



# Toward Performance & Portability & Productivity in Parallel Programming

### A Holistic Code *Generation*, *Optimization*, and *Execution* Approach for Data-Parallel Computations Targeting Modern Parallel Architectures

Ari Rasch University of Münster, Germany

## **Introductory Remark**



# Parallel Programming in Today's World

## Parallel programming is hard:



#### **v,z**+1113

# Challenges: Performance & Portability & Productivity

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### The Performance challenge:



Runtime (lower is better) of unoptimized vs optimized matrix multiplication



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# **Challenges:** Performance & Portability & Productivity

## The Portability challenge:



Runtime (lower is better) of GPU/CPU-optimized matrix multiplication on GPU (left) and CPU (right).



# **Challenges: Performance & Portability & Productivity**

## The Productivity challenge:

1	<pre>kernel void MatMul(global const float A[M][K] ,</pre>											
2	<pre>global const float B[K][N] ,</pre>											
3	<pre>global float C[M][N] )</pre>											
4	{											
5	<pre>int i = get_global_id(0);</pre>											
6	int $j = get_global_id(1);$											
7												
8	for( int k=0 ; k <k )<="" ++k="" ;="" td=""></k>											
9	C[i][j] += A[i][k] * B[k][j];											
10	}											

Naive OpenCL implementation of matrix multiplication

\_\_kernel void MatMul( /\* ... \*/ ) 1 { 2 const size\_t i\_wq\_l\_1 = get\_group\_id(2); 3 // ... 5 lines skipped 4 5 \_\_private TYPE\_TS res\_p[/\*...\*/][/\*...\*/]; 6 { 8 // ... 7 lines skipped for (size\_t p\_iteration\_l\_1 = 0; p\_iteration\_l\_1 < (2);</pre> 9 ++p\_iteration\_l\_1) { for (size\_t p\_iteration\_l\_2 = 0; p\_iteration\_l\_2 < (1)</pre> 10 ; ++p\_iteration\_l\_2) { size\_t p\_iteration\_r\_1 = 0; 11 res\_p[p\_step\_l\_1][((p\_iteration\_l\_1) \* 1 + 0)][(0)][ 12  $p_step_l_2][((p_iteration_l_2) * 1 + 0)] = f($ a[(((l\_step\_l\_1 x\* (32 / 1) + (((p\_step\_l\_1 \* 13  $(2) + (((p_iteration_l_1) * 1 + 0)) / 1) * 1$ + i\_wi\_l\_1 \* 1 + ((((p\_iteration\_l\_1) \* 1 +  $0)) % 1))) / 1) * (64 * 1) + i_wq_l_1 * 1 +$  $((((p_step_l_1 * (2) + (((p_iteration_l_1)$ \* 1 + 0)) / 1) \* 1 + i\_wi\_l\_1 \* 1 + (((( p\_iteration\_l\_1) \* 1 + 0)) % 1))) % 1))) \*  $1024 + (((l_step_r_1 * (2 / 1) + ((($ p\_step\_r\_1 \* (1) + (((p\_iteration\_r\_1) \* 1 +  $(0)) / 1) * 1 + i_wi_r_1 * 1 + (((($ p\_iteration\_r\_1) \* 1 + 0)) % 1))) / 1) \* (2 \* 1) + i\_wq\_r\_1 \* 1 + ((((p\_step\_r\_1 \* (1) + (((p\_iteration\_r\_1) \* 1 + 0)) / 1) \* 1 + i\_wi\_r\_1 \* 1 + ((((p\_iteration\_r\_1) \* 1 + 0) ) % 1))) % 1)))], // ... 107 lines skipped 14 } 15

**Optimized OpenCL implementation of matrix multiplication** 

High Productivity requires automatic optimization

# **Contributions of this Thesis**

This thesis introduces a novel, holistic approach to Generating & Optimizing & Executing code:



The ultimate goal of MDH+ATF+HCA is to simultaneously achieve <u>Performance</u> & <u>Portability</u> & <u>Productivity</u>

# Outline

### This talk(/thesis) is structured into three main parts:





Overview Getting Started Code Examples Publications Citations Contact



#### Multi-Dimensional Homomorphisms (MDH)

An Algebraic Approach Toward <u>Performance</u> & <u>Portability</u> & <u>Productivity</u> for Data-Parallel Computations

#### Overview

The approach of Multi-Dimensional Homomorphisms (MDH) is an algebraic formalism for systematically reasoning about *de-composition* and *re-composition* strategies of data-parallel computations (such as linear algebra routines and stencil computations) for the memory and core hierarchies of state-of-the-art parallel architectures (GPUs, multi-core CPU, multi-device and multi-node systems, etc).

