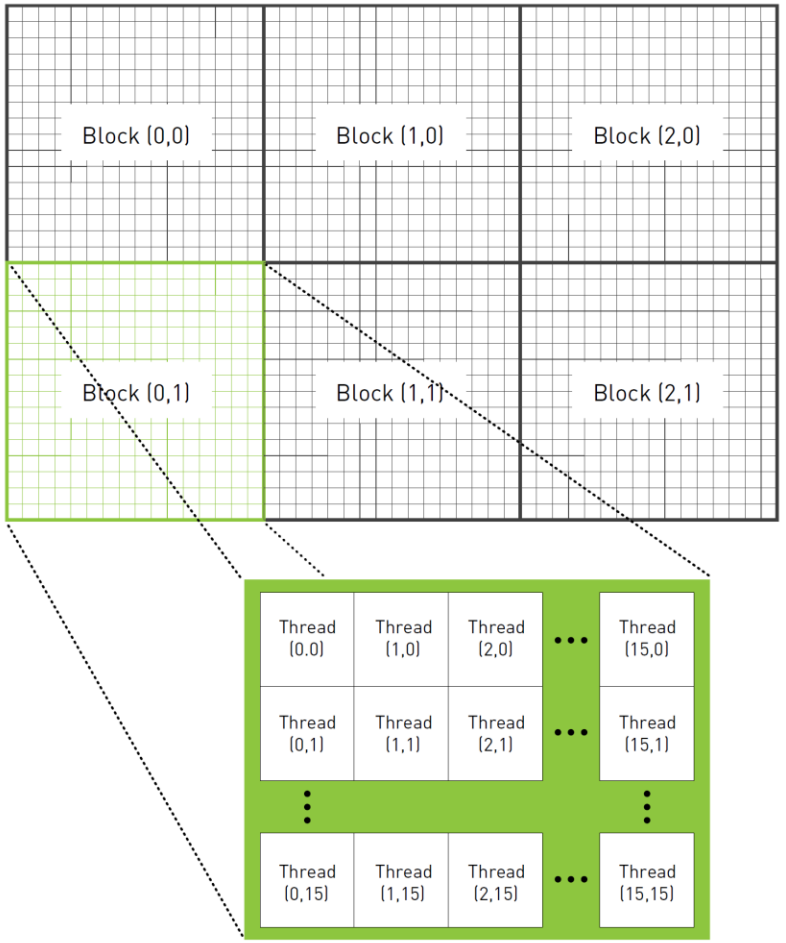
Summary

- For compiling CUDA kernels, Kernel Tuner uses either **PyCUDA** or **CuPy**
  - **PyCUDA** forces kernels to have `extern "C"` linkage
    - Limited support for templates by on-the-fly wrapper generation by Kernel Tuner
  - **CuPy** fully supports C++ and templates, but no host code is allowed
- General recommendations:
  - Use simple types for kernel arguments
  - Isolate device code from host code to simplify separate compilation
  - Using arrays of structs is not recommended

Grid and Thread block dimensions

CUDA Thread Hierarchy

- Launching a kernel starts many **threads** in parallel on the GPU
- Threads are grouped into fixed-sized 1D/2D/3D **thread blocks**
- Thread blocks are arranged in a 1D/2D/3D **grid**

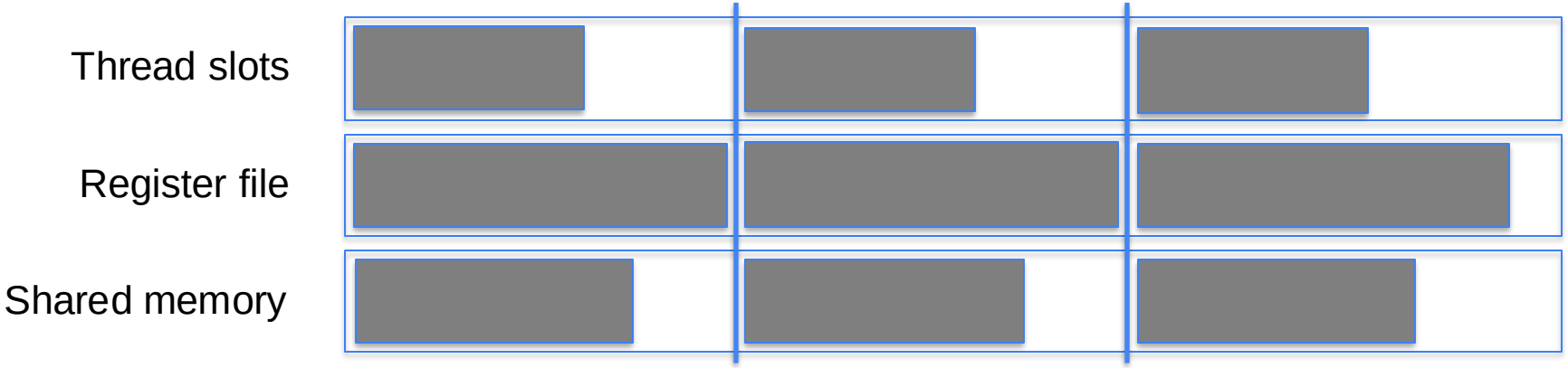


Choosing thread block dimensions

- Almost all GPU kernels can be written to allow for **varying thread block dimensions**
- Usually, changing thread block dimensions affects **performance**, but not the result
- The question is: how to determine the **optimal setting**?

Why do thread block dimensions matter so much?

