Masaryk University Faculty of Informatics



Framework for Parallel Kernels Auto-tuning

Master's Thesis

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Declaration

Hereby I declare that this paper is my original authorial work, which I have worked out on my own. All sources, references, and literature used or excerpted during elaboration of this work are properly cited and listed in complete reference to the due source.

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Abstract

The result of this thesis is a framework for auto-tuning of parallel kernels which are written in either OpenCL or CUDA language. The framework includes advanced functionality such as support for composite kernels and online auto-tuning. The thesis describes API and internal structure of the framework and presents several examples of its utilization for kernel optimization.

Keywords

auto-tuning, parallel programming, OpenCL, CUDA, kernel, optimization

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1 Introduction

In recent years, acceleration of complex computations using multi-core processors, graphics cards and other types of accelerators has become much more common. Currently, there are many devices developed by multiple vendors which differ in hardware architecture, performance and other attributes. In order to support application development for these devices, several software APIs (application programming interfaces) such as OpenCL (Open Computing Language) or CUDA (Compute Unified Device Architecture) were designed. Code written in these APIs can be run on various devices while producing the same result. However, there is a problem with portability of performance due to different hardware characteristics of these devices. For example, code which was optimized for a GPU may run poorly on a regular multi-core processor. The problem may also exist among different generations of devices developed by the same vendor, even if they have comparable parameters and theoretical performance.

A costly solution to this problem is to manually optimize code for each utilized device. This has several significant disadvantages such as a necessity to dedicate large amount of resources to write different versions of code and test which one performs best on a given device. Furthermore, new devices are released frequently and in order to efficiently utilize their capabilities, it is often necessary to rewrite old versions of code and repeat the optimization process again.

An alternative solution is a technique called auto-tuning where a system, which supports this technique, is capable of empirically optimizing its parameters in order to perform its task more efficiently. Auto-tuning is a general technique with broad range of applications, which include areas such as network protocols, compilers and database systems. This thesis focuses on a specific form of auto-tuning called code variant auto-tuning and its application on programs written in OpenCL and CUDA. In this version of auto-tuning, program code contains parameters which, depending on their value, affect performance of a computation on particular device. For example, there might be a parameter which controls length of a vector type of some variable. Optimal values of these parameters might differ for various devices based on their hardware capabilities. Parametrized code is then launched

repeatedly using different combinations of parameters in order to find the best configuration for a particular device empirically.

To make the code variant auto-tuning process easier to implement in previously mentioned APIs, several frameworks were created. However, large number of these are focused on domain-specific computations. There are some frameworks which are more general, but their features are limited and usually only support simpler usage scenarios. The aim of this thesis was to develop an auto-tuning framework which would support more complex use cases, such as situations where computation is split into several smaller functions. Additionally, the framework should be written in a way which would allow its easy integration into existing software and make it possible to perform online auto-tuning – combination of auto-tuning and regular computation.

Apart from introduction and conclusion, the thesis is split into five main chapters. Chapter two provides description of the compute APIs supported by the new framework. It also includes possible areas of auto-tuning utilization in these APIs. The third chapter serves as an introduction to auto-tuning, it presents several existing auto-tuning frameworks and compares their strengths and weaknesses.

The following two chapters are dedicated to KTT (Kernel Tuning Toolkit) framework, which was developed in this thesis. The former provides motivation for development of a new framework and focuses on describing its public API. The latter includes an overview of its internal structure. The sixth chapter presents several scenarios of the new framework utilization. The conclusion provides a summary of thesis results and lists several possible areas for future work.

2 Compute APIs and possibilities for auto-tuning

This chapter includes description of compute APIs which are utilized by KTT framework – OpenCL and CUDA. Because both APIs provide relatively similar functionality, only OpenCL is described here in greater detail. Section about CUDA is mostly focused on explaining features which differ from OpenCL. It is worth mentioning that CUDA actually consists of two different APIs – low-level driver API and high-level runtime API built on top of the driver API. This thesis includes description of the driver API only, because the runtime API lacks features which are necessary to implement auto-tuning in CUDA.

The final section of this chapter provides examples of auto-tuning opportunities in these APIs.

2.1 OpenCL

OpenCL is an API for developing primarily parallel applications which can be executed on a range of different devices such as CPUs, GPUs and certain types of accelerators such as Intel MIC (Many Integrated Core) devices or FPGAs (field-programmable gate arrays). It is developed by Khronos Group, which is a consortium of several independent companies. OpenCL is therefore designed to support hardware devices from multiple vendors. An OpenCL application consists of two main parts. First part is a host program, which is typically executed on a CPU and is responsible for OpenCL device configuration, memory management and launching of kernels. Second part is a kernel, which is a function executed on an OpenCL device and usually contains computationally intensive part of a program. Kernels are written in OpenCL C which is based on C programming language.

2.1.1 Host program in OpenCL

Host program is written in a standard programming language, for example C or C++. It can handle regular inexpensive tasks such as data preparation, input processing, network communication and others. In relation to OpenCL, its objectives include configuration of kernels,

their launch, synchronization and retrieval of results. OpenCL API defines several important structures which can be utilized to fulfill this goal:

- *cl_platform* References an OpenCL platform. Platforms represent an implementation of OpenCL standard by a specific vendor (e.g., AMD, Intel, Nvidia).
- *cl_device* References an OpenCL device (e.g., Intel Core i5-4690, Nvidia GeForce GTX 970). Devices are usually tied to a single platform, they are used for executing kernels.
- cl_context Serves as a holder of resources, similar in functionality to an operating system process. Majority of other OpenCL structures have to be tied to a specific context. Context is created for one or more OpenCL devices.
- cl_command_queue All commands which are executed directly on an OpenCL device have to be submitted to a command queue. It is possible to initialize multiple command queues within a single context in order to overlap independent operations.
- cl_mem Data which is directly accessed by a kernel has to be bound to an OpenCL buffer, which is referenced by a cl_mem variable. This includes both scalar and vector arguments. It is possible to specify buffer memory location (device or host memory) and access type (read-only, read-write, write-only).
- *cl_program* A variable which references an OpenCL device program compiled from an OpenCL C source file. Program can be shared by multiple kernel objects.
- cl_kernel An object used to reference a specific kernel. Holds information about OpenCL program, kernel function name (single program can contain definitions of multiple kernel functions) and buffers which are utilized by a kernel.
- *cl_event* Serves as a synchronization primitive for individual commands submitted to an OpenCL device. It can be used to

retrieve information about the corresponding command, such as status or execution duration.

Execution of an OpenCL application then typically consists of the following main steps:

- selection of platform and device
- initialization of OpenCL context and one or more command queues
- initialization of OpenCL buffers (either in host or dedicated device memory)
- compilation and execution of kernel function
- retrieval of data produced by kernel from OpenCL buffers into host memory (if data is located in dedicated device memory)

2.1.2 Kernel in OpenCL

Code in a kernel source file is written from a perspective of single work-item, which is the smallest OpenCL execution unit. Each work-item has its own *private memory* (memory which is mapped to e.g., CPU or GPU register).

Work-items are organized into a larger structure called *work-group*, from which they all have access to *local memory* (e.g., GPU shared memory). Work-group is executed on a single *compute unit* (e.g., CPU core, GPU streaming multiprocessor). It is possible for multiple work-groups to be executed on the same compute unit. OpenCL work-group can have up to three dimensions. Number and size of dimensions affect work-item indexing within a work-group.

Individual work-groups are organized into *NDRange* (N-Dimensional Range). At NDRange level, it is possible to address two types of memory – *global memory* and *constant memory*. Global memory (e.g., CPU main memory, GPU global memory) is usually very large but has high latency. On the other hand, constant memory generally has a small capacity but lower latency. It can be utilized to store read-only data. Certain devices such as CPUs do not have hardware support for constant memory and usually store variables marked with constant

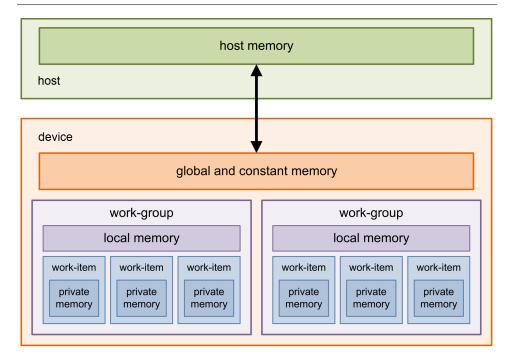


Figure 2.1: OpenCL memory hierarchy, source: [15].

memory keyword in global memory. Organization and indexing of work-groups inside an NDRange works in the same way as for work-items within a work-group. The entire hierarchy is illustrated in Figure 2.1.

Hierarchical organization into NDRange, work-groups and work-items allows for more flexible mapping of computation tasks onto heterogeneous hardware devices, which can have different architectures. Furthermore, it may also make it easier to map tasks onto OpenCL kernels. Whole tasks are defined at the NDRange level, work-groups represent large computation chunks which are executed in arbitrary order. The smallest operations (e.g., addition of two numbers) are mapped onto work-items.

Figure 2.2 contains a simple OpenCL kernel, which performs addition of elements from arrays *a* and *b*, then stores the result in array *c*. Qualifier __global specified for the arguments means that they are stored in global memory. Function get_global_id(int) is used to retrieve

Figure 2.2: Vector addition in OpenCL.

work-item index unique for the entire NDRange in specified dimension.

2.2 CUDA, comparison with OpenCL

CUDA is a parallel compute API developed by Nvidia Corporation. It works similarly to OpenCL, but there are also several differences which played an important role during the framework development:

- CUDA is officially available only for graphics cards released by Nvidia Corporation and CPUs¹. GPUs developed by other vendors and other types of accelerators are not supported.
- Differences in terminology identical or similar concepts have different terms in OpenCL and CUDA.
- Global indexing (i.e., NDRange indexing in OpenCL) works differently in CUDA.

Table 2.1 contains terms used in OpenCL and their counterparts in CUDA. Due to several differences in design, some terms do not have an equivalent term in the other API.

Difference in global indexing plays an important role during addition of tuning parameters which affect either grid dimensions or block dimensions. In OpenCL, an NDRange size in a given dimension is specified as size of a work-group multiplied by number of work-groups. However, in CUDA a grid size is specified only as a number of blocks. This is rather inconvenient for porting auto-tuned programs

^{1.} PGI compiler provides CUDA support for CPUs.

OpenCL term	CUDA term
compute unit	streaming multiprocessor
processing element	CUDA core
NDRange	grid
work-group	thread block
work-item	thread
global memory	global memory
constant memory	constant memory
local memory	shared memory
private memory	local memory
cl_platform	N/A
cl_device_id	CUdevice
cl_context	CUcontext
cl_command_queue	CUstream
cl_mem	CUdeviceptr
cl_program	nvrtcProgram, CUmodule
cl_kernel	CUfunction
cl_event	CUevent

Table 2.1: Comparison between OpenCL and CUDA terminology.

from one API to the other. The problem will be further elaborated upon in Chapter 4.

2.3 Possibilities for auto-tuning in compute APIs

Design of previously described APIs allows for a wide range of optimization opportunities, both inside kernel and host code. These optimizations can be implemented with usage of tuning parameters. While some of the parameters can be utilized only in a limited range of applications, there are also several ones which are relevant for larger number of computation tasks. This section provides a list of some of

the most common optimization parameters which are used in code variant auto-tuning.