The MDH approach (formally) introduces:

- 1. *High-Level Program Representation (Contribution 1)* that enables the user conveniently implementing data-parallel computations, agnostic from hardware and optimization details;
- 2. Low-Level Program Representation (Contribution 2) that expresses device- and data-optimized de- and re-composition strategies of computations;
- 3. *Lowering Process (Contribution 3)* that fully automatically lowers a data-parallel computation expressed in its high-level program representation to an optimized instance in its low-level representation, based on concepts from automatic performance optimization (a.k.a. *auto-tuning*), using the Auto-Tuning Framework (ATF).

The MDH's low-level representation is designed such that Code Generation from it (e.g., in OpenMP for CPUs, CUDA for NVIDIA GPUs, or OpenCL for multiple kinds of architectures) becomes straightforward.



Our Experiments report encouraging results on GPUs and CPUs for MDH as compared to state-of-practice approaches, including NVIDIA cuBLAS/cuDNN and Intel oneMKL/oneDNN which are hand-optimized libraries provided by vendors.

### https://mdh-lang.org

#### ACM TOPLAS 2024

#### (De/Re)-Composition of Data-Parallel Computations via Multi-Dimensional Homomorphisms

ARI RASCH, University of Muenster, Germany

Data-parallel computations, such as linear algebra routines and stencil computations, constitute one of the most relevant classes in parallel computing, e.g., due to their importance for deep learning. Efficiently de-composing such computations for the memory and core hierarchies of modern architectures and re-composing the computed intermediate results back to the final result—we say (*de/re*)-composition for short—is key to achieve high performance for these computations on, e.g., GPU and CPU. Current high-level approaches to generating data-parallel code are often restricted to a particular subclass of data-parallel computations and architectures (e.g., only linear algebra routines on only GPU or only stencil computations), and/or the approaches rely on a user-guided optimization process for a well-performing (de/re)-composition of computations, which is complex and error prone for the user.

We formally introduce a systematic (de/re)-composition approach, based on the algebraic formalism of Multi-Dimensional Homomorphisms (MDHs). Our approach is designed as general enough to be applicable to a wide range of data-parallel computations and for various kinds of target parallel architectures. To efficiently target the deep and complex memory and core hierarchies of contemporary architectures, we exploit our introduced (de/re)-composition approach for a correct-by-construction, parametrized cache blocking, and parallelization strategy. We show that our approach is powerful enough to express, in the same formalism, the (de/re)-composition strategies of different classes of state-of-the-art approaches (scheduling-based, polyhedral, etc.), and we demonstrate that the parameters of our strategies enable systematically generating code that can be fully automatically optimized (auto-tuned) for the particular target architecture and characteristics of the input and output data (e.g., their sizes and memory layouts). Particularly, our experiments confirm that via auto-tuning, we achieve higher performance than state-of-the-art approaches, including hand-optimized solutions provided by vendors (such as NVIDIA cuBLAS/cuDNN and Intel oneMKL/oneDNN), on real-world datasets and for a variety of data-parallel computations, including linear algebra routines, stencil and quantum chemistry computations, data mining algorithms, and computations that recently gained high attention due to their relevance for deep learning.

CCS Concepts: • Computing methodologies → Parallel computing methodologies; *Machine learning*; • Theory of computation → Program semantics; • Software and its engineering → Compilers;

Additional Key Words and Phrases: Code generation, data parallelism, auto-tuning, GPU, CPU, OpenMP, CUDA, OpenCL, linear algebra, stencils computation, quantum chemistry, data mining, deep learning

A full version of this article is provided by Rasch [2024], which presents our novel concepts with all of their formal details. In contrast to the full version, this article relies on a simplified formal foundation for better illustration and easier understanding. We often refer the interested reader to Rasch [2024] for formal details that should not be required for understanding the basic ideas and concepts of our approach.