- The GPU consists of several (1 to 80) *streaming multiprocessors* (SMs)
- The SMs are fully independent and contain several resources:
  - Register file, Shared memory, Thread Slots, and Thread Block slots
- SM resources are dynamically partitioned among the thread blocks that execute concurrently on the SM, resulting in a certain *occupancy*



Specifying thread block dimensions to tune_kernel

- In Kernel Tuner, you specify the possible values for thread block dimensions of your kernel using special tunable parameters:
  - `block_size_x, block_size_y, block_size_z`
- For each, you may pass a list of values this parameter can take:
  - `params["block_size_x"] = [32, 64, 128, 256]`

- You can use different names for these by passing the `block_size_names` option using a list of strings
- Note: when you change the thread block dimensions, the number of thread blocks used to launch the kernel generally changes as well

Specify thread block dimensions at compile-time

- Kernel Tuner automatically inserts a block of `#define` statements to set values for `block_size_x, block_size_y, and block_size_z`
- You can use these values in your code to access the thread block dimensions as compile-time constants
- This is generally a good idea for performance, because
  - Loop conditions may use the thread block dimensions, fixing the number of iterations at compile-time allows the compiler to optimize the code by unrolling the loop
  - Shared memory declarations can use the thread block dimensions, e.g. for compile-time sizes multi-dimensional data

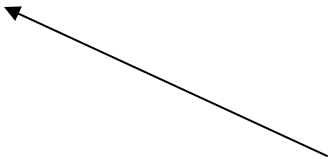
Vector add example

```
import numpy
from kernel_tuner import tune_kernel

kernel_string = """
__global__ void vector_add(float *c, float *a, float *b, int n) {
    int i = blockIdx.x * block_size_x + threadIdx.x;
    if (i<n) {
        c[i] = a[i] + b[i];
    }
}"""

n = numpy.int32(1e7)
a = numpy.random.randn(n).astype(numpy.float32)
b = numpy.random.randn(n).astype(numpy.float32)
c = numpy.zeros_like(b)
args = [c, a, b, n]
tune_params = {"block_size_x": [32, 64, 128, 256, 512]}

tune_kernel("vector_add", kernel_string, n, args, tune_params)
```



Notice how we can use **`block_size_x`** in our **`vector_add`** kernel code, while it is not defined (yet)

Vector add example

```
import numpy
from kernel_tuner import tune_kernel

kernel_string = """
__global__ void vector_add(float *c, float *a, float *b, int n) {
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c = numpy.zeros_like(b)
args = [c, a, b, n]
tune_params = {"block_size_x": [32, 64, 128, 256, 512]}

tune_kernel("vector_add", kernel_string, n, args, tune_params)
```
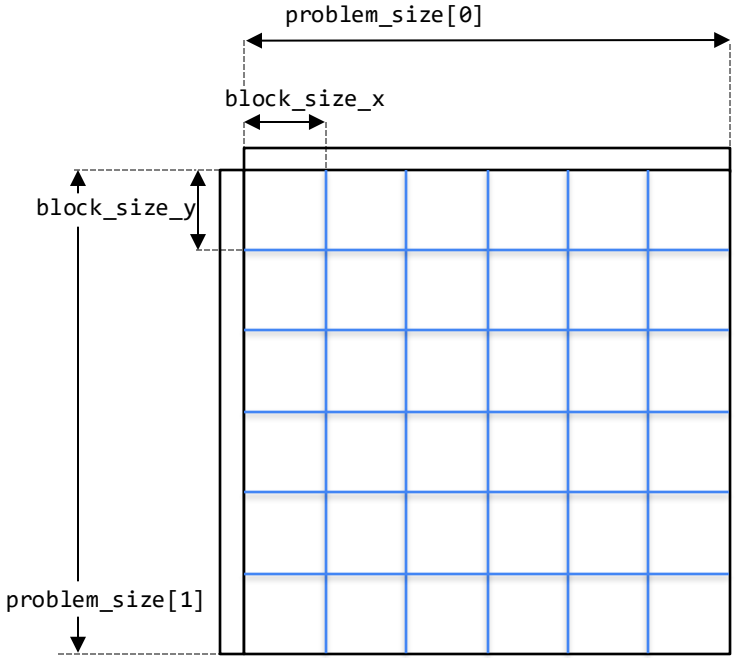

n is the number of elements in our array, the number of thread blocks depends on both **n** and **block_size_x**

Specifying grid dimensions

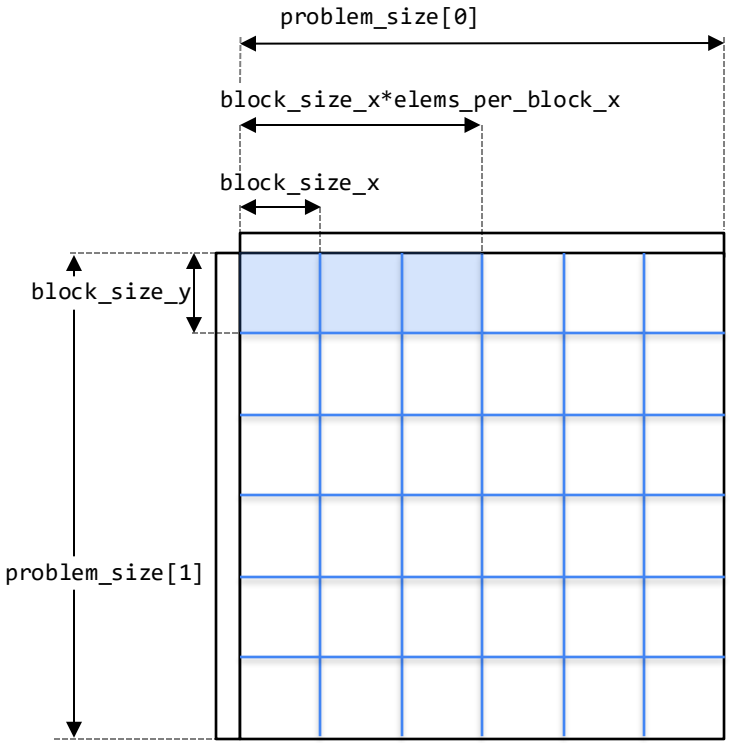
- You specify the `problem_size`
- `problem_size` describes the dimensions across which threads are created
- By default, the grid dimensions are computed as:
  - `grid_size_x = ceil(problem_size_x / block_size_x)`