2.3.1 Work-group (thread block) dimensions

Work-group dimensions specify how many work-items are included in a single work-group. Work-groups are executed on compute units, which are mapped onto, for example CPU cores or GPU multiprocessors. Performance of these devices may be vastly different and manually finding an optimal work-group size in combination with other tuning parameters is difficult. The dimensions also indirectly affect cache locality of data, which is a reason why this parameter usually makes an ideal candidate for auto-tuning.

2.3.2 Usage of vector data types

Modern processors contain vector registers that allow concurrent execution of a single instruction over multiple data which leads to a significant speed-up of certain types of computations. Kernel compilers attempt to automatically utilize these registers in order to speed up computation without manual code modification. However, automatic vectorization is not always optimal. There is an option to perform manual vectorization by using vector data types which are available in both OpenCL and CUDA. It is possible to control vector length with a tuning parameter, e.g., by using type aliases.

2.3.3 Data placement in different types of memory

Section 2.1.2 described various memory types available in OpenCL, similar memory hierarchy can also be found in CUDA. In many cases, there are more valid memory types to choose from for data placement. The choice can have an effect on performance, for example accessing data from OpenCL local memory is usually faster than using global memory. The problem is that local memory capacity is limited and while on certain devices the data could fit into it, on other devices it would be necessary to use global memory instead. Having a single version of kernel which would utilize only global memory would be

inefficient for large number of devices. This can be solved by using tuning parameter which controls the data memory placement.

2.3.4 Data layout in memory

Composite data can be organized into memory in multiple ways. For example, data storing 3D vertex coordinates can be split into three separate arrays which are then stored in memory consecutively. Another way to organize the same data is to first put all information about a vertex into a structure and then create an array of these structures. The former layout is commonly referred to as structure of arrays (SoA), while the latter is called array of structures (AoS). The difference is illustrated with Figure 2.3.

The benefit of SoA is that variables with the same data type are stored in contiguous memory, which enables certain devices (e.g., Intel CPUs) to more efficiently utilize vector instructions. Other types of devices such as GPUs support native vector addressing and usage of SoA layout may lead to performance degradation.

2.3.5 Combining multiple parameters

In many situations, multiple tuning parameters can be utilized at once in order to further increase performance. However, certain parameters may affect each other. For example, optimal work-group size can be different when data is stored in global memory compared to a situation where it is placed in local memory. This makes it difficult to obtain the best combination manually, especially when many tuning parameters are used. Feasible solution is to automatize this process.

Figure 2.3: Comparison of array of structures and structure of arrays layouts.

3 Code variant auto-tuning and related frameworks

This chapter describes common terms used in relation to auto-tuning and provides a list of desired features which should be supported by auto-tuning frameworks. Afterwards, several generic frameworks are presented, including their advantages, disadvantages, usage examples and comparison. Frameworks which are domain-specific or not publicly available are not discussed here.

3.1 Auto-tuning glossary

The following terms are commonly encountered in subsequent chapters and their knowledge is required for better understanding of autotuning process:

- tuning parameter Parameter which, depending on its value, affects performance of a computation. For example, a parameter which controls length of a vector type of some variable. The exact way parameter comes into effect depends on a specific framework. Common option is a utilization of just-in-time compilation and preprocessor macros.
- configuration space Space which is created as a Cartesian product of all tuning parameters and their values. Certain elements

of configuration space may be eliminated by utilizing constraints.

- *tuning configuration* Single element of configuration space.
- *traversal of configuration space* A process where tuned program is launched repeatedly with different tuning configurations and its running time is measured.
- search method A method employed to explore individual tuning configurations. Because configuration space may become very large, exhaustive search is not always a viable option. It is possible to explore the space randomly or utilize an optimization method.

3.2 Features of auto-tuning frameworks

While there are no strict requirements over functionality that should be available in auto-tuning frameworks, there are several features which are either commonly implemented by existing frameworks or desired by users. They include the following:

- Scope of tuning parameters While definition of tuning parameters is supported by essentially all frameworks, not all of them allow parameters to affect all parts of a program. For example, some frameworks support only parameters which affect kernel code but not host code.
- Parameter constraints Ability to mark certain tuning configurations as invalid due to incompatible combinations of tuning parameter values. Such configurations should be excluded from configuration space traversal, which can lead to improved usability and performance.
- Advanced search methods Support for different methods which offer reasonable performance and quality of results.
- Output validation Certain tuning configurations might include code which is experimental or still in development. Tuner

should offer an ability to compare the produced output with precomputed reference output and detect differences.

- Usage of kernel compositions A computation may utilize multiple kernels in order to produce complete result. The kernels may share some tuning parameters and a framework should be able to generate tuning configurations which support such scenarios.
- Online auto-tuning Ability to combine configuration space traversal with regular computation. Output from tested tuning configurations can be immediately utilized in other parts of a program. This is valuable in situations where tuning cannot be done prior to program execution, for example when optimal selection of tuning parameters depends on input.
- Integration into existing software Framework should not significantly restrict usage of features which are available in compute APIs. Ideally, users should be able to port native applications into framework without losing access to some of the corresponding compute API functionality.
- User-friendliness and ease of use Availability of documentation, tutorials, clean and stable API. Availability of utility methods such as printing of tuning results in common format, debugging support and others.

3.3 CLTune

CLTune [1] is a framework for auto-tuning of OpenCL and CUDA kernels. It is freely available in a form of library and provides C++ interface for writing host programs. It is relatively easy to use and provides capabilities for tuning of separate kernels, multiple configuration search strategies, including several optimization-based approaches and result validation in a form of reference kernels.

However, it also has several limitations. Among the most significant ones are lack of support for kernel compositions, limited argument handling options (all kernels must accept the same kernel arguments, argument placement in memory is impossible to control) and poor

support for integration into existing software (code which launches kernels is internal part of the framework and cannot be modified). This results in a need to write separate applications for tuning and computation. The framework is no longer actively developed, so it is unlikely that new features will be introduced.

Tuner configuration in CLTune consists of several main steps which are listed below. KTT functionality in its basic form is based on the same idea. Figure 3.1 contains part of a program written in CLTune, which includes all of the following steps:

- 1. Initialization of tuner by specifying target platform and device.
- 2. Addition of tuned kernel.
- 3. Addition of reference kernel for output validation.
- 4. Definition of tuning parameters.
- 5. Setup of kernel arguments.
- 6. Launch of the tuning process.
- 7. Retrieval of results.

In order to support tuning parameters, kernel source file needs to be modified. In case of CLTune, the tuner exports parameter values from given configuration to kernel source code by using preprocessor macros. Kernel code has to be modified by user, so that the exported values have intended effect on computation. Simple example of such modification is shown in Figure 3.2.

3.4 Kernel Tuner

Kernel Tuner [2] is another open-source auto-tuning framework. It supports tuning of OpenCL and CUDA kernels as well as regular C functions, though in the last case, user is responsible for measuring execution duration. API is provided in Python language. Compared to CLTune, it provides more utility methods, for example ability to set kernel compiler options, measuring execution duration in multiple

Figure 3.1: Host program written in CLTune.

Figure 3.2: Adding support for auto-tuning to kernel via preprocessor macros.

iterations to increase accuracy and validating output with user-defined precomputed answer rather than being restricted to reference kernel.

As in case of CLTune, disadvantages include lack of support for kernel compositions and inability for integration into existing software. However, Kernel Tuner is still actively developed and some of these shortcomings may be eventually amended.

Host program has to be written in similar fashion to CLTune, definitions of tuning parameters are exported in the same way. Figure 3.3 contains major portion of a host program written in Kernel Tuner.

```
def tune():
  with open('stencil.cl', 'r') as f:
  kernel_string = f.read()
6 problem_size = (4096, 2048)
   size = numpy.prod(problem_size)
  x_old = numpy.random.randn(size).astype(numpy.float32)
  x_{new} = numpy.copy(x_old)
   args = [x_new, x_old]
11
12
13 tune_params = OrderedDict()
tune_params["block_size_x"] = [32*i for i in range(1,9)]
  tune_params["block_size_y"] = [2**i for i in range(6)]
  grid_div_x = ["block_size_x"]
  grid_div_y = ["block_size_y"]
  return kernel_tuner.tune_kernel("stencil_kernel", kernel_string, problem_size,
20
      args, tune_params, grid_div_x=grid_div_x, grid_div_y=grid_div_y)
21
  if __name__ == "__main__":
      tune()
23
```

Figure 3.3: Host program written in Kernel Tuner, source: [10].

3.5 OpenTuner

Unlike other mentioned tuners, OpenTuner [3] is an auto-tuning framework which can be used to tune programs written in essentially any language. It supports multiple forms of auto-tuning, for example tuning of compiler flags or CPU frequencies as well as code variant auto-tuning. The API is provided in Python language. Due to tuner's more generic nature, users are responsible for writing more sections of code themselves. In case of code variant auto-tuning, this involves writing a method which adds parameter definitions from tuner-generated configurations to tuned program and compiles it. The other listed frameworks have this functionality already built-in. Other shortcomings include problems with integration into software and lack of complete API documentation. Framework does not seem to be actively developed anymore with majority of the development being done before 2017.

While the other frameworks use preprocessor definitions to export tuning parameters into code, OpenTuner does not have any specific way of parameter handling. The way parameters become visible in tuned code depends on capabilities of target programming language and on the user-written method for parameter export. Figure 3.4 contains an example of OpenTuner configuration for tuning of C code. Tuning parameters are added to code through compiler flags.

3.6 ATF

ATF (Auto-Tuning Framework) [4] is a recently released framework which offers several improvements over the previous solutions. Similarly to OpenTuner, it supports several forms of auto-tuning and multiple languages. Unlike other mentioned frameworks, it relies on annotating user code with directives and there is therefore no need to write separate tuning program. Another advantage is the ability to generate configuration space more efficiently by utilizing multithreading and pre-filtering of parameter values based on constraints. This improves tuner performance in situations where many tuning parameters with a large number of valid values are used.

```
class GccFlagsTuner(MeasurementInterface):
  def manipulator(self):
      manipulator = ConfigurationManipulator()
      manipulator.add_parameter(IntegerParameter('vectorType', 1, 2, 4, 8))
      return manipulator
  def run(self, desired_result, input, limit):
8
      cfg = desired result.configuration.data
9
10
  gcc_cmd = 'g++ tuned_program.cpp '
  gcc_cmd += '-VECTOR_TYPE='+ cfg['vectorType']
  gcc_cmd += ' -o ./tmp.bin'
   compile_result = self.call_program(gcc_cmd)
   assert compile_result['returncode'] == 0
16
17
18 run_cmd = './tmp.bin'
  run_result = self.call_program(run_cmd)
  assert run result['returncode'] == 0
  return Result(time=run_result['time'])
22
  def save_final_config(self, configuration):
24
      print "Optimal vector type written to final_config.json:",
25
          configuration.data
      self.manipulator().save_to_file(configuration.data, 'final_config.json')
```

Figure 3.4: Configuration of OpenTuner, source: [3].

ATF also supports various abort conditions to end exploration of search space during offline tuning. These include conditions based on absolute tuning time, number of explored configurations and relative speedup within several recently tested configurations. However, several shortcomings which were present in previous frameworks also remain in ATF. There is no support for online tuning and no explicit support for kernel compositions. The framework currently also lacks documentation and provides only a handful of usage examples. Another inconvenience is the necessity to ask for usage permission.

