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Autotuning
Introduction to autotuning, overview of our research

Jiří Filipovič et al.

Fall 2024

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Program development workflow

Implementation questions

- which algorithm to use?
- how to implement the algorithm efficiently?
- how to set-up a compiler?

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Program development workflow

Compiler's questions

- how to map variables to registers?
- which unrolling factor to use for a loop?
- which functions should be inlined?
- and many others...

Program development workflow

Execution

- how many nodes and threads assign to the program?
- should accelerators be used?
- how to mix MPI and OpenMP threads?

Program development workflow

Execution

- how many nodes and threads assign to the program?
- should accelerators be used?
- how to mix MPI and OpenMP threads?

A compiler works with **heuristics**, people usually too.

Tuning of the program

We can empirically tune those possibilities

- use different algorithm

- change code optimizations

- use different compiler flags

- execute in a different number of threads

- etc.

Tuning of the program

A tuning allows us to outperform heuristics – we just test what works better.

- however, we have to invest more time into development
- there are vertical dependencies, so we cannot perform tuning steps in isolation
- the optimum usually **depends on hardware and input**

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Autotuning

The tuning can be automated

- then we talk about **autotuning**

Autotuning

- in design time, we define the space of *tuning parameters*
- each tuning parameter defines some property of the tuned application
- during autotuing, a search method is used to traverse assign optimal values for tuning parameters
- performed according to some objective, usually performance

Taxonomy of Autotuning

Tuning scope

- what properties of the application are changed by autotuner
- e.g. compiler flags, number of threads, source code optimizations parameters

Tuning time

- offline autotuning (performed once, e.g., after SW installation)
- dynamic autotuning (performed in runtime)

Developer involvement

- transparent, or requiring only minor developer assist (e.g. compiler flags tuning)
- application-level, requiring an expert programmer to identify tunning opportunities (e.g. code optimizations parameters tuning)

Our focus

We target autotuning of code optimization parameters

- the source code is changed during a tuning process
- the user defines how tuning parameters influence the code
- very powerful (source code may control nearly everything)
- autotuning framework implementation is difficult
  - requires recompilation
  - runtime checks of correctness/precision
  - non-trivial expression of tuning parameters
  - we have no implicit assumptions about tuning space
- heterogeneous computing (we are tuning OpenCL or CUDA code)
- offline and dynamic autotuning

Motivation Example

Let's solve a simple problem – vectors addition

- we will use CUDA
- we want to optimize the code

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Motivation Example

```
__global__ void add(float* const a, float* b) {
    int i = blockIdx.x*blockDim.x + threadIdx.x;
    b[i] += a[i];
}
```

It should not be difficult to write different variants of the code...

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Optimization

```
__global__ void add(float4* const a, float4* b) {
    int i = blockIdx.x*blockDim.x + threadIdx.x;
    b[i] += a[i];
}
```

Kernel has to be executed with n/4 threads.

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Optimization

```
__global__ void add(float2* const a, float2* b) {
    int i = blockIdx.x*blockDim.x + threadIdx.x;
    b[i] += a[i];
}
```

Kernel has to be executed with n/2 threads.

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Optimization

```
__global__ void add(float* const a, float* b, const int n) {
    int i = blockIdx.x*blockDim.x + threadIdx.x;
    for (; i < n; i += blockDim.x*gridDim.x)
        b[i] += a[i];
}
```

Kernel has to be executed with n/m threads, where *m* can be anything.

What to Optimize?

Mixture of:

- thread-block size
- vector variables
- serial work

i.e. 3D space – and this is trivial example...

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Autotuning

Autotuning tools explore code parameters automatically

```
__global__ void
add(VECTYPE* const a, VECTYPE* b, const int n) {
    int i = blockIdx.x*blockDim.x + threadIdx.x;
#if SERIAL_WORK > 1
    for (; i < n; i += blockDim.x*gridDim.x)
#endif
        b[i] += a[i];
}
```

The code executing kernel add has to configure parallelism
according to values of VECTYPE and SERIAL_WORK tuning
parameters.