Grid divisor lists

- Other parameters, or none at all, may also affect the grid dimensions
- **Grid divisor lists** control how `problem_size` is divided to compute the grid size
- Use the optional arguments:
  - `grid_div_x, grid_div_y, and grid_div_z`

- You may disable this feature by explicitly passing empty lists as grid divisors, in which case `problem_size` directly sets the grid dimensions



problem_size

- The problem size is usually a single integer or a tuple of integers
- But you may also use strings to use a tunable parameter
- `problem_size` may also be a (lambda) function that takes a dictionary of tunable parameters and returns a tuple of integers
- For example `reduction.py`:

```
size = 800000000
tune_params["block_size_x"] = [32, 64, 128, 256, 512, 1024]
tune_params["num_blocks"] = [32, 64, 128, 256, 512, 1024, 2048, 4096, 8192, 16384, 32768]
problem_size = "num_blocks"
grid_div_x = []
```

User-defined metrics

Metrics

- Kernel Tuner measures and reports time during tuning in milliseconds (ms)
  - This is the averaged time of (by default) 7 iterations, you can change the number of iterations using the `iterations` optional argument
  - Actually, all individual execution times will be returned by `tune_kernel`, but only the average is printed to screen
- You may want to use a metric different from time to compare kernel configurations

User-defined metrics

- Are composable, and therefore the order matters, so they are passed using a Python `dict`
- The `key` is the name of the metric, and the `value` is a function that computes it
- For example:

```
metrics = dict()
metrics["time_s"] = lambda p : (p["time"] / 1000)
```

Second hands-on

Second hands-on

- The second hands-on notebook is:
  - https://github.com/KernelTuner/kernel_tuner_tutorial/blob/master/hands-on/esiwace3/01_Kernel_Tuner_Basic.ipynb

- The goal of this hands-on is to experiment with tunable grid dimensions and user defined metrics

- Please follow the instructions in the Notebook

- Feel free to ask questions to instructors and mentors

GPU Optimizations and the Search Space

GPU code optimizations

- Modify the kernel code in an attempt to improve performance or tunability
- Effects on performance can be **different** on **different GPUs** or **different input data**
- You can tune
  - enabling or disabling an optimization
  - the parameters introduced by certain optimizations
- You often need to **combine** multiple different optimizations with specific tunable parameter values to arrive at **optimal performance**

Overview of GPU Optimizations

- Coalescing memory accesses
- Host/device communication
- Kernel fusion
- Loop blocking
- Loop unrolling
- Prefetching
- Recomputing values
- Reducing atomics
- Reducing branch divergence
- Reducing redundant work
- Reducing register usage
- Reformatting input data
- Using a specific memory space
- Using warp shuffle instructions
- Varying work per thread
- Vectorization

Overview of GPU Optimizations

- Coalescing memory accesses
- Host/device communication
- Kernel fusion
- Loop blocking
- **Loop unrolling**
- Prefetching
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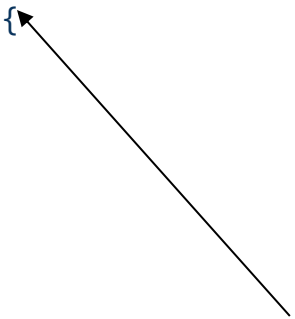
- Reducing atomics
- Reducing branch divergence
- Reducing redundant work
- **Reducing register usage**
- Reformatting input data
- Using a specific memory space
- Using warp shuffle instructions
- **Varying work per thread**
- **Vectorization**

(Partial) Loop Unrolling

- Why?
  - Increases instruction-level-parallelism
  - Reduces loop overhead instructions
- How?
  - In the early days, only manually or with a code generator
  - Compiler does this now: `#pragma unroll <value>`
  - In CUDA, value has to be integer constant expression
    - 0 is not allowed, 1 means unrolling is disabled
  - Remember, Kernel Tuner inserts parameters with `#define`
  - Parameters that start with `loop_unroll_factor_` are inserted as integer constant expressions instead, on 0 KT removes line with pragma

Partial loop unrolling

```
...

#pragma unroll loop_unroll_factor_k
for (int k=0; k<n; k++) {
    ...
}
```



The compiler can unroll this loop if `n` is known at compile-time. The `loop_unroll_factor_k` parameter should be a divisor of the loop counter `n`

Reducing register usage

- Why?
  - Registers are an important and limited SM resource and are likely to limit occupancy
  - Allows to increase the tunable range of thread block dimensions
- How?
  - Compiling constant values into your code rather than keeping them in registers (e.g. using templates or tunable parameters)
  - Limiting or disabling loop unrolling are very effective ways of reducing register usage
  - In kernels that do many different things, splitting the kernel may reduce register usage
  - Tell the compiler the thread block dimensions using `__launch_bounds__`