Example of tuning OpenCL SAXPY (single-precision a * x + y) kernel with ATF framework can be seen in Figure 3.5.

```
1 int main() {
const int N = 1024;
4 const ::std::string saxpy = R"cl__(
  __kernel void saxpy(const int N, const float a, const __global float* x,
       __global float* y)
      for(int w = 0; w < WPT; ++w) {
          const int id = w * get_global_size(0)
          + get_global_id(0);
          y[id] += a * x[id];
10
11
12 }
13 )cl__";
14
  auto WPT = atf::tp("WPT", atf::interval<int>(1, N), atf::divides(N));
   auto LS = atf::tp("LS", atf::interval<int>(1, N), atf::divides(N / WPT));
18
19 auto cf_saxpy =
atf::cf::ocl({0, atf::cf::device_info::GPU, 1}, {saxpy, "saxpy"},
inputs(atf::scalar<int>(N), // N
22 atf::scalar<float>(), // a
23 atf::buffer<float>(N), // x
24 atf::buffer<float>(N)), // y
25 atf::cf::GS(N / WPT), atf::cf::LS(LS));
27 auto best_config = atf::annealing(
atf::cond::duration<std::chrono::minutes>(2))(WPT, LS)(cf_saxpy);
29 }
```

Figure 3.5: Example of tuning SAXPY kernel with ATF, source: [11].

3.7 Comparison of frameworks

Table 3.6 showcases state of features in previously discussed frameworks. Note that the state of supported features may change as several mentioned frameworks are still actively developed.

Feature	CLTune	Kernel Tuner	OpenTuner	ATF
Supported APIs	CUDA, OpenCL	CUDA, OpenCL	any language or API	any language or API
Tuning parameters	kernel code only	kernel and host code	kernel and host code	kernel and host code
Parameter constraints	>	>	requires additional user effort	>
Search methods	multiple optimiza- tion methods sup- ported			
Output validation	reference kernel only	reference kernel or precomputed buffer	×	×
Kernel compositions	×	×	requires additional user effort	×
Online auto-tuning	×	×	×	×
Full API documenta- tion	>	>	×	×

Figure 3.6: Comparison of features in auto-tuning frameworks.

4 KTT framework

While the previously mentioned frameworks handle auto-tuning of single kernels well and provide fairly wide range of utility methods, they all lack support for tuning of kernel compositions and online auto-tuning. They were designed for tuning of separate programs combined with explicit exporting of optimized parameter values into production code without possibility of integration into existing software. These are the main features which should be included in the new auto-tuning framework.

Originally, CLTune was planned to be used as a basis for the new framework. Extra functionality was to be added on top of the existing code structure. However, this has proved to be rather problematic. While CLTune API is written in a clean and user-friendly manner, its internal structure made it difficult to extend its functionality. Large part of the internal code is placed into a small number of very long methods which mix together operations such as argument handling and result validation with access to compute API functions. This made it difficult to introduce new features without refactoring large portion of code.

It was eventually decided to write a completely new framework named Kernel Tuning Toolkit. Baseline portion of KTT API remained similar to CLTune, so it would be easy to port existing programs. However, the internal structure was completely rewritten from scratch, with only very small portions of CLTune code for the following features being reused:

- generating of tuning configurations
- definition of tuning parameter constraints
- search methods based on simulated annealing and particle swarm optimization techniques

The new tuner structure is further discussed in chapter 5.

4.1 Overview of KTT functionality

This section describes different usage scenarios supported by KTT framework and provides a high-level overview of the steps performed in each scenario.

4.1.1 Single kernel tuning

The simplest scenario which is also supported by all of the previously discussed frameworks is offline tuning of a single kernel. The tuning process in this case is similar to that of CLTune framework. Addition of tuned kernel and its arguments to tuner is followed by definition of tuning parameters. Framework then performs the tuning, including handling of kernel execution and buffer management. Tuning results are reported once the operation is finished. The entire workflow is illustrated in Figure 4.1. A concrete example of this usage scenario is described in Section 4.6.

4.1.2 Kernel compositions and host code tuning

A more complex situation is tuning of a computation which involves execution of multiple kernels and performs portion of a computation on a CPU (e.g., output from one kernel organized in structure of arrays layout is transformed in a CPU code into array of structures layout and then used as input for other kernel). Solution provided by KTT framework for such scenarios is called tuning manipulator, which enables users to customize portion of the framework's code that is responsible for kernel execution and buffer management, and optionally perform some part of computation directly in C++ code. The API also provides methods for changing and updating kernel arguments as these can be different for individual kernel executions, which is in contrast to single kernel tuning where all the executions happen under the same conditions. The general usage is shown in Figure 4.2. Further information about manipulators can be found in Section 4.5. Specific examples utilizing kernel compositions and tuning manipulators are located in Chapter 6.

4.1.3 Online tuning and software integration

The two previous sections described situations which involved tuning of standalone computations. However, KTT framework also supports integration into other applications. There are two possible usage scenarios:

- Tuning is performed at the start of application, which can then transparently continue its computation. Tuning is integrated directly with the application and there is no need for separate tuning program.
- Tuning is performed at the time of computation. Application executes kernels and uses their output while KTT transparently changes tuning parameters and searches for the best configuration. This scenario is referred to as online tuning and is beneficial in cases when kernel running time dominates over tuning overhead as all of the kernel executions contribute to final result. An example of this way of usage is in Chapter 6.

Both of these scenarios require the framework to provide access to underlying compute API functionality without too many restrictions as that would make the direct integration into software difficult, if not impossible. Additionally, the second scenario requires the framework overhead to be minimal so that the speedup gained by utilizing online tuning is more significant than the time lost performing internal framework operations.

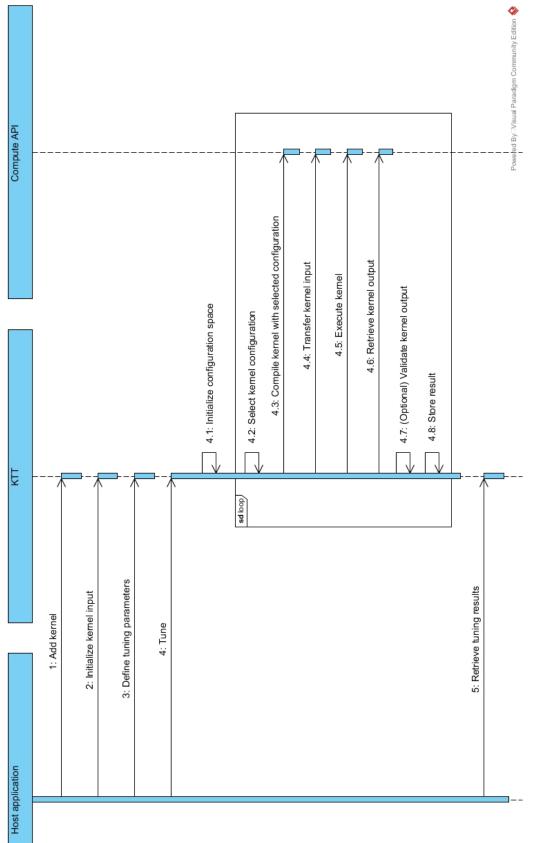


Figure 4.1: Diagram showcasing offline tuning of a single kernel.

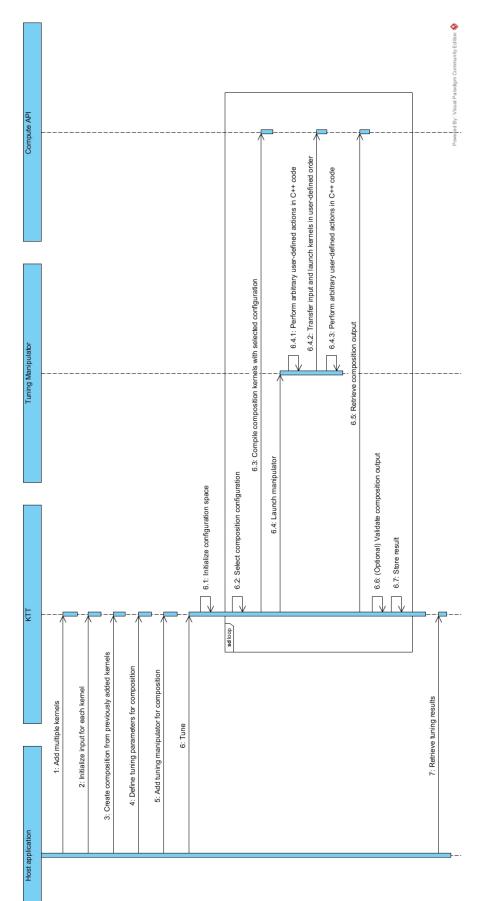


Figure 4.2: Diagram showcasing offline tuning of a kernel composition utilizing tuning manipulator.

4.2 KTT API

KTT framework API provides users with methods which can be used to develop and tune OpenCL or CUDA applications. It is split into three major classes, some basic methods were inspired by CLTune. It is written in C++ language.

KTT framework can be acquired from GitHub¹ as an open-source library with prebuilt binaries being available for certain platforms. Manual library compilation is also possible by using a build tool premake5, C++14 compiler and CUDA or OpenCL distribution. Supported operating systems include Linux and Windows.

The described API corresponds to version 0.6 of KTT framework. It is the first release candidate version and contains all of the functionality that was planned to be implemented as a part of this thesis.

4.3 Tuner class

Tuner class makes up the main part of KTT API. It includes methods which implement following functionality:

- handling of kernels and kernel compositions
- handling of kernel arguments
- addition of tuning parameters and constraints
- kernel running and tuning
- kernel output validation
- retrieval of tuning results
- retrieval of information about available platforms and devices

4.3.1 Tuner creation

In order to access the API methods, tuner object has to be created. There are currently three versions of tuner constructors available (Figure 4.3). They allow specification of compute API (either OpenCL or

^{1.} Repository link: https://github.com/Fillo7/KTT

CUDA), platform index, device index and number of utilized compute queues. OpenCL API with one compute queue is the default setting. Indices are assigned to platforms and devices by KTT framework, they can be retrieved with a tuner method.

```
Tuner(const PlatformIndex platform, const DeviceIndex device)
Tuner(const PlatformIndex platform, const DeviceIndex device, const ComputeAPI API)
Tuner(const PlatformIndex platform, const DeviceIndex device, const ComputeAPI API, const uint32_t computeQueueCount)
```

Figure 4.3: Tuner constructors.

4.3.2 Kernel handling

Kernels can be added to tuner from a file or a C++ string (Figure 4.4). Users furthermore need to specify kernel function name and default global and local sizes (i.e., dimensions for NDRange / grid and workgroup / thread block). The sizes are stored inside *DimensionVector* objects, which are a part of KTT framework. They allow easy thread size manipulation and support up to three dimensions. Existing kernels can be referenced by using a handle returned by tuner. Kernel compositions can be added by specifying handles of kernels which should be included inside a composition. In order to use compositions, user additionally has to define a tuning manipulator whose usage is detailed in Section 4.5.

4.3.3 Kernel argument handling

There are three types of kernel arguments supported by KTT – vector, scalar and local memory (OpenCL) arguments. All arguments are referenced by using a handle provided by tuner. Argument addition methods are templated and support primitive data types (e.g., int, float) as well as user-defined data types (e.g., struct, class). Arguments are bound to kernels by using a method which accepts kernel handle and corresponding argument handles. This allows them to be shared among multiple kernels. The mentioned methods can be seen in Figure 4.5.