Kernel Tuning Toolkit

We have developed a Kernel Tuning Toolkit (KTT) [5]

- a framework allowing to tune code parameters for OpenCL and CUDA
- allows both offline and dynamic tuning
- enables cross-kernel optimizations
- tuning problem described in C++, python, or JSON input
- mature implementation, documented, with examples
- https://github.com/HiPerCoRe/KTT

[5] Filip Petrovič and Jiří Filipovič. "Kernel Tuning Toolkit". In: SoftwareX 22 (2023), p. 101385

Kernel Tuning Toolkit

Typical workflow in C++ similar to CUDA/OpenCL

- initialize the tuner for a specified device
- create an input/output of the kernel
- create a kernel
- create a tuning space for the kernel
- assign input/output to the kernel
- execute or tune the kernel

KTT creates a layer between an application and OpenCL/CUDA.

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KTT Sample Code

```
// Initialize tuner and kernel definition
ktt::Tuner tuner(platformIndex, deviceIndex);

const ktt::DimensionVector ndRangeDimensions(inputSize);
const ktt::DimensionVector workGroupDimensions(128);
ktt::KernelId fooDef = tuner.AddKernelDefinitionFromFile("foo",
  ndRangeDimensions, workGroupDimensions);

// Creation and assign of kernel arguments
ktt::ArgumentId a = tuner.AddArgumentVector(srcA,
  ktt::ArgumentAccessType::ReadOnly);
ktt::ArgumentId b = tuner.AddArgumentVector(srcB,
  ktt::ArgumentAccessType::WriteOnly);
tuner.SetArguments(fooDef, {a, b});

// Create kernel and its tuning space
ktt::KernelId foo = tuner.CreateSimpleKernel("foo", fooDef);
tuner.AddParameter(foo, "UNROLL", {1, 2, 4, 8});

tuner.Tune(foo);
tuner.SaveResult(foo, "foo-output", ktt::PrintFormat::JSON);
```

Alternative KTT usage

Python

- similar to C++ (use C++ bindings)
- input/output as numpy arrays
- easier rapid experimenting

JSON

- declarative way
    - defines input/output (generated, binary)
    - defines tuning space
    - configures tuning space
- can be loaded in C++/python, or run by provided miniapp
- allows interoperability between KTT and Kernel Tuner (and hopefuly more autotuners in future)

Kernel Tuning Toolkit

In practise, we usually need more functionality

- tuning parameters can affect parallelism configuration (e.g. block and grid size in CUDA)
    - by pre-defined functions (e.g. multiply specified block/grid dimmension)
    - by lambda function provided by programmer
- some combinations of tuning parameters can be discarded *a priori*
    - lambda functions constraining tuning space
- KTT can check, if tuned kernel runs successfully
    - automatic check of successful execution
    - user can provide reference kernel, or reference class, and comparing function, KTT compares results automatically

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Advanced features of KTT

Cross-kernel optimizations

- the user can define a *kernel launcher*: the code defining how are kernel(s) executed
  - default launcher just execute a kernel
- can query tuning parameters
- can call multiple kernels or the same kernel multiple times
- can execute host code, and host-device memory transfers
- allows tuning code parameters with wider influence, as tuned kernels do not need to be functionally equivalent

Reduction

new kernel

atomic
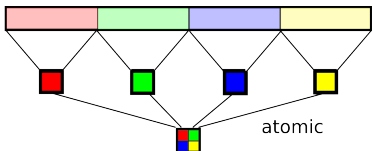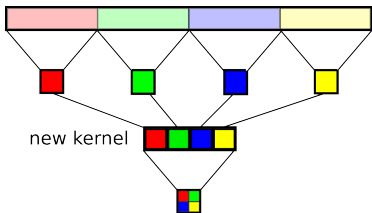
Advanced features of KTT

Dynamic autotuning [6]

- dynamic tuning performs autotuning during application runtime
- KTT can execute the best kernel known so far to perform kernel's task
- or try different combination of tuning parameters before the execution
- tuning is transparent for the application
- tuning can be queried in any time

[6] F. Petrovič et al. "A benchmark set of highly-efficient CUDA and OpenCL kernels and its dynamic autotuning with Kernel Tuning Toolkit". In: *Future Generation Computer Systems* 108 (2020), pp. 161–177. DOI: 10.1016/j.future.2020.02.069