Reducing register usage

```
__global__ void
some_kernel(...)
{
    ...
}
```

```
__global__ void
__launch_bounds__(
   block_size_x * block_size_y * block_size_z,
                  blocks_per_sm
)
some_kernel(...)
{
    ...
}
```

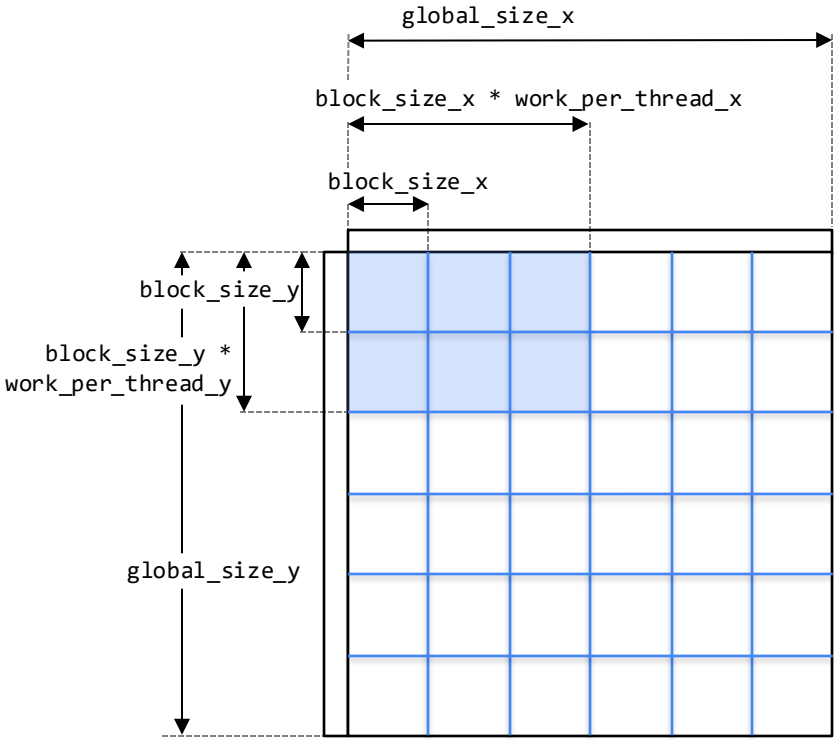
Varying work per thread

- Why?
  - Increasing **work per thread** often increases **data reuse** and **locality**
  - Reduces **redundant instructions** previously executed by other threads
  - Increases **instruction-level parallelism** (ILP), but also increases **register usage**
- How?
  - Reduce number of threads blocks in total, but increase the work per thread block
  - Bring down number of threads within the block, but keep the amount of work equal

Varying work per thread

```
...
#pragma unroll
for (kb = 0; kb < block_size_x; kb++) {

    sum += sA[ty][kb] * sB[kb][tx];

}
```

```
...
#pragma unroll
for (kb = 0; kb < block_size_x; kb++) {

    #pragma unroll
    for (int j = 0; j < work_per_thread_x; j++) {
        sum[j] += sA[ty][kb] * sB[kb][tx + j * block_size_x];
    }

}
```



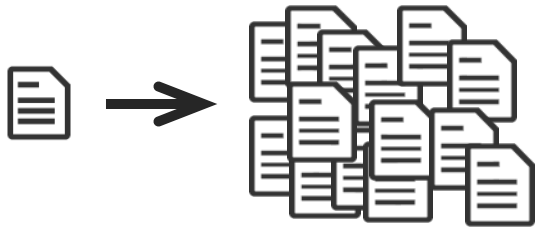
Vectorization

- Why?
  - Reduces the instructions needed to fetch data from global memory
  - Improves memory throughput
  - Often also increases work per thread and instruction-level parallelism
  - May increase register usage
- How?
  - Using wider data types (e.g. `float2` or `float4` instead of `float`)
  - Vector length can be tuned

Output verification

Programming tunable applications

- When working with tunable code you are essentially maintaining **many different versions** of the same program in a single source
- It may happen that certain combinations of tunable parameters lead to versions that produce **incorrect results**
- Kernel Tuner can **verify** the output of kernels while tuning!



Output verification

- When you pass a reference `answer` to `tune_kernel`:
  - Kernel Tuner will run the kernel once before benchmarking and compare the kernel output against the reference `answer`
  - The `answer` is a list that matches the kernel arguments in number, shape, and type
  - By default, Kernel Tuner will use `np.allclose()` with an absolute tolerance of `1e-6` to compare the state of all kernel arguments in GPU memory
  - The `answer` may contain `None` for kernel arguments that don't need verification
- And of course, you can modify this behavior, but first a simple example

Simple answer example

```
args = [c, a, b, n]
answer = [a+b, None, None, None]

tune_kernel("vector_add", kernel_string, size, args, tune_params,
            answer=answer, atol=1e-3)
```

Search space restrictions

Restricting the search

- By default, the search space is the **Cartesian product** of all possible combinations of tunable parameter values

- However, for some tunable kernels:
  - there are tunable parameters that depend on each other
  - only certain combinations of tunable parameter values are valid

Dependent parameters example

```
tune_params["block_size_x"] = [32, 64, 128, 256, 512]
tune_params["block_size_y"] = [1, 2, 3, 4, 5, 6, 7, 8]
tune_params["block_size_z"] = [1, 2, 3, 4, 5, 6, 7, 8]
```

- The parameters controls the block size: `block_size_{x, y, z}`
- But the total threads per block cannot exceed a maximum

- What if we only want configurations in which the number of threads per block does not exceed 512?