Figure 4.4: Kernel addition methods.

```
ArgumentId addArgumentVector(const std::vector<T>& data, const
ArgumentAccessType accessType)

ArgumentId addArgumentVector(std::vector<T>& data, const ArgumentAccessType
accessType, const ArgumentMemoryLocation location, const bool copyData)

ArgumentId addArgumentScalar(const T& data)

ArgumentId addArgumentLocal(const size_t localMemoryElementsCount)

void setKernelArguments(const KernelId id, const std::vector<ArgumentId>& argumentIds)
```

Figure 4.5: Argument handling methods.

Vector arguments are added from C++ vector containers. It is possible to specify access type (read, write or combined), memory location from where argument data is accessed by kernel (device or host) and whether argument copy should be made by the tuner. By default, copies of all vector arguments are made by tuner, so the original vectors remain modifiable by a user without interfering with the tuning process. In case argument is placed in host memory, it is possible to utilize zero-copy feature, which means that kernel has direct access to buffer which was initialized from host code. This functionality is supported by both CUDA and OpenCL. All of the vector argument handling options are illustrated with Figure 4.6.

4.3.4 Tuning parameters and constraints

Tuning parameters are specified for kernels with a name and list of valid values (Figure 4.7). Both integer and floating-point values are

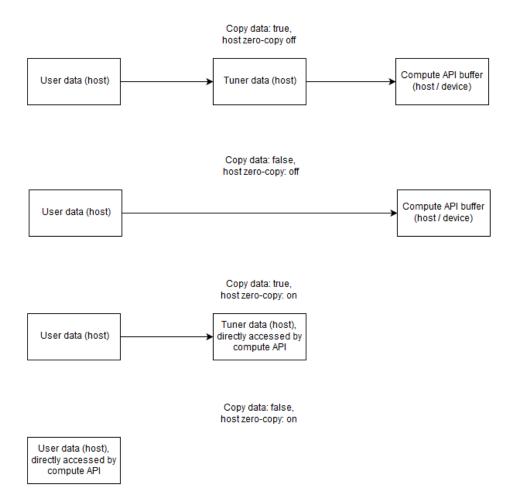


Figure 4.6: Vector argument handling options in KTT framework. Each box represents one copy of a buffer.

```
void addParameter(const KernelId id, const std::string& parameterName, const
    std::vector<size_t>& parameterValues)

void addParameterDouble(const KernelId id, const std::string& parameterName,
    const std::vector<double>& parameterValues)

void addParameter(const KernelId id, const std::string& parameterName, const
    std::vector<size_t>& parameterValues, const ModifierType type, const
    ModifierAction action, const ModifierDimension dimension)

void addConstraint(const KernelId id, const
    std::function<bod(std::vector<size_t>)>& constraintFunction, const
    std::vector<std::string>& parameterNames)
```

Figure 4.7: Tuning parameter and constraint addition methods.

supported. Before kernel tuning begins, configurations for each combination of kernel parameter values are generated. For example, adding parameter A with values 1 and 2, and parameter B with values 5 and 10 will result in four configurations being generated – $\{1, 5\}$, $\{1, 10\}$, $\{2, 5\}$ and $\{2, 10\}$. Tuned kernel is then launched with parameter definitions prepended to kernel source code based on the current configuration.

Some tuning parameters may additionally affect global and local sizes of tuned kernel. This is useful, for example, in cases where parameter in kernel source code modifies amount of work done by a single work-item and therefore changes total number of needed work-items. Each dimension can be modified separately, supported modifiers include addition, subtraction, multiplication and division.

If certain combinations of tuning parameters are invalid or unsupported by a kernel source code, they can be eliminated by using parameter constraints. Constraint is a function which accepts list of parameter values for specified parameters and returns a boolean result which signifies whether the combination is valid or not. Constraint conditions are defined by users.

Tuning parameters for kernel compositions are added separately and are shared by all kernels inside a composition. Individual kernels outside compositions are not affected by composition parameters either.

4.3.5 Kernel tuning and running

KTT supports offline and online kernel tuning as well as regular kernel running. In offline tuning, kernel configurations are tested iteratively one after another without interruption. This mode is strictly focused on finding the best performing configuration, retrieval of kernel output by user and swapping of kernel argument data between configurations is not possible. On the other hand, it allows efficient validation of output. Because the argument data remains the same for all configurations, the reference output needs to be computed only once.

In online tuning, single configuration is tested at time, enabling combination with kernel running. It also allows kernel output retrieval using KTT built-in structure *OutputDescriptor*. This structure specifies handle of argument to be retrieved, memory location for output data and optionally size of the retrieved data, which is useful in case only part of the argument is needed. Online tuning also supports swapping of argument data between each configuration, though if validation is enabled, reference output needs to be recomputed every time a new configuration is run. It is important to note that the input size should remain the same across all tested configurations during tuning so that the measured durations can be objectively compared. The optimal configurations are not necessarily identical for different input sizes either.

In both modes, the order and number of tested configurations depends on utilized search method. KTT currently supports five search methods – full search, random search, simulated annealing, particle swarm optimization and Markov chain Monte Carlo. Full search simply explores all configurations iteratively. The other four methods allow specification of a fraction parameter which controls number of explored configurations (e.g., setting fraction to 0.5 will result in 50% of all configurations being tested). In random search, the explored configurations are chosen randomly, while the last three methods employ probabilistic techniques in order to find configurations with good performance more quickly.

Output retrieval is supported for kernel running in the same fashion as for online tuning. Kernels can be run in any valid tuning configuration which is specified by a user. Output validation is not performed during kernel running. Kernels can be run using the best found con-

```
void tuneKernel(const KernelId id)
void tuneKernelByStep(const KernelId id, const std::vector<OutputDescriptor>&
    output)
void runKernel(const KernelId id, const std::vector<ParameterPair>&
    configuration, const std::vector<OutputDescriptor>& output)
void setSearchMethod(const SearchMethod method, const std::vector<double>&
    arguments)
void setTuningManipulator(const KernelId id,
    std::unique_ptr<TuningManipulator> manipulator)
```

Figure 4.8: Kernel tuning and running methods.

figuration immediately after the tuning has finished which means that splitting auto-tuning and production applications is not necessary.

In basic case, launch of a kernel is handled automatically by a tuner after the initial setup. However, for scenarios where part of a computation happens in C++ code or kernel compositions are utilized, it is necessary to implement a *TuningManipulator* and then bind it to corresponding kernel. Tuning manipulators are discussed in greater detail in Section 4.5.

Figure 4.8 contains all of the previously described methods related to kernel tuning and running.

4.3.6 Output validation

Kernel output can be validated in two ways – with a reference class or a reference kernel (Figure 4.9). In the former case, user has to implement a class which includes a method that computes reference output on a CPU. Tuner then compares this output with result produced by tuned kernels. If difference in tuned output at certain index is detected, given kernel configuration is considered invalid. More details about reference class can be found in Section 4.4. The latter case works similarly, difference being that reference output is computed by a kernel with user-specified configuration. Both methods support validation of multiple kernel arguments. It is also possible to only check subpart of the argument, which is useful when result is shorter than length of an entire argument.

```
void setReferenceKernel(const KernelId id, const KernelId referenceId, const
    std::vector<ParameterPair>& referenceConfiguration, const
    std::vector<ArgumentId>& validatedArgumentIds)

void setReferenceClass(const KernelId id, std::unique_ptr<ReferenceClass>
    referenceClass, const std::vector<ArgumentId>& validatedArgumentIds)

void setValidationMethod(const ValidationMethod method, const double
    toleranceThreshold)

void setValidationRange(const ArgumentId id, const size_t range)

void setArgumentComparator(const ArgumentId id, const std::function<bool(const
    void*, const void*)>& comparator)
```

Figure 4.9: Output validation methods.

When kernel arguments with floating-point data type are validated, user can choose one of the multiple validation techniques and a tolerance threshold. If tuned output differs slightly from reference output, but remains within the threshold, it is still considered correct. Validation techniques include side by side comparison where result difference is calculated and compared to threshold for each pair of elements with corresponding index in reference and tuned output. Other technique is absolute difference, where the differences between individual pairs are summed up and only the resulting sum is compared to threshold.

Users additionally have an option to add a custom comparator for specified argument. Comparator is a method which receives two elements with the same data type and decides whether they are equal. Comparators are mandatory for arguments with user-defined data types as the tuner is only able to automatically validate arguments with built-in data types.

4.3.7 Tuning results retrieval

Each tuning result includes a list of parameter values, global and local sizes and corresponding duration of computation. List of all tuning results for specified kernel can be printed either to a C++ output stream or a file. Supported print formats include verbose format intended for log files or terminals and CSV (comma-separated values) format which is useful for subsequent processing and analysis of results.

Figure 4.10: Result retrieval methods.

List of parameter values for the best known configuration can also be retrieved through an API method, which is useful for combining online auto-tuning with kernel running. The available methods can be seen in Figure 4.10.

4.3.8 Platform and device information retrieval

When using KTT framework for the first time on a system, it is useful to retrieve indices for available platforms and devices, which are then used during proper tuner initialization. The assigned indices and corresponding platform and device names can be printed to specified C++ output stream. It is furthermore possible to retrieve more detailed information about individual platforms and devices, such as list of supported extensions, memory capacities, number of compute units and others (Figure 4.11).

```
void printComputeAPIInfo(std::ostream& outputTarget)
std::vector<PlatformInfo> getPlatformInfo()
std::vector<DeviceInfo> getDeviceInfo(const PlatformIndex index)
DeviceInfo getCurrentDeviceInfo()
```

Figure 4.11: Information retrieval methods.

4.3.9 Other notable methods

Other notable API methods include a method for specification of kernel compiler options, choice of a global size notation and an option to enable automatic global size correction (Figure 4.12). Compiler

```
void setCompilerOptions(const std::string& options)
void setGlobalSizeType(const GlobalSizeType type)
void setAutomaticGlobalSizeCorrection(const bool flag)
```

Figure 4.12: Other notable methods.

options can be specified as a string of individual flags separated by a white space.

Choice of a global size notation allows using OpenCL NDRange dimension specification for CUDA grid and vice versa. This allows elimination of one of the notable differences between OpenCL and CUDA API in host code and makes it easier to port programs written in one API to the other.

Automatic global size correction ensures that global size is always a multiple of local size, which is a necessary requirement for running kernels in OpenCL, and also in CUDA, if OpenCL global size notation option is used. Framework performs automatic roundup of a global size to the nearest higher multiple of a local size. Enabling this behaviour is useful when multiple tuning parameters which affect thread sizes are present.

4.3.10 Error handling

There are two basic types of errors that are handled by KTT framework – errors caused by incorrect API usage (e.g., using invalid kernel or argument handle) and kernel execution errors (e.g., a kernel under specific configuration cannot be launched due to insufficient amount of device resources or computes incorrect result). In the first case, the framework prints a message describing cause of error and then throws an exception, aborting the entire tuning process. The error has to be then corrected by a user.

In the second case, it is undesirable that a single faulty kernel would cause the entire tuning process to be terminated. When a kernel error is encountered, a message describing the cause is printed, but the tuning process then continues with next configuration. This works well during offline tuning where kernel output is discarded after validation. Moreover, when the tuner is configured to hold input and

output buffers (see Section 4.3.3), it completely rewrites input and output buffers held by compute API, so potential data corruption caused by kernel malfunction is eliminated.