Dynamic Tuning Sample

```
// Main application loop
while (application_run) {
  ...
  if (tuningRequired)
    tuner.TuneIteration(foo, output);
  else {
    ktt::KernelConfiguration best =
      tuner->GetBestConfiguration(foo);
    tuner.Run(foo, best, output);
  }
  ...
}
```
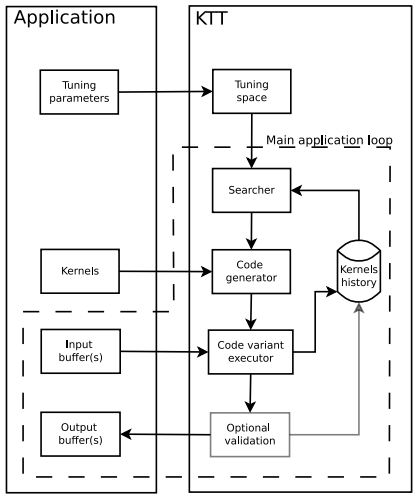
Dynamic tuning

Dynamic autotuning is challenging

- when the kernel is executed, there must be no significant performance drop
- automatic memory management has to move only necessary data
- KTT has to support asynchronous execution of
  - memory copy, host and device code execution
  - simultaneous execution of multiple kernels

Parallelism in KTT

- intra-launcher: parallelism inside kernel launcher
- global parallelism: asynchronous execution of multiple launcher instances

During autotuning, global parallelism has to be disabled.

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KTT Architecture

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Benchmark set

Benchmark	dimensions	configurations
BiCG	11	5,122
Convolution	10	5,248
Coulomb 3D	8	1,260
GEMM	15	241,600
GEMM batched	11	424
Hotspot	6	480
Transpose	9	10,752
N-body	8	9,408
Reduction	5	175
Fourier	6	360

Table: A list of the benchmarks and the size and dimensionality (i.e., the number of tuning parameters) of their tuning spaces.

Testbed setup

Device	Architecture	SP perf.	BW
2× Xeon E5-2650	Sandy Bridge	512	102
Xeon Phi 5110P	Knights Corner	2,022	320
Tesla K20	Kepler	3,524	208
GeForce GTX 750	Maxwell	1,044	80
GeForce GTX 1070	Pascal	5,783	256
Radeon RX Vega 56	GCN 5	8,286	410
GeForce RTX 2080Ti	Turing	11,750	616

Table: Devices used in our benchmarks. Arithmetic performance (SP perf.) is measured in single-precision GFlops, memory bandwidth (BW) is measured in GB/s.

Performance

Benchmark	2080Ti	1070	750	K20	Vega56	E5-2650	5110P
BiCG	88.3%	84.7%	81.7%	50.4%	75.6%	46.0%	6.45%
Coulomb 3D	91.8%	91.4%	84.3%	43.2%	65.3%	74.2%	22.2%
GEMM	79.8%	80.6%	91.1%	51.3%	96.3%	37.5%	19.7%
GEMM batched	86.8%	81.4%	90.0%	49.6%	86.0%	27.7%	20.9%
Transpose	87.1%	80.2%	86.3%	64.2%	86.1%	62.5%	10.0%
N-body	89.7%	86.6%	87.7%	40.6%	82.2%	77.7%	29.9%
Reduction	68.7%	87.5%	89.4%	64.1%	71.6%	33.9%	10.1%
Hotspot	1.35×	1.94×	2.06×	1.4×	2.88×	1.2×	12.8×

Table: Performance of benchmarks autotuned for various hardware devices. The performance relative to the theoretical peak of devices.

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Performance portability

Benchmark	GPU→GPU		
	avg±stdev	worst	failed
BiCG	89.0%±12.3%	57%	1
Convolution	79.4%±14.9%	55%	3
Coulomb 3D	95.8%±6.5%	67%	0
GEMM	83.6%±16.4%	31%	0
GEMM batched	85.4%±17%	37%	0
Hotspot	80.3%±17.5%	46%	3
Transpose	85.0%±21.9%	8%	3
N-body	78.8%±24.2%	2%	3
Reduction	88.4%±24%	12%	3
Fourier	74.5%±30%	31%	0

Table: Relative performance of benchmarks ported across GPU
architectures without re-tuning.

Dynamic autotuining of Batched GEMM
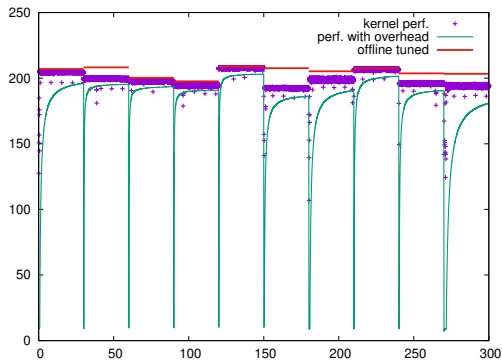
Figure: Batched GEMM on GeForce GTX 1070.