Dependent parameters example

```
tune_params["block_size_x"] = [32, 64, 128, 256, 512]
tune_params["block_size_y"] = [1, 2, 3, 4, 5, 6, 7, 8]
tune_params["block_size_z"] = [1, 2, 3, 4, 5, 6, 7, 8]

restrict = ["block_size_x * block_size_y * block_size_z <= 512"]

kernel_tuner.tune_kernel(..., restrictions=restrict, ...)
```

Caching tuning results

Caching

- Tuning **large search spaces** can take very long
- You might need to stop and continue later
- **Caching** is enabled by passing a filename to the `cache` option
- Kernel Tuner will append new results to the cache directly after benchmarking a kernel configuration
- Kernel Tuner detects existing (possibly incomplete) cache files and automatically resumes tuning where it had left off

Third hands-on

Third hands-on

- The third hands-on notebook is:
  - https://github.com/KernelTuner/kernel_tuner_tutorial/blob/master/hands-on/esiwace3/02_Kernel_Tuner_Intermediate.ipynb

- The goal of this hands-on is to experiment with search space restrictions, caching, and output verification

- Please follow the instructions in the Notebook
- Feel free to ask questions to instructors and mentors

Performance Portable Applications and Search Strategies

Performance portability

- The property that the same application has **similar performance** on **different hardware**
- Auto-tuning may be used to achieve performance portability, if an application has been tuned on different hardware and we select a kernel based on the hardware at hand
- Kernel configuration selection can be done compile-time or run-time, based on earlier obtained tuning results

store_results

- The `store_results` function can be used to store information about the best performing configurations of a tunable kernel

```
from kernel_tuner.integration import store_results

store_results("vector_add_results.json", "vector_add", "vector_add.cu",
              tune_params, size, results, env, top=3)
```

- Stores the (e.g.) top 3% of tuning results for the specified combination of `problem_size` and GPU (retrieved from `env`) to the JSON file
  - The new results are appended to the JSON file
  - Results for the same `problem_size` and GPU are updated

Compile-time kernel selection

- Performs kernel selection at compile time
- Main advantage:
  - Can be done with very limited changes to the host application
- Limitation:
  - Limited to only selecting kernels based on properties known at compile-time, e.g. the target GPU

Compile-time kernel selection example

```
from kernel_tuner.integration import store_results, create_device_targets

store_results("results.json", "vector_add", "vector_add.cu", tune_params, size, results, env)
create_device_targets("vector_add.h", "results.json")
```

vector_add.h

```
/* header file generated by Kernel Tuner, do not modify by hand */
#pragma once
#ifndef kernel_tuner /* only use these when not tuning */

#ifdef TARGET_A100_PCIE_40GB
#define block_size_x 672

#elif TARGET_RTX_A6000
#define block_size_x 160

#else /* default configuration */
#define block_size_x 352
#endif /* GPU TARGETS */

#endif /* kernel_tuner */
```

Compile-time kernel selection example

```
from kernel_tuner.integration import store_results, create_device_targets

store_results("results.json", "vector_add", "vector_add.cu", tune_params, size, results, env)
create_device_targets("vector_add.h", "results.json")
```

Kernel Tuner always inserts
`#define kernel_tuner`
When compiling kernels for benchmarking

vector_add.h

```
/* header file generated by Kernel Tuner, do not modify by hand */
#pragma once
#ifndef kernel_tuner /* only use these when not tuning */

#ifdef TARGET_A100_PCIE_40GB
#define block_size_x 672

#elif TARGET_RTX_A6000
#define block_size_x 160

#else /* default configuration */
#define block_size_x 352
#endif /* GPU TARGETS */

#endif /* kernel_tuner */
```

Compile-time kernel selection example

```
from kernel_tuner.integration import store_results, create_device_targets

store_results("results.json", "vector_add", "vector_add.cu", tune_params, size, results, env)
create_device_targets("vector_add.h", "results.json")
```

This `block_size_x` value showed best performance on the A100

vector_add.h

```
/* header file generated by Kernel Tuner, do not modify by hand */
#pragma once
#ifndef kernel_tuner /* only use these when not tuning */

#ifdef TARGET_A100_PCIE_40GB
#define block_size_x 672

#elif TARGET_RTX_A6000
#define block_size_x 160

#else /* default configuration */
#define block_size_x 352
#endif /* GPU TARGETS */

#endif /* kernel_tuner */
```

Compile-time kernel selection example

```
from kernel_tuner.integration import store_results, create_device_targets

store_results("results.json", "vector_add", "vector_add.cu", tune_params, size, results, env)
create_device_targets("vector_add.h", "results.json")
```

This `block_size_x` value showed best performance on the A6000

vector_add.h

```
/* header file generated by Kernel Tuner, do not modify by hand */
#pragma once
#ifndef kernel_tuner /* only use these when not tuning */

#ifdef TARGET_A100_PCIE_40GB
#define block_size_x 672

#elif TARGET_RTX_A6000
#define block_size_x 160

#else /* default configuration */
#define block_size_x 352
#endif /* GPU TARGETS */

#endif /* kernel_tuner */
```