However, the situation is more complicated during online tuning, as kernel output can be utilized by a host application between kernel invocations. In this case, it is necessary for a host application to check whether computation was successful and possibly recompute the corresponding portion of a result under different configuration (by repeating kernel invocation with different combination of tuning parameters). If the kernel is executed but results are incorrect, the error is detected only if reference kernel or reference class is defined. However, result validation may not be suitable during online tuning where performance of the tuning process is crucial. Therefore, it is best to ensure correctness of computation using different combinations of tuning parameters during offline tuning when kernels are developed. If all the combinations yield correct results, the only type of error should be caused by a lack of resources on particular device, which can be detected by the tuner without usage of reference kernel or class.

4.4 Reference class

Reference class is an interface provided by KTT framework used for validating kernel output via implementation of a C++ method. In order to utilize it, a new class which publicly inherits from *ReferenceClass* interface must be defined by a user. For the resulting class to be valid, it is necessary to implement two virtual methods and optionally override one more method (Figure 4.13).

The first method should implement computation of a reference output. The second method is then used to retrieve the prepared output. The third, optional method can be overriden if the resulting output size is smaller than the size of corresponding validated kernel argument. This is useful in situations where only a part of the argument is validated.

Implemented class can be then assigned to tuner by using a method from tuner API described in Section 4.3.6. The implemented methods are utilized by tuner during output validation phase.

```
virtual void computeResult() = 0
virtual void* getData(const ArgumentId id) = 0
virtual size_t getNumberOfElements(const ArgumentId id)
```

Figure 4.13: Reference class methods.

4.5 Tuning manipulator class

Tuning manipulator is an interface for customizing the way kernels are launched inside KTT framework. This is useful in several scenarios:

- Tuned kernel is launched iteratively in order to produce complete result.
- Part of a computation happens on a CPU side in C++ code.
- Tuning parameters which affect host code are present.
- Kernel compositions are utilized.
- Framework is integrated into another software which needs to perform additional operations between individual kernel launches.

Because in all of the above-mentioned scenarios, the exact way kernel is launched depends on a specific use case, it is up to user to define their own tuning manipulator. The definition works in a similar way as for reference class – a new class inheriting from *TuningManipulator* interface has to be created and a virtual method which launches a kernel and performs any user-defined operations needs to be implemented.

Tuning manipulator interface also includes several other methods which can be used by a user within the kernel launch method. These include methods for work with multiple compute queues, asynchronous operations, buffer management and methods which make handling of tuning parameters affecting host code easier.

4.5.1 Kernel running and host code tuning

The basic task which needs to be fulfilled by the implemented method is to run a kernel with corresponding tuning configuration. If the

Figure 4.14: Kernel running and configuration retrieval methods.

implemented method executes only this one task, then the resulting behaviour is the same as if no tuning manipulator was used at all.

Kernel inside a tuning manipulator can be run either with global and local sizes that correspond to current configuration or with user-specified sizes. The second option can be used in addition to or as an alternative to thread size modifying parameters described in Section 4.3.4. Methods for thread size and parameter value retrieval are available as well. Those can be used to implement tuning parameters which affect host code. The list of all tuning manipulator methods related to kernel running can be seen in Figure 4.14.

4.5.2 Kernel argument and buffer management

When a kernel is run iteratively to produce a complete result, it is often desirable to modify input data between iterations. Tuning manipulator interface provides methods for this scenario. It is possible to modify both scalar and vector arguments. It is also possible to retrieve data of vector arguments, which is useful, for example when the data has to be preprocessed on a CPU in-between iterative kernel launches (Figure 4.15).

All of the modifications performed on kernel arguments and corresponding buffers are isolated to a single tuning manipulator instance call. This makes it possible to utilize manipulators in offline tuning, where the initial state of kernel arguments before testing of each tuning configuration needs to remain the same.

```
void updateArgumentScalar(const ArgumentId id, const void* argumentData)
void updateArgumentVector(const ArgumentId id, const void* argumentData, const
size_t numberOfElements)
void getArgumentVector(const ArgumentId id, void* destination, const size_t
numberOfElements)
void copyArgumentVector(const ArgumentId destination, const ArgumentId source,
const size_t numberOfElements)
void changeKernelArguments(const KernelId id, const std::vector<ArgumentId>&
argumentIds)
```

Figure 4.15: Kernel argument and buffer handling methods.

4.5.3 Compute queues and asynchronous operations

In real-world computations, multiple compute queues are often utilized in order to overlap independent parts of a computation and thus increase performance. For this purpose, manipulator interface includes methods for executing asynchronous operations in a specified queue and for device synchronization. Number of queues which are available corresponds to a user-specified amount during tuner initialization. Queues are referenced with handles provided by KTT. Methods which can be run asynchronously include kernel running and operations with vector kernel arguments. It is possible to synchronize either only specified queue or all queues which effectively synchronizes the entire device (Figure 4.16).

Figure 4.16: Compute queue handling and asynchronous methods.

4.6 Example of API usage

Figures 4.17 and 4.18 contain a simple example of using KTT to tune OpenCL vector addition kernel (shown in Figure 2.2).

Output validation is done via reference class interface which is defined in the first figure. User-defined constructor (lines 4-9) initializes all the data that is needed to compute reference result. Method which computes the result (lines 11-17) performs a simple addition of elements inside two vector containers in a for loop. The final method (lines 19-26) is called internally by KTT framework to retrieve computed reference result. Since KTT validation component works directly with computed data, the method needs to return pointer to a buffer which contains this data rather than pointer to the entire vector container. Because it is possible to validate multiple arguments with single reference class, this method also checks for which argument the reference result should be returned.

Second figure then shows the main part of a host program. Kernel in this example is tuned using a single tuning parameter which controls size of a work-group – four possible parameter values are specified. Lines 5-16 contain initialization of data, global and local sizes. NDRange size is initialized to a total number of elements inside vector so that each element is processed by a single work-item. For simplicity's sake, it is assumed that number of elements is a multiple of 32. Work-group size is initialized to one because it will be controlled with tuning parameter, which is added later. Tuner is initialized (line 18) by specifying platform and device index, followed by addition of tuned kernel and its arguments (lines 19-24). The next line includes instantiation of previously defined reference class and its addition to tuner. Line 28 contains definition of a tuning parameter which multiplies work-group size in dimension x. Since the default size was defined as 1, this effectively sets the resulting size to the parameter's value. Once all the configuration is done, tuning of kernel can be started (line 29) and is followed by printing of results to standard output stream (line 30).

More complex examples, including usage of tuning manipulator interface, are covered in Chapter 6.

```
class SimpleValidator : public ktt::ReferenceClass
2 {
g public:
      SimpleValidator(const ktt::ArgumentId validatedArgument, const
           std::vector<float>& a, const std::vector<float>& b, const
           std::vector<float>& result) :
          validatedArgument(validatedArgument),
5
          a(a),
          b(b),
          result(result)
       {}
10
      void computeResult() override
11
12
          for (size_t i = 0; i < result.size(); i++)</pre>
              result.at(i) = a.at(i) + b.at(i);
15
          }
      }
      void* getData(const ktt::ArgumentId id) override
19
20
          if (validatedArgument == id)
          {
              return result.data();
          }
          return nullptr;
25
      }
26
27
  private:
28
      ktt::ArgumentId validatedArgument;
29
       const std::vector<float>& a;
       const std::vector<float>& b;
31
       std::vector<float> result;
32
   };
```

Figure 4.17: KTT usage example – reference class definition.

```
int main(int argc, char** argv)
   {
2
      // Initialize platform / device index and path to kernel file.
      const size t numberOfElements = 1024 * 1024;
      const ktt::DimensionVector ndRangeDimensions(numberOfElements);
      const ktt::DimensionVector workGroupDimensions(1);
      std::vector<float> a(numberOfElements);
      std::vector<float> b(numberOfElements);
      std::vector<float> result(numberOfElements, 0.0f);
10
      for (size_t i = 0; i < numberOfElements; i++)</pre>
          a.at(i) = static_cast<float>(i);
          b.at(i) = static_cast<float>(i + 1);
16
      ktt::Tuner tuner(platformIndex, deviceIndex);
18
      ktt::KernelId kernelId = tuner.addKernelFromFile(kernelFile,
          "vectorAddition", ndRangeDimensions, workGroupDimensions);
      ktt::ArgumentId aId = tuner.addArgumentVector(a,
          ktt::ArgumentAccessType::ReadOnly);
      ktt::ArgumentId bId = tuner.addArgumentVector(b,
          ktt::ArgumentAccessType::ReadOnly);
      ktt::ArgumentId resultId = tuner.addArgumentVector(result,
23
          ktt::ArgumentAccessType::WriteOnly);
      tuner.setKernelArguments(kernelId, std::vector<ktt::ArgumentId>{aId, bId,
          resultId});
      tuner.setReferenceClass(kernelId,
          std::make_unique<SimpleValidator>(resultId, a, b, result),
          std::vector<ktt::ArgumentId>{resultId});
      tuner.addParameter(kernelId, "multiply_work_group_size",
          std::vector<size_t>{32, 64, 128, 256}, ktt::ModifierType::Local,
          ktt::ModifierAction::Multiply, ktt::ModifierDimension::X);
      tuner.tuneKernel(kernelId);
      tuner.printResult(kernelId, std::cout, ktt::PrintFormat::Verbose);
      return 0;
31
32
  }
```

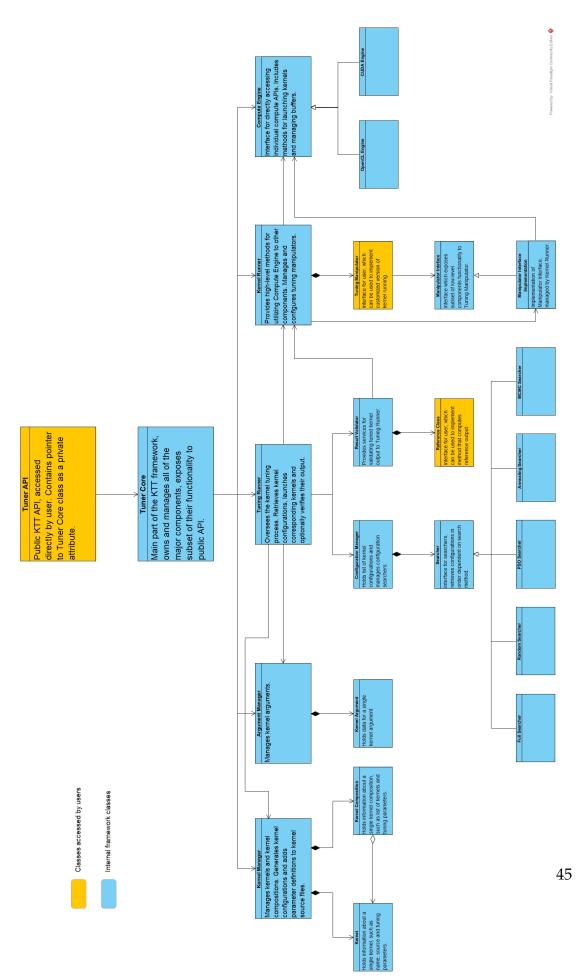
Figure 4.18: KTT usage example – main part of the host program.