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Dynamic autotuining of Batched GEMM
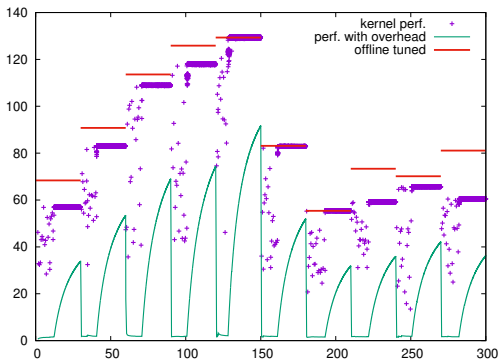
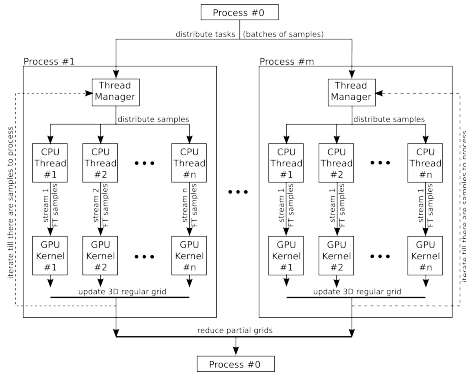Figure: Batched GEMM on Tesla K20.

3D Fourier Reconstruction

Figure: Performance of dynamic tuned 3D Fourier reconstruction [8] .

[8] D. Střelák et al. "A GPU Acceleration of 3D Fourier Reconstruction in Cryo-EM". In: *The International Journal of High Performance Computing Applications* 0 (0 2019). DOI: 10.1177/1094342019832958

3D Fourier Reconstruction

	2080Ti	1070	750	680
2080Ti	100%	99%	31%	49%
1070	99%	100%	31%	50%
750	43%	67%	100%	94%
680	60%	72%	71%	100%

Table: Performance portability of 3D Fourier reconstruction with 128×128 samples.

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3D Fourier Reconstruction

	128x128	91x91	64x64	50x50	32x32
128x128	100%	100%	77%	70%	32%
91x91	100%	100%	76%	68%	33%
64x64	94%	94%	100%	91%	67%
50x50	79%	78%	98%	100%	86%
32x32	65%	67%	80%	92%	100%

Table: Performance portability on GeForce GTX1070 for different samples.

3D Fourier Reconstruction

	best runtime	tuning 50	tuning full
2080Ti	1m40s	88% $\pm$ 3%	54%
1070	5m49s	96% $\pm$ 2%	79%
750	16m59s	92% $\pm$ 4%	72%
680	15m12s	94% $\pm$ 2%	75%

Table: The relative performance of dynamically-tuned 3D Fourier reconstruction.

Dynamic autotuning of SpMV

SpMV is important kernel in many applications

- perform multiplication of sparse matrix with dense vector
- system of equations solving, graph processing, . . .

Challenging to compute efficiently

- optimization decisions strongly dependent on input structure

Dynamic autotuning of SpMV

Multiple libraries available

- cuSPARSE – closed-source library actively developed by NVIDIA
- CUSP – open-source library released by NVIDIA, slower compared to cuSPARSE

Our goal

- insert dynamic autotuning into CUSP for DIA, ELL [2] , COO and CSR [1] formats
- minimize required changes in code using CUSP

[2] M. Demek. "Dynamic autotuning of SpMV kernel in CUSP library". MA thesis. Masaryk University, 2023

[1] F. Bráblík. "Dynamic autotuning of SpMV kernel in CUSP library". MA thesis. Masaryk University, 2024

Dynamic autotuining of SpMV
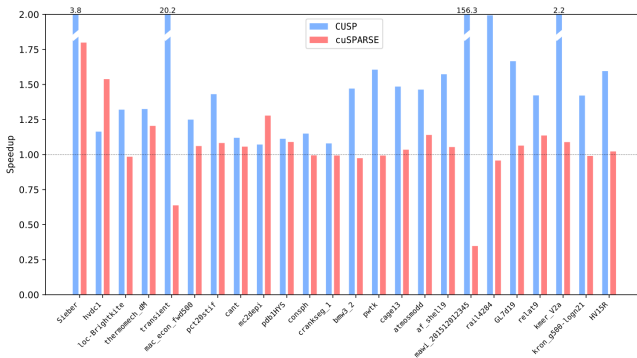
Figure: SpMV benchmark for CSR format.