Compile-time kernel selection example

```
from kernel_tuner.integration import store_results, create_device_targets

store_results("results.json", "vector_add", "vector_add.cu", tune_params, size, results, env)
create_device_targets("vector_add.h", "results.json")
```

This `block_size_x` value showed best performance overall, on all GPUs

vector_add.h

```
/* header file generated by Kernel Tuner, do not modify by hand */
#pragma once
#ifndef kernel_tuner /* only use these when not tuning */

#ifdef TARGET_A100_PCIE_40GB
#define block_size_x 672

#elif TARGET_RTX_A6000
#define block_size_x 160

#else /* default configuration */
#define block_size_x 352
#endif /* GPU TARGETS */

#endif /* kernel_tuner */
```

Compile-time kernel selection example

In vector_add.cu:

```
#include "vector_add.h"
```

In Makefile:

```
TARGET_GPU = `nvidia-smi --query-gpu="gpu_name" --format=csv,noheader | sed -E 's/[^[:alnum:]]+/_/g'`
CU_FLAGS = -DTARGET_${TARGET_GPU}

vector_add.o: vector_add.cu
	nvcc ${CU_FLAGS} -c $< -o $@
```

Typing ‘make’ will now use different `block_size_x` values on A100, A6000, and on other GPUs

Run-time kernel selection

- More flexible, allows also to select kernels based on data size or other properties
- Requires more significant modification of the host application
- Depends on the programming language of the host application

Run-time kernel selection in Python

```
In Python:
from kernel_tuner.integration import store_results

store_results("vector_add_results.json", "vector_add", "vector_add.cu", tune_params, size, results, env)
```

```
In the Python host application:

from kernel_tuner import kernelbuilder

# create a kernel using the stored results
vector_add = kernelbuilder.PythonKernel(kernel_name, kernel_string, n, args,
                                        results_file=test_results_file)

# call the kernel
vector_add(c, a, b, n)
```

Run-time kernel selection in C++

```
In Python:
from kernel_tuner.integration import store_results

store_results("vector_add_results.json", "vector_add", "vector_add.cu", tune_params, size, results, env)
```

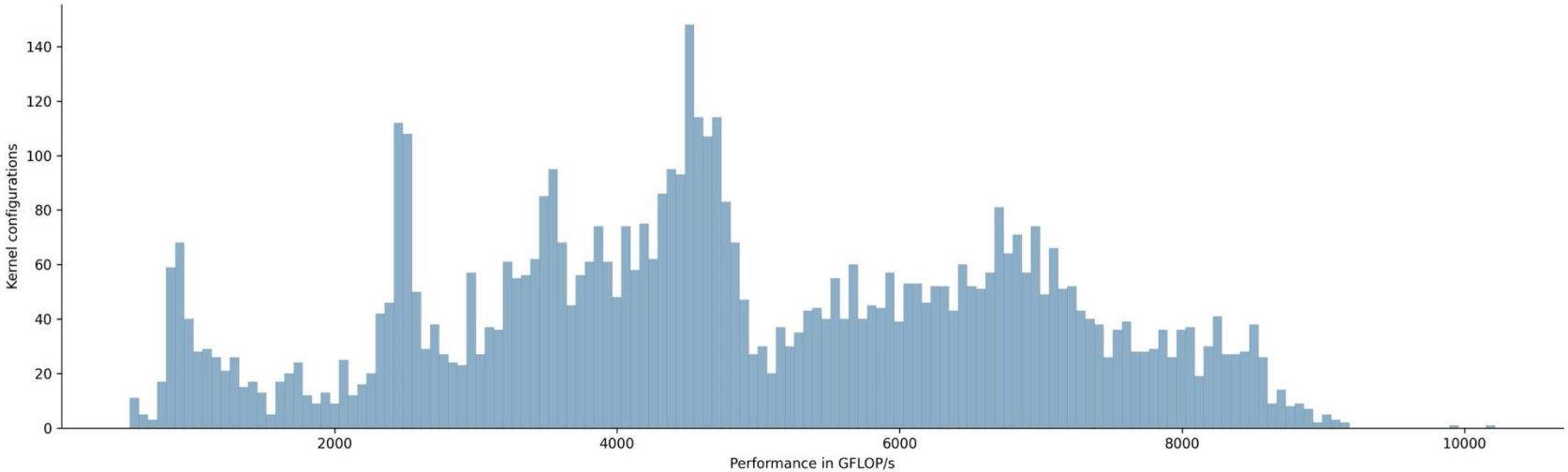
```
In vector_add.cpp:

#include "kernel_launcher.h"
using namespace kernel_launcher;


auto vector_add = CudaKernel<float*, float*, float*, int>::compile_best_for_current_device(
            "vector_add_results.json", 800000000, "vector_add.cu", {"-std=c++11"});

int grid_size = (n + vector_add.get_block_dim().x - 1) / vector_add.get_block_dim().x;

vector_add(grid_size)(dev_C, dev_A, dev_B, n);
```

Uses Kernel Launcher header-only C++ library: https://github.com/KernelTuner/kernel_launcher

Optimization strategies

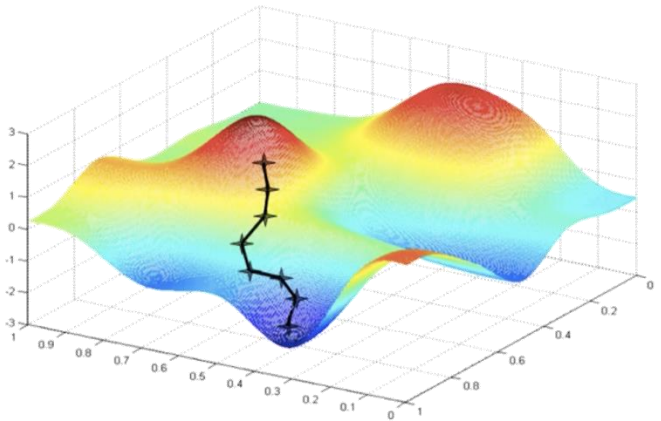
Large search space of kernel configurations