5 KTT structure

KTT structure is loosely based on layered architecture pattern [5], which is often employed for developing enterprise applications. Individual functionality is split into multiple components across several layers. On the lowest layer, each component is independent and focuses on a single task (e.g., managing of kernels), which makes it easier to extend existing functionality and introduce new features. Functionality of individual components is interconnected on upper layers with the topmost layer serving as a public API. Figure 5.1 contains high-level class diagram of KTT framework, which includes all of the major components and dependencies between them. Some smaller components and utility classes such as result printer are not included in order to improve readability.

Functionality of the following components is further described in this chapter:

- Tuner
- Tuner core
- Kernel manager
- Argument manager
- Tuning runner
- Configuration manager
- Result validator
- Compute engine
- Kernel runner
- Manipulator interface



and kernel runner / argument manager were omitted in order to improve readability without severely Figure 5.1: KTT class diagram. Note that two dependencies between kernel runner / kernel manager impacting diagram accuracy.

5.1 Tuner and tuner core

Tuner component represents the main part of public API. Its methods were described in Chapter 4. In order to hide internal framework components from users, it utilizes pointer to implementation idiom. The public header (.h) file contains only declaration of implementation class (i.e., tuner core) and a pointer to its instance. However, the actual tuner core header with method definitions is directly included only in tuner implementation (.cpp) file. This file is needed during compilation, but the built library can be then distributed with tuner header only. There is no need to include internal headers for components such as tuner core, which makes upgrading to newer versions of the framework easier in certain situations (e.g., if methods in tuner core are modified in newer versions of the framework, but methods in tuner API remain the same, software which utilizes the framework only needs to replace library file without recompilation).

Tuner core makes up the main internal part of the framework. It owns and manages several smaller components and exposes subset of their functionality to public API. In some cases, it combines functionality of methods from multiple components into a single public API method.

5.2 Kernel manager

Primary task of a kernel manager is storage and management of kernels and kernel compositions. Other responsibilities include assigning unique handles for new kernels and compositions, adding tuning parameter definitions to kernel source code and generating kernel configurations which are then used by other components.

Configurations are generated recursively with parameters being processed one by one. The method which generates configurations contains a loop which launches a new instance of the same method for each parameter value. The new instances then repeat the process for subsequent parameters until the resulting configuration contains definitions of all parameters. When a configuration is complete, it is checked whether it satisfies all user-defined constraints. Configurations which pass the check are then placed inside a shared vector

container which is visible from all instances of recursively called methods, invalid configurations are discarded. Kernel configurations also include global and local sizes, which are updated when a thread-modifying tuning parameter is processed. With multiple such parameters, the modification happens in the order of their addition.

Kernel compositions are components which contain references to all kernels that they include. Addition of tuning parameters works in a similar fashion as for regular kernels, difference being that when a parameter is added to a composition, its definition is added to source codes of all utilized kernels. If there is a kernel, which does not utilize certain parameter, the definition can be safely ignored. However, it is still possible to add thread-modifying parameters which only affect thread sizes of a specific kernel inside a composition.

5.3 Argument manager

Argument manager stores and generates unique handles for kernel arguments. Arguments inside KTT can store elements with user-defined data types as well as built-in data types. This is made possible by storing the argument elements as raw data and converting to proper data type only when needed (e.g., during result validation). Restriction is that the used data type has to be trivially copyable¹. However, this is not much of a problem because data which is copied into e.g., GPU memory should be trivially copyable either way.

5.4 Tuning runner, configuration manager and result validator

Tuning runner and its two subcomponents – configuration manager and result validator, oversee both offline and online tuning. During offline tuning, result validator first computes reference output using a reference class or a kernel. Configurations generated by a kernel manager are then handed over to a configuration manager which

^{1.} Trivially copyable data type cannot have user-defined copy / move constructors, destructor or assignment operators and cannot contain virtual methods, which effectively makes it safe to copy with low-level functions such as std::memcpy.

instantiates a searcher based on user-specified search method. Kernels or kernel compositions are then launched in a loop using different configurations. The loop consists of the following steps:

- 1. Tuning runner retrieves next configuration from configuration manager. Order of tested configurations depends on a searcher which is a subcomponent of configuration manager.
- 2. Tuning runner launches a computation using previously retrieved configuration.
- 3. When computation is finished, the output is compared with previously generated reference output.
- 4. Computation duration is reported back to configuration manager, the duration can be utilized by a searcher to optimize exploration of configuration space. Durations for failed computations or invalid results are reported as infinity.

Once the loop has finished, tuning runner performs cleanup and the tuning results are stored for later retrieval.

Online tuning contains similar steps as offline tuning, except that it performs only single iteration of the previously described loop per online tuning method invocation. The other important difference is that if result validation is enabled, the reference output has to be recomputed for each configuration as the output between launches of individual configurations may change. Since online tuning method can be launched more times than the total number of available configurations, tuner always launches computation with the best found configuration after completing the traversal of configuration space.

5.5 Compute engine

Compute engine serves as an interface for implementing support for multiple compute APIs into KTT framework. It abstracts relatively complicated low-level compute API functions into smaller number of easier-to-use methods. It also provides automatic management of certain resources such as context, command queues, kernels and events. Other framework components then do not need to utilize the specific compute API functions but rather use unified compute engine interface. This simplifies addition of new compute APIs into KTT and makes it possible to support multiple APIs in a single version of KTT library.

Compute engine interface declares several virtual methods which need to be implemented by inheriting class that provides support for specific compute API. These include methods for running kernels, managing buffers, retrieving results, synchronizing command queues and querying for information about platforms and devices.

5.6 Kernel runner and manipulator interface

Kernel runner provides simplified methods for using compute engine to higher-level components such as tuner core or tuning runner. It handles running of kernels both with and without tuning manipulators. It also allows running of kernel compositions which always have to use tuning manipulator. Manipulators for individual kernels and compositions are stored inside this component as well.

Motivation for developing tuning manipulator API was to allow users to have greater control over the process of running kernel computations. For example, certain computations require running the same kernel multiple times in a loop, computing portion of the result directly in C++ code or utilizing multiple kernels. The main KTT API alone does not allow for such functionality because it provides only high-level kernel running methods which are easier to use but only support simpler use cases. In order to handle the complex scenarios, users need to have access to more fine-grained functionality, similar to what is offered by a previously described compute engine component.

However, exposing compute engine methods to public API directly would be problematic for two reasons. Firstly, as KTT framework is further developed, declarations of compute engine methods often change in order to support new functionality. This would force users to frequently update their code during transitions to newer versions of the framework. Secondly, significant number of compute engine methods are intended to be used together as a part of single computation (e.g., uploading kernel arguments into buffers followed by a

launch of kernel) and having these methods declared in the main API along with the high-level methods would cause confusion.

Because of these reasons, tuning manipulator and the related component called manipulator interface were developed. Users can define a class which inherits from tuning manipulator and consequently gain access to its methods, which provide functionality similar to compute engine. Tuning manipulator contains a private pointer to manipulator interface and internally calls its methods. Implementing class for the manipulator interface is a part of kernel runner and has direct access to compute engine. When a kernel or a composition utilizing tuning manipulator is run, kernel runner sets the manipulator interface pointer inside tuning manipulator to the implementing class and computation may then normally proceed. This way users have access to functionality of internal framework components without a need to directly expose these components to public API.

6 Advanced KTT usage examples

This chapter presents several examples which utilize advanced features of KTT framework. These include utilization of tuning manipulator, kernel compositions, online auto-tuning and integration of KTT into existing software. The examples were contributed to KTT framework by multiple authors.

6.1 Reduction example with tuning manipulator

This example demonstrates tuning of a kernel which performs summation of floating-point numbers contained in an array. It is possible to either finish the entire computation in a single kernel invocation utilizing atomic instructions or compute the result iteratively over multiple kernel launches. The second scenario requires usage of tuning manipulator. The example was originally published in [8].

It is split into three figures – Figure 6.1 contains the main part of a host program. Tuning parameters and constraints are defined in Figure 6.2 and Figure 6.3 includes definition of a manipulator.

Host program begins with initialization of data and kernel dimensions (lines 6-17), default NDRange size corresponds to a total number of elements rounded up to the nearest higher multiple of 512, which is the largest possible work-group size that kernel in this example utilizes. The following lines (19-27) contain initialization of tuner, addition of kernel and its arguments. Kernel output is validated using reference class (line 32). Since result of the computation is only a single number, validation range is set to one (line 33). Tuning manipulator is added to tuner in a similar fashion as a reference class (line 34). The manipulator in this example modifies certain kernel arguments whose ids are passed into its constructor. The remaining code section (lines 36-37) contains start of a tuning process and printing of results.

Tuning parameters are defined in Figure 6.2 (lines 5-9). The first parameter controls size of a work-group, same as in the simple example from Section 4.6. The next two parameters are used to control number of work-groups. Parameter "UNBOUNDED_WG" controls whether number of work-groups scales based on input size. If the scaling is disabled, then their number is controlled with parameter "WG_NUM"

whose values are set to a multiple of available compute units. The number of compute units and several other device parameters can be retrieved through KTT API (lines 2-3). Parameter "VECTOR_SIZE" controls which vector data type is used for input buffer. This parameter also divides the global size because more elements are processed by a single work-item when longer vector types are used. The last parameter determines whether the computation is done in a single kernel execution or iterative kernel launches are utilized. The example also makes use of multiple parameter constraints (lines 11-16). For example, the first constraint ensures that only one of the parameters which affect number of work-groups remains active inside a configuration.

Tuning manipulator is defined in Figure 6.3. Apart from constructor, it contains definition of a method which performs the computation. First, it retrieves information about current configuration (lines 6-9), including parameters and modified kernel dimensions. If "UN-BOUNDED_WG" parameter is inactive, it sets NDRange size based on a value of "WG_NUM" parameter (lines 10-12). The kernel is then launched (line 13) using the corresponding global and local size. In case atomic operations are used, the computation is then finished and tuning manipulator ends. Otherwise kernel is launched repeatedly in O(log(n)) iterations, input size shrinking by a factor of work-group size multiplied by vector length in each iteration (lines 15-36). Because an output from one iteration is used as an input in next iteration, the source and destination buffers keep getting swapped (line 22). As the input size continuously shrinks, NDRange size and several kernel arguments have to be updated in each iteration (lines 23-28). Once the input size reaches 1, the computation is finished. One extra iteration is sometimes performed in order to ensure that result is inside the original destination buffer.

```
int main(int argc, char** argv)
  {
2
      // Initialize platform / device index and path to kernel file.
      const int n = 32 * 1024 * 1024;
      const int nAlloc = ((n + 16 - 1) / 16) * 16;
      std::vector<float> src(nAlloc, 0.0f);
      std::vector<float> dst(nAlloc, 0.0f);
      int nUp = ((n + 512 - 1) / 512) * 512;
10
      ktt::DimensionVector ndRangeDimensions(nUp);
      ktt::DimensionVector workGroupDimensions(1);
12
13
      for (int i = 0; i < n; i++)</pre>
          src[i] = 1000.0f * ((float)rand()) / ((float)RAND_MAX);
16
17
18
      ktt::Tuner tuner(platformIndex, deviceIndex);
      ktt::KernelId kernelId = tuner.addKernelFromFile(kernelFile, "reduce",
20
          ndRangeDimensions, workGroupDimensions);
      ktt::ArgumentId srcId = tuner.addArgumentVector(src, ktt::ReadWrite);
      ktt::ArgumentId dstId = tuner.addArgumentVector(dst, ktt::ReadWrite);
      ktt::ArgumentId nId = tuner.addArgumentScalar(n);
23
      int offset = 0;
24
      ktt::ArgumentId inOffsetId = tuner.addArgumentScalar(offset);
25
      ktt::ArgumentId outOffsetId = tuner.addArgumentScalar(offset);
      tuner.setKernelArguments(kernelId, std::vector<ktt::ArgumentId>{srcId,
          dstId, nId, inOffsetId, outOffsetId});
      // Definition of tuning parameters and constraints is in separate figure.
30
31
      tuner.setReferenceClass(kernelId, std::make_unique<ReferenceReduction>(src,
          dstId), std::vector<ktt::ArgumentId>{dstId});
      tuner.setValidationRange(dstId, 1);
      tuner.setTuningManipulator(kernelId,
34
           std::make_unique<TunableReduction>(srcId, dstId, nId, inOffsetId,
           outOffsetId));
35
      tuner.tuneKernel(kernelId);
36
      tuner.printResult(kernelId, "reduction_output.csv", ktt::PrintFormat::CSV);
37
      return 0;
38
  }
39
```