What do we use KTT for?

So we have developed fancy autotuning framework...

- which is interesting work anyway, but we can do even more...

In GPU-accelerated applications

- used during program development (exploration of possible optimizations)
- manually added into applications to enable dynamic tuning
- used in cryo-electron microscopy suite Xmipp

What do we use KTT for?

Some more theoretical (but still with clear practical usage) tasks

- searching tuning space
- tuning budget estimation
- interoperability with other tools

Searching tuning space

Why is searching tuning spaces important and difficult?

- important to speed-up autotuning convergence
- discrete many-dimensional non-convex spaces are hard to optimize with mathematical optimization
- as spaces changes with hardware or input, it is also hard task for machine learning (if ML model relates tuning parameters to runtime, it becomes invalid)

We proposed a novel method [3]

- decomposing relation between tuning parameters and runtime: ML used for relating tuning parameters to performance counters, expert system used steer optimization method
- ML model is independent on HW and input

[3] J. Filipovič et al. "Using hardware performance counters to speed up autotuning convergence on GPUs".
In: *Journal of Parallel and Distributed Computing* 160 (2022), pp. 16–35. ISSN: 0743-7315. DOI:
https://doi.org/10.1016/j.jpdc.2021.10.003

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Searching tuning space
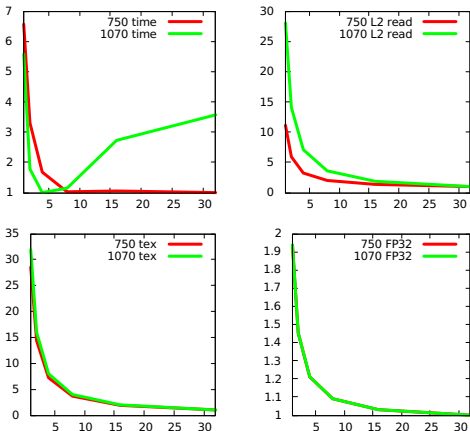
Figure: Dependence between a tuning parameter and various properties of the Coulomb 3D kernel running with large gridbox on GeForce GTX 750 and with small gridbox on GeForce GTX 1070. The x-axis shows a tuning parameter changing thread coarsening. The y-axis shows normalized values of selected properties: kernel runtime, L2 cache read transactions, texture cache read transactions and 32-bit floating-point operations.

Searching tuning space

Main idea behind the searcher

- relation between tuning parameters and performance counters measuring amount of operations remains stable – can be captured by ML model

- relation between tuning parameters and performance counters measuring stress of GPU subsystems depend on GPU and input – can be observed during tuning and used to identify bottlenecks

- an expert system asks ML model which tuning parameters to change to supress bottlenecks

- mimics what programmers are doing
  - they profile the code to observe bottlenecks, and use their understanding of the code to introduce changes supressing the bottlenecks

Searching tuning space
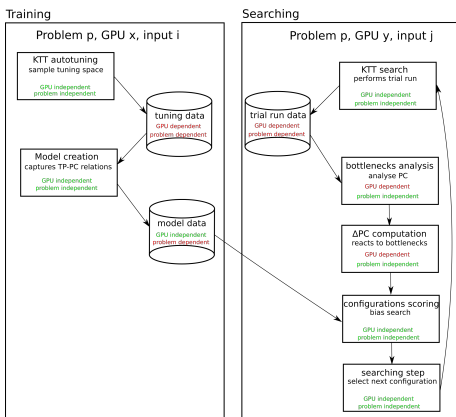
Figure: Schematic view of the searcher workflow. The boxes show program components, cylinders show data objects.

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Searching tuning space
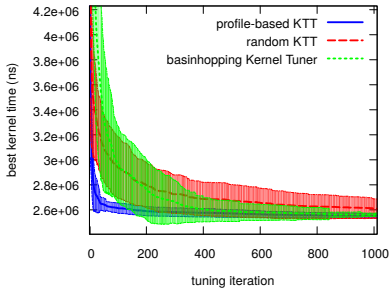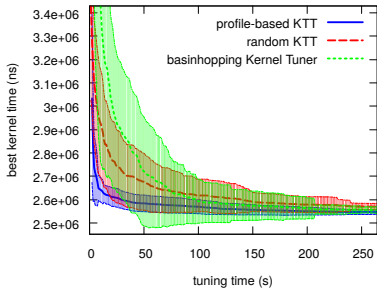
Figure: Convergence of the GEMM benchmark using KTT and Kernel
Tuner. Left: convergence speed in time. Right: comparison of iterations
(empirical tests).