Auto-tuning a Convolution kernel on Nvidia A100

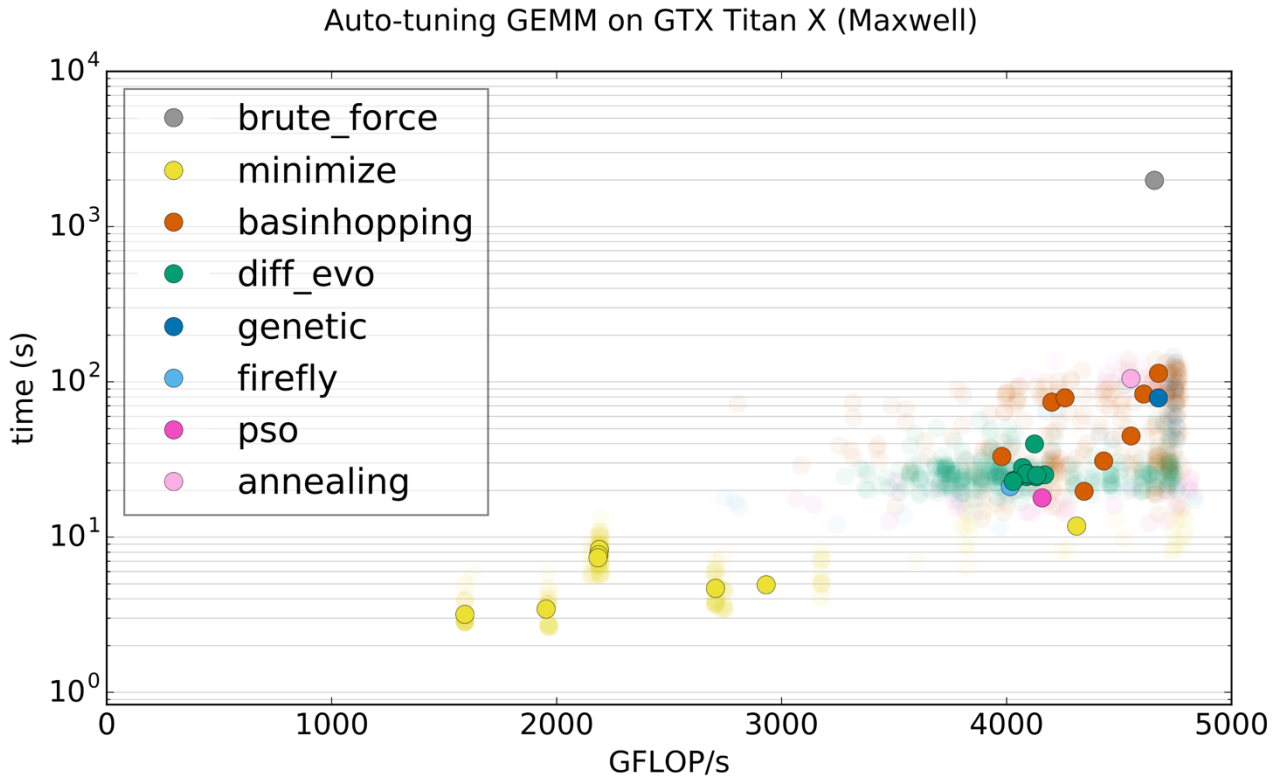


Optimization strategies in Kernel Tuner

- Local optimization
  - Nelder-Mead, Powell, CG, BFGS, L-BFGS-B, TNC, COBYLA, and SLSQP
- Global optimization
  - Basin Hopping
  - Simulated Annealing
  - Differential Evolution
  - Genetic Algorithm
  - Particle Swarm Optimization
  - Firefly Algorithm
  - Bayesian Optimization
  - Multi-start local search
  - …



Speeding up auto-tuning



Your mileage may vary

- Active topic of research
- Different optimizers seem to behave very differently for different combinations of **kernel + GPU + input**
- Nearly all methods are **stochastic**, meaning that they do not always return the global optimum or even the same result
- It is all a matter of how much time you have versus how strongly you want guarantees of finding an optimal configuration
- **Experiment**!

How to use a search strategy

- By passing `strategy="string_name"`, where `"string_name"` is any of:
  - `"brute_force"`: Brute force search
  - `"random_sample"`: random search
  - `"minimize"`: minimize using a local optimization method
  - `"basinhopping"`: basinhopping with a local optimization method
  - `"diff_evo"`: differential evolution
  - `"genetic_algorithm"`: genetic algorithm optimizer
  - `"mls"`: multi-start local search
  - `"pso"`: particle swarm optimization
  - `"simulated_annealing"`: simulated annealing optimizer
  - `"firefly_algorithm"`: firefly algorithm optimizer
  - `"bayes_opt"`: Bayesian Optimization
- Note that nearly all methods have specific options or hyperparameters that can be set using the `strategy_options` argument of `tune_kernel`

Observers

Observers introduction

- Observers allow to modify the behavior during benchmarking and measure quantities other than time
- Follows the ‘observer’ programming pattern, allowing an object to observe events
- Also used internally for measuring time in the various backends