Figure 6.1: Main part of the reduction host program.

```
1
      const ktt::DeviceInfo di = tuner.getCurrentDeviceInfo();
      size_t cus = di.getMaxComputeUnits();
      tuner.addParameter(kernelId, "WORK_GROUP_SIZE_X", {32, 64, 128, 256, 512},
          ktt::ModifierType::Local, ktt::ModifierAction::Multiply,
          ktt::ModifierDimension::X);
      tuner.addParameter(kernelId, "UNBOUNDED_WG", {0, 1});
      tuner.addParameter(kernelId, "WG_NUM", {0, cus, cus * 2, cus * 4, cus * 8,
          cus * 16});
      tuner.addParameter(kernelId, "VECTOR_SIZE", {1, 2, 4, 8, 16},
          ktt::ModifierType::Global, ktt::ModifierAction::Divide,
          ktt::ModifierDimension::X);
      tuner.addParameter(kernelId, "USE_ATOMICS", {0, 1});
10
      auto persistConstraint = [](std::vector<size_t> v) {return (v[0] == 1 &&
          v[1] == 0) \mid \mid (v[0] == 0 \&\& v[1] > 0);;
      tuner.addConstraint(kernelId, persistConstraint, {"UNBOUNDED_WG",
          "WG_NUM"});
      auto persistentAtomic = [](std::vector<size_t> v) {return (v[0] == 1) ||
13
          (v[0] == 0 \&\& v[1] == 1);;
      tuner.addConstraint(kernelId, persistentAtomic, {"UNBOUNDED_WG",
          "USE_ATOMICS"});
      auto unboundedWG = [](std::vector<size_t> v) {return (v[0] == 0 || v[1] >=
          32);};
      tuner.addConstraint(kernelId, unboundedWG, {"UNBOUNDED_WG",
          "WORK_GROUP_SIZE_X"});
17
       . . .
```

Figure 6.2: Definition of tuning parameters and constraints in reduction host program.

```
class TunableReduction : public ktt::TuningManipulator {
   public:
    // Constructor initializes private manipulator attributes.
    void launchComputation(const ktt::KernelId kernelId) override {
          ktt::DimensionVector globalSize = getCurrentGlobalSize(kernelId);
          ktt::DimensionVector myGlobalSize = globalSize;
          ktt::DimensionVector localSize = getCurrentLocalSize(kernelId);
          auto parameterValues = getCurrentConfiguration();
          if (getParameterValue("UNBOUNDED_WG", parameterValues) == 0) {
10
              myGlobalSize = ktt::DimensionVector(getParameterValue("WG_NUM",
                  parameterValues) * localSize.getSizeX());
12
          runKernel(kernelId, myGlobalSize, localSize);
          if (getParameterValue("USE_ATOMICS", parameterValues) == 0) {
15
              size_t n = globalSize.getSizeX() / localSize.getSizeX();
16
              size_t inOffset = 0, outOffset = n, iterations = 0;
              size_t vectorSize = getParameterValue("VECTOR_SIZE",
                  parameterValues);
              size_t wgSize = localSize.getSizeX();
19
              while (n > 1 \mid | \text{ iterations } \% 2 == 1) {
                  swapKernelArguments(kernelId, srcId, dstId);
22
                  myGlobalSize.setSizeX((n + vectorSize - 1) / vectorSize);
23
                  myGlobalSize.setSizeX(((myGlobalSize.getSizeX() - 1) / wgSize +
24
                      1) * wgSize);
                  if (myGlobalSize == localSize) outOffset = 0;
25
                  updateArgumentScalar(nId, &n);
                  updateArgumentScalar(outOffsetId, &outOffset);
                  updateArgumentScalar(inOffsetId, &inOffset);
29
                  runKernel(kernelId, myGlobalSize, localSize);
30
                  n = (n + wgSize * vectorSize - 1) / (wgSize * vectorSize);
                  inOffset = outOffset / vectorSize;
                  outOffset += n;
                  iterations++;
              }
          }
36
      }
37
38
  private:
      // Attributes are ids of kernel arguments passed to manipulator constructor.
40
  };
41
```

Figure 6.3: Tuning manipulator for reduction kernel.

6.2 Sorting example with kernel compositions

This example showcases tuning of a radix sort computation on an array of integers which utilizes three separate kernels. The first kernel builds a per-block histogram of each digit. The histograms are then used as an input for the second kernel which performs a top-level exclusive scan on them. The scanned histograms are then processed by the final kernel which also writes a final result into global memory. The original kernels without tuning parameters were taken from SHOC Benchmark Suite [12].

The example is split into two figures – Figure 6.4 contains a host program and Figure 6.5 includes a definition of launchComputation() method inside tuning manipulator.

The host program begins with initialization of tuner and kernel dimensions (lines 4-7). Since both NDRange and work-group size for all kernels are controlled with tuning manipulator, they are set here to 1. Next, individual kernels (lines 9-11) and their arguments are added to tuner. The argument addition is not included in this example due to its length, however it happens in a similar way as in previous examples. Line 15 contains addition of kernel composition with specification of included kernels and creation of composition manipulator. The ids of kernel arguments that will be updated are once again passed into its constructor. Kernel arguments are then set individually for each kernel inside the newly defined composition (lines 16-18). The kernels in this example support three different tuning parameters (lines 20-22). They are all fairly standard – the first parameter controls utilization of vector data types, the second one affects size of a work-group and the final parameter changes NDRange size and therefore affects number of work-groups required to compute the result. Parameters are defined at composition level and are visible to all of the included kernels. It remains for user to decide exactly which kernels are affected by individual parameters inside kernel source code. There is a single combination of "LOCAL_SIZE" and "GLOBAL_SIZE" parameters that is unsupported by implemented kernels. It is eliminated with a definition of constraint (line 24). The figure ends with an addition of reference class that performs the sorting on a CPU, launch of a tuning and printing of results (lines 26-28).

Figure 6.5 contains a computation launch method inside manipulator. The method first retrieves configuration and sets the kernel dimensions accordingly (lines 2-7). Afterwards, several arguments are updated based on the previously set dimensions (lines 9-16). Currently there is a limitation for updating vector arguments – it is not possible to simply resize the argument without also providing a new data. Here it is solved by creating an artificial buffer with size corresponding to new argument size (lines 15-16). In this case, it does not have a significant negative impact on performance, but vector argument resize method is planned to be added to manipulator API nonetheless. Result is then computed in iterations with three composition kernels being launched with previously set kernel dimensions (lines 28-30). The work in second kernel is done by a single work-group. Additionally, the first and third kernels have their input and output buffers swapped on each iteration (lines 21-26, 32). If the final output ends up in input buffer after last iteration, it is moved into the correct output buffer and computation is finished (lines 36-37).

6.3 Integrating KTT into software and online auto-tuning

This section briefly introduces a software for 3D Fourier reconstruction. The introduction is followed by motivation for implementing online auto-tuning into this software, description of implementation and evaluation of auto-tuning impact.

6.3.1 3D Fourier reconstruction in Xmipp

Xmipp¹ is a software for cryo-electron microscopy (cryo-EM). It contains several tools used for processing different steps of cryo-EM image reconstruction pipeline. The pipeline has several computational bottlenecks, one of them being 3D Fourier reconstruction [6]. The 3D Fourier reconstruction builds a 3D volume in Fourier space from a set of Fourier transforms of specimen's 2D projections. Essentially, the reconstruction algorithm inserts 2D images with different rotations into a 3D grid using an interpolation kernel.

^{1.} Website: http://xmipp.cnb.csic.es

```
int main(int argc, char** argv) {
      // Initialize platform / device index and path to kernel file.
2
      ktt::Tuner tuner(platformIndex, deviceIndex);
      std::vector<ktt::KernelId> kernelIds(3);
      const ktt::DimensionVector ndRangeDimensions(1);
      const ktt::DimensionVector workGroupDimensions(1);
      kernelIds[0] = tuner.addKernelFromFile(kernelFile, std::string("reduce"),
          ndRangeDimensions, workGroupDimensions);
      kernelIds[1] = tuner.addKernelFromFile(kernelFile, std::string("top_scan"),
10
          workGroupDimensions, workGroupDimensions);
      kernelIds[2] = tuner.addKernelFromFile(kernelFile,
          std::string("bottom_scan"), ndRangeDimensions, workGroupDimensions);
      // Addition of kernel arguments.
13
14
      ktt::KernelId compositionId = tuner.addComposition("sort", kernelIds,
15
          std::make_unique<TunableSort>(kernelIds, size, inId, outId, isumsId,
          sizeId, localMem1Id, localMem2Id, localMem3Id, numberOfGroupsId,
          shiftId)):
      tuner.setCompositionKernelArguments(compositionId, kernelIds[0],
16
          std::vector<size_t>{inId, isumsId, sizeId, localMem1Id, shiftId});
      tuner.setCompositionKernelArguments(compositionId, kernelIds[1],
17
          std::vector<size_t>{isumsId, numberOfGroupsId, localMem2Id});
      tuner.setCompositionKernelArguments(compositionId, kernelIds[2],
18
          std::vector<size_t>{inId, isumsId, outId, sizeId, localMem3Id,
          shiftId});
19
      tuner.addParameter(compositionId, "FPVECTNUM", {4, 8, 16});
20
      tuner.addParameter(compositionId, "LOCAL_SIZE", {128, 256, 512});
      tuner.addParameter(compositionId, "GLOBAL_SIZE", {512, 1024, 2048, 4096,
          8192, 16384, 32768});
      auto workGroupConstraint = [](std::vector<size_t> vector) {return
          vector.at(0) != 128 || vector.at(1) != 32768;};
      tuner.addConstraint(compositionId, workGroupConstraint, {"LOCAL_SIZE",
24
          "GLOBAL_SIZE"});
      tuner.setReferenceClass(compositionId,
          std::make_unique<ReferenceSort>(input),
          std::vector<ktt::ArgumentId>{outId});
      tuner.tuneKernel(compositionId);
      tuner.printResult(compositionId, std::string("sort result.csv"),
28
          ktt::PrintFormat::CSV);
      return 0;
29
   }
30
```