Tuning budget estimation

Tuning budget estimation

- the problem: as autotuning itself requires computational resources, it is also subject of optimization
- therefore, estimating when to stop autotuning is crucial, as it balances
  - overhead of tuning process (number of tuning steps $\times$ average time of tuned kernel with re-compilation)
  - expected improvement of speed of tuned kernel
- we shown it is possible to guess from historical data and regression of tuning searching convergence [4]

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[4] Jaroslav Ol'ha et al. "Estimating resource budgets to ensure autotuning efficiency". In: *Available at SSRN 4661862* (2024)

Tuning budget estimation
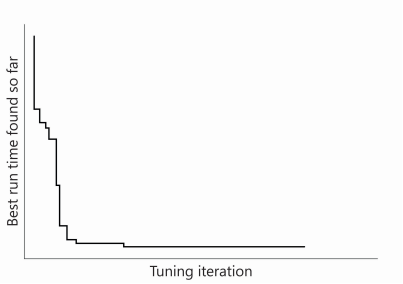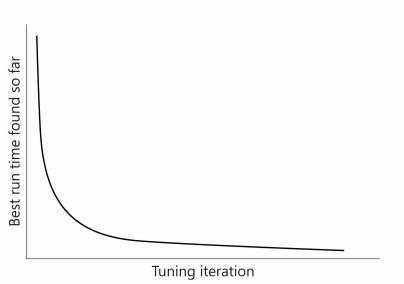
Figure: Example of tuning space searcher convergence.
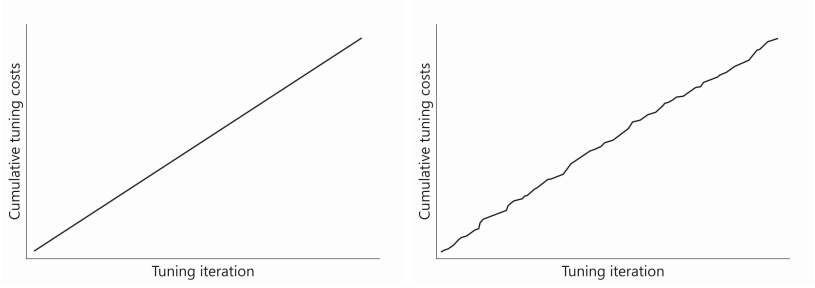
Tuning budget estimation

Figure: Example of tuning cost.
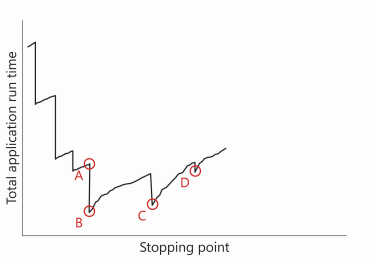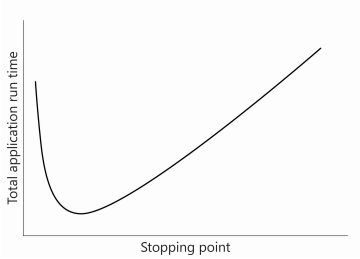
Tuning budget estimation

Figure: Example of total runtime depending on performed tuning steps.

KTT interoperability

KTT can be connected with different frameworks

- programming heterogeneous nodes is generaly challenging: distribution of work among multiple accelerators and CPU, data distribution
- StarPU implements task-based parallelism, it executes DAG of data-dependent tasks on heterogeneous nodes
    - alternative implementation of tasks
    - StarPU schedules data movement and task execution across the node
- connection of KTT and StarPU makes tasks tunable [7]
    - tuning transparent to user
    - decoples codes of domain and HPC experts

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[7] D. Střelák et al. "Umpalumpa: a framework for efficient execution of complex image processing workloads on heterogeneous nodes". In: *Computing* (2023), pp. 1–29

Future work

Still many interesting topics untouched

- autotuning for energy efficiency
- optimizing optimization spaces
- high-level programming of autotuned code
- non-trivial applications

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