Observer base class

```
class BenchmarkObserver(ABC):
    """Base class for Benchmark Observers"""

  def register_device(self, dev):
    """Sets self.dev, for inspection by the observer at various points during benchmarking"""
    self.dev = dev

  def before_start(self):
    """before start is called every iteration before the kernel starts"""
    pass

  def after_start(self):
    """after start is called every iteration directly after the kernel was launched"""
    pass

  def during(self):
    """during is called as often as possible while the kernel is running"""
    pass

  def after_finish(self):
    """after finish is called once every iteration after the kernel has finished execution"""
    pass

  @abstractmethod
  def get_results(self):
    """ get_results should return a dict with results that adds to the benchmarking data
    get_results is called only once per benchmarking of a single kernel configuration and
    generally returns averaged values over multiple iterations.
    """
    pass
```

NVMLObserver

- NVML is the NVIDIA Management Library for monitoring and managing GPUs
- Kernel Tuner's NVMLObserver supports the following observable quantities: `"power_readings", "nvml_power", "nvml_energy", "core_freq", "mem_freq", "temperature"`
- If you pass an NVMLObserver, you can also use the following special tunable parameters to benchmark GPU kernels under certain conditions: `nvml_pwr_limit, nvml_gr_clock, nvml_mem_clock`
- Requires NVML, nvidia-ml-py, and certain features may require root access

NVMLObserver example

```
...
tune_params["nvml_pwr_limit"] = [250, 225, 200, 175]

nvmlobserver = NVMLObserver(["nvml_energy", "temperature"])

metrics = OrderedDict()
metrics["GFLOPS/W"] = lambda p: (size/1e9) / p["nvml_energy"]

results, env = tune_kernel("vector_add", kernel_string, size, args,
                           tune_params, observers=[nvmlobserver],
                           metrics=metrics, iterations=32)
```

Fourth hands-on

Advanced hands-on

- The fourth hands-on notebook is:
  - https://github.com/KernelTuner/kernel_tuner_tutorial/blob/master/hands-on/esiwace3/03_Kernel_Tuner_Advanced.ipynb

- The goal of this hands-on is to experiment with search optimization strategies and custom observers

- Please follow the instructions in the Notebook
- Feel free to ask questions to instructors and mentors

Closing Remarks

Learning objectives

- Familiarize with the concept of auto-tuning
- Get to know the fundamentals of Kernel Tuner
- Tune the CUDA block dimensions
- Specify user-defined metrics and verify the output of tuned kernels
- Explore the interplay between code optimizations and auto-tuning
- Speedup tuning with search-space restrictions and optimization algorithms
- Integrate the tuning results into your application

Kernel Tuner – developed open source

- Kernel Tuner is developed as an open-source project
- GitHub repository:
  - https://github.com/KernelTuner/kernel_tuner
  - License: Apache 2.0

- If you use Kernel Tuner in a project, please cite the paper:
  - B. van Werkhoven, Kernel Tuner: A search-optimizing GPU code auto-tuner, *Future Generation Computer Systems*, 2019

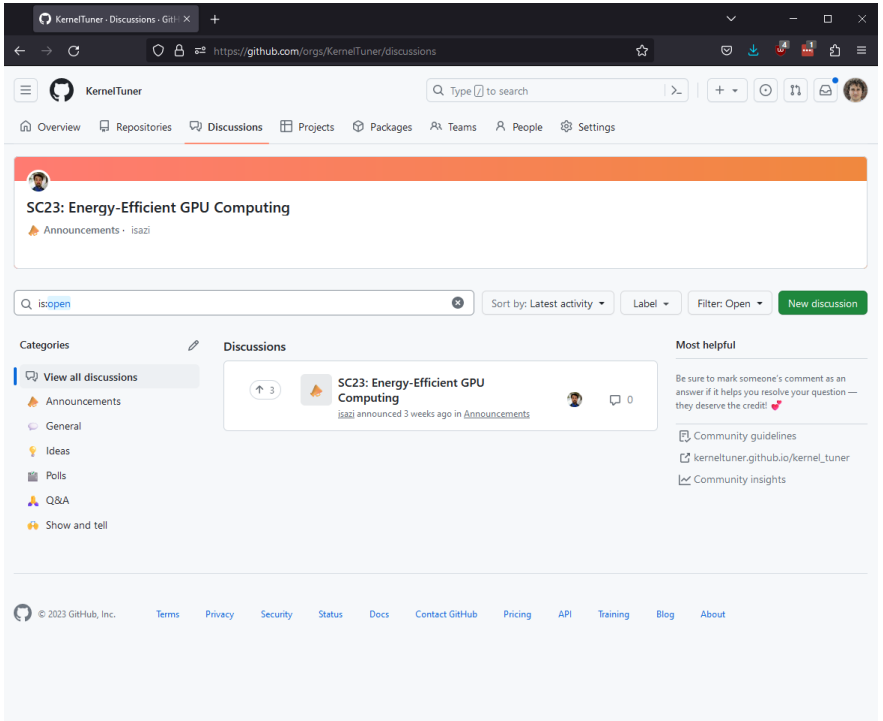
Contributions are welcome!

- Contributions can come in many forms: tweets, blog posts, issues, pull requests
- Before making larger changes, please create an issue to discuss

- For the full contribution guide, please see: https://kerneltuner.github.io/kernel_tuner/stable/contributing.html

Join the discussion!

- We have a discussion board on GitHub!



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