58

Figure 6.4: Sorting host program.

```
void launchComputation(const ktt::KernelId) override {
      const int radixWidth = 4;
      std::vector<ktt::ParameterPair> parameterValues = getCurrentConfiguration();
      size_t localSize = getParameterValue("LOCAL_SIZE", parameterValues);
      const ktt::DimensionVector workGroupDimensions(localSize);
      size_t globalSize = getParameterValue("GLOBAL_SIZE", parameterValues);
      const ktt::DimensionVector ndRangeDimensions(globalSize);
      size_t numberOfGroups = globalSize / localSize;
      updateArgumentScalar(numberOfGroupsId, &numberOfGroups);
10
      updateArgumentLocal(localMem1Id, localSize);
      updateArgumentLocal(localMem2Id, 2 * localSize);
      updateArgumentLocal(localMem3Id, 2 * localSize);
      size_t isumsSize = (numberOfGroups * 16 * sizeof(unsigned int));
      std::vector<unsigned int> is(isumsSize);
      updateArgumentVector(isumsId, is.data(), isumsSize);
16
      bool inOutSwapped = false;
18
      for (int shift = 0; shift < sizeof(unsigned int) * 8; shift+=radix_width) {</pre>
          updateArgumentScalar(shiftId, &shift);
20
          bool even = ((shift / radix_width) % 2 == 0) ? true : false;
          if (even) {
              changeKernelArguments(kernelIds[0], {inId, isumsId, sizeId,
                  localMem1Id, shiftId});
          } else {
24
              changeKernelArguments(kernelIds[0], {outId, isumsId, sizeId,
25
                  localMem1Id, shiftId});
          runKernel(kernelIds[0], ndRangeDimensions, workGroupDimensions);
          runKernel(kernelIds[1], workGroupDimensions, workGroupDimensions);
          runKernel(kernelIds[2], ndRangeDimensions, workGroupDimensions);
30
31
          swapKernelArguments(kernelIds[2], inId, outId);
          if (shift + radix_width < sizeof(unsigned int) * 8)</pre>
              inOutSwapped = !inOutSwapped;
      }
      if (inOutSwapped)
          copyArgumentVector(outId, inId, size);
37
   }
38
```

Figure 6.5: Computation method inside tuning manipulator in sorting example.

The CUDA-based GPU acceleration of 3D Fourier reconstruction has been introduced in [7]. The algorithm uses a gather memory access pattern, which parallelizes the computation over a 3D domain, so there are no race conditions in updating voxel data. In contrast to previously used scatter pattern, the gather-based implementation is faster but relatively complex, exposing several tuning parameters which are listed in Table 6.1.

Originally, KTT 0.5 has been integrated into 3D Fourier reconstruction for offline tuning and values of tuning parameters for various hardware have been manually exported into the code. The tuning results showed poor performance portability across GPUs, even within the same generation (the worst performance portability has been measured between Maxwell generation GeForce GTX750 and Pascal generation Tesla P100 – the code tuned for P100 and executed on GTX750 performed at 31% of the fastest GTX750 implementation). Moreover, the size of samples inserted into 3D domain influences selection of optimal tuning parameters. The tuning has to be repeated for samples of different size, otherwise suboptimal performance is obtained, as can be seen in Table 6.2.

The disadvantage of offline tuning in this scenario is that it is impractical for all combinations of hardware and input sizes. Furthermore, it is also possible to configure interpolation window size, which has an influence on the optimal selection of tuning parameter values. These problems can be solved by introducing online tuning.

6.3.2 Online tuning implementation

When utilizing online tuning, implementation of the kernel can be changed during program execution. In order to support it, all CUDA code which directly accesses a GPU has to be removed from 3D Fourier reconstruction code and replaced with calls to KTT framework. A pseudocode of the reconstruction is shown in Algorithm 1. The output volumes *G* (Fourier transform of the volume) and *W* (weights for 3D voxels) are initialized at the beginning of the computation. In loop at line 3, the samples are added into 3D volume. More precisely, the samples are packed into buffers of predefined size, their Fourier transform is computed on a CPU, copied into GPU memory and then GPU kernel is executed to insert the samples into volumes *G*, *W*. During offline

Parameter	Values	Description	
BLOCK_DIM	8, 12, 16, 20, 24, 28, 32	dimensions of a thread block	
ATOMICS	0, 1	allows (1) or prohibits (0) usage of atomic updates for accessing 3D volume	
GRID_DIM_Z	1, 4, 8, 16	number of samples processed in parallel, must be 1 if ATOMICS=0	
PRECOMP_INT	0, 1	use on-the-fly computation (0) or precomputation (1) of interpolation weights	
SHARED_INT	0, 1	cache precomputed interpolation weight in shared memory (1) or read it directly from global memory (0), set only when PRECOMP_INT=1	
SHARED_IMG	0, 1	cache input sample in shared memory (1) or read it directly from global memory (0), may be 1 only if SHARED_INT=0 due to limited shared memory capacity in current GPUs	
TILE_SIZE	1, 2, 4, 8	size of a tile formed from threads, TILE>1 is allowed only when SHARED_IMG=0, it must divide BLOCK_DIM	

Table 6.1: Tuning parameters used in 3D Fourier reconstruction, taken from [7].

Tesla P100	256x256	128x128	64x64	50x50
256x256	100%	100%	50%	32%
128x128	100%	100%	50%	32%
64x64	64%	82%	100%	90%
50x50	56%	67%	91%	100%

Table 6.2: Performance portability on Tesla P100, where code is tuned for (rows) / executed (columns) with different image sizes.

tuning, only one buffer has to be prepared and used with altering kernel implementations in order to find the fastest one.

Online tuning has to perform both tuning and computation at the same time. Therefore, all input and output data have to be managed by KTT during the whole program execution. In the loop in line 3, the data are prepared on CPU, then a KTT method which launches online tuning is executed. The method selects a new combination of tuning parameters and executes a tuning manipulator. The manipulator first copies buffer s_f into GPU memory and then executes a kernel, which inserts samples from s_f into volumes G, W. The kernel execution is asynchronous, so CPU may compute FFT of another buffer while kernel is still running. The manipulator may execute kernel iteratively or just once, depending on whether atomic operations are switched off or on with a tuning parameter.

Algorithm 1 3D reconstruction

- 1: initialize output volumes *G*, *W* in GPU memory to zero
- 2: initialize buffer of sample's Fourier Transform s_f in GPU memory
- 3: for all $s \in S$ do
- 4: $s_f \leftarrow FFT(s)$ on CPU
- 5: upload s_f to GPU
- 6: insert trans. samples from s_f into G, W
- 7: end for
- 8: download *G*, *W* to CPU memory
- 9: apply weights *W* to *G* and perform inverse transform of *G*

6.3.3 Evaluation

In order to evaluate online auto-tuning with 3D Fourier reconstruction, two experiments were designed:

- tuner overhead measurement;
- amortized performance measurement.

The first experiment measures an overhead added by the tuner. The space of tuning parameters was modified to contain only one configuration. In such case, KTT performs a single kernel compilation, concludes the tuning and then just executes the computation. The timing of such computation is compared against the original implementation which accessed CUDA API directly. If there was any significant overhead created by the tuner (e.g., an overhead in some tuning method or a limitation of KTT design, requiring to use a GPU in less efficient way), the timing of online-tuned implementation would be significantly worse. Otherwise, the version with online tuning would perform similarly to the original version.

The second experiment evaluates the benefit of online tuning. The experiment consists of the following steps:

- execution of code which was tuned offline for different hardware and samples resolution (so it would be suboptimal with current setup);
- execution of code which was tuned offline for the same hardware but different samples resolution (reflects current Xmipp implementation);
- execution of code which was tuned offline for utilized hardware and samples resolution (this is an upper-bound for online tuning, as the tuning overhead is completely removed by offline tuning);
- execution of code utilizing online tuning which is not tuned for any specific hardware or samples resolution.

This experiment highly depends on a given computation problem, selection of tuning parameters and optimization method. However, a

convergence of performances of online and offline tuned code should still be seen after sufficient amount of time, once tuning overhead (kernel compilation, execution of suboptimal kernels) is amortized.

To conduct the experiments, a desktop computer equipped with Intel Core i7-3820 (4 cores at 3.6 GHz) and GeForce GTX 1070 was utilized. The benchmark has been performed using projection images of the Brome Mosaic Virus [9] in resolution 83×83 pixels.

The first experiment has been performed using 15,697 images. The runtime of the original, offline tuned code is 49.81 s, the online tuned code with only one combination of tuning parameters is 51.06 s, so the overhead of added online tuning is 2.5%. This overhead is negligible compared to performance differences in tuned code (see Table 6.2).

The second experiment tests how the overall performance (including all the overhead of the initial tuning) is changing in time. Images in resolution 83 × 83 pixels were used and online tuning was configured in such a way that it performs tuning during first 50 kernel executions and computation with the fastest kernel afterwards. The tuning uses Markov chain Monte Carlo search method. As the search method is stochastic, 10 individual tunings were performed, the results are shown for the best and worst-performing one. The performance is measured in millions of images added to 3D space per second. As can be seen in Figure 6.6, the performance of online tuning is poor during first 25 seconds where new kernels are compiled and tested. Afterwards, the overhead of initial tuning process is amortized quite quickly. The original code version tuned for Maxwell GPU and images of resolution 128×128 is outperformed after 43-54 seconds. The code tuned for GeForce GTX 1070 and image resolution 128×128 is outperformed after 98-192 seconds. Note that the fastest kernel is executed immediately after tuning has finished (approximately after 25 seconds). However, it takes some time to amortize the overhead of the initial tuning. The original code tuned offline for GeForce GTX 1070 and image size 83×83 shows an upper-bound for the test. It cannot be achieved by online auto-tuning, as all combinations of tuning parameters are explored in offline tuning, but its overhead is not included in measurement.

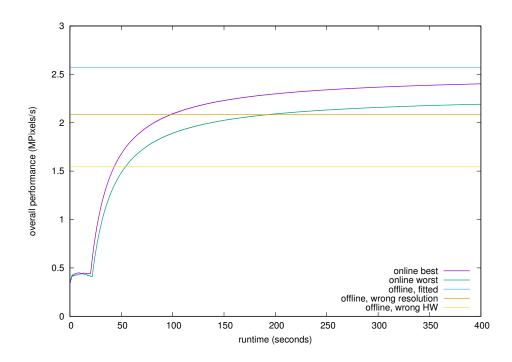


Figure 6.6: Performance comparison of offline and online tuned code.

7 Conclusion

The framework developed as a part of this thesis contains all the functionality needed to fulfill the assignment. Certain features such as tuning manipulators or possibility of online tuning are not yet supported by any other publicly available framework and KTT therefore offers improvements over current state-of-the-art auto-tuning software. Furthermore, it was demonstrated that the stated features can be used in practice in scenarios such as auto-tuning of non-trivial computations which utilize multiple kernels or integration into other software where it can be used to combine online tuning with regular computation.

However, there is still a lot of room left for improvements and many ways in which the framework could be extended. It would be interesting to explore viability of auto-tuning in area of graphics applications and shaders with addition of support for APIs such as Vulkan or OpenGL. Another improvement could be made in the area of tuning for different input sizes since the tuner currently assumes that the input size does not change significantly during exploration of configuration space. The exploration itself could use some additional improvements as well with support for more search optimization techniques. It would be also useful to develop a tool which analyses the impact of individual tuning parameters and their combinations on performance on specific devices or a tool for tuning results visualization.

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A Electronic attachment

Electronic attachment for the thesis is available in Information System of Masaryk University. It contains the following materials:

- thesis text in PDF format
- full source code for version 0.6 of KTT framework
- supplementary KTT framework materials such as API documentation, tutorials and example projects