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### **MDH** is a (formal) framework for expressing & optimizing data-parallel computations:



- 1. **Contribution 1 (HL-REP):** defines *data parallelism* & introduces *higher-order functions* for expressing dataparallel computations, agnostic from hardware and optimization details while still capturing high-level information relevant for generating high-performing code
- 2. **Contribution 2 (LL-REP):** allows *expressing and reasoning about optimizations* for the memory and core hierarchies of contemporary parallel architectures & generalizes these optimizations to apply to arbitrary combinations of data-parallel computations and architectures
- 3. **Contribution 3** (→): introduces a structured optimization process for arbitrary combinations of dataparallel computations and parallel architectures — that allows *fully automatic* optimization (auto-tuning)



Example: MatVec expressed in MDH



High-Level Representation of MatVec

### What is happening here:

- inp\_view captures the accesses to input data
- md\_hom expresses the data-parallel computation
- **out\_view** captures the accesses to output data



 $\otimes_6 \otimes_7 \otimes_8 \otimes_9$ 

+

							inp_	out_view	
md_hom	f	$\otimes_1$	$\otimes_2$	$\otimes_3$	$\otimes_4$	Views	А	В	C
Dot	*	+	/	/	/	Dot	$(k) \mapsto (k)$	$(k) \mapsto (k)$	(k) → ()
MatVec	*	++	+	/	/	MatVec	$(i,k) \mapsto (i,k)$	$(i,k) \mapsto (k)$	(i,k) → (i)
MatMul	*	++	++	+	/	MatMul	$(i,j,k) \mapsto (i,k)$	$(i,j,k) \mapsto (k,j)$	$(i,j,k) \mapsto (i,j)$
$MatMul^T$	*	++	++	+	/	$MatMul^T$	$(i,j,k) \mapsto (k,i)$	$(i,j,k) \mapsto (j,k)$	$(i,j,k) \mapsto (j,i)$
bMatMul	*	++	++	++	+	bMatMul	$(b,i,j,k) \mapsto (b,i,k)$	$(b,i,j,k) \mapsto (b,k,j)$	$(b,i,j,k) \mapsto (b,i,j)$

1) Linear Algebra Routines

					inp_vi	out_view	
				Views	I	F	0
	inp_view out_view		out_view	Conv2D	$(p,q,r,s) \mapsto (p+r,q+s)$	$(p,q,r,s) \mapsto (r,s)$	$(p,q,r,s) \mapsto (p,q)$
md_hom $\  f \  \otimes_1 \  \otimes_2$	Views	А	Out	MCC	$(n,p,\ldots) \mapsto (n,p+r,q+s,c)$	$(n,p,\ldots) \mapsto (k,r,s,c)$	$(n,p,\ldots) \mapsto (n,p,q,k)$
MBBS id ++prefix-sum(+) +	MBBS	(i,j) → (i,j)	(i) → (i)	MCC_Capsule	$(n,p,\ldots) \mapsto (n,p+r,q+s,c,cm,ck)$	$(n,p,\ldots) \mapsto (k,r,s,c,ck,cn)$	$(n,p,\ldots) \mapsto (n,p,q,k,cm,cn)$

8) Maximum Bottom Box Sum

2) Convolution Stencils

md\_hom

Conv2D

MCC\_Capsule

MCC

		inp_view	out_view						
md_hom $\  \mathbf{f} \  \otimes_1 \  \otimes_2 \mathbf{V}$	/iews	I	0				inp_	view	out_view
Jacobi1D J <sub>1D</sub> ++ / Ja	Jacobi1D	(i) $\mapsto$ (i+0) , (i) $\mapsto$ (i+1) , (i) $\mapsto$ (i+2)	(i) → (i)	md_hom f	$\otimes_1$ $\otimes_2$	Views		E	М
Jacobi2D J <sub>2D</sub> ++ ++ J	Jacobi2D	$(i,j) \mapsto (i,j+1)$ , $(i,j) \mapsto (i+1,j)$ ,	$(i,j) \mapsto (i,j)$	PRL wght	++ max <sub>PRL</sub>	PRL	$(i,j) \mapsto (i)$	$(i,j) \mapsto (j)$	$(i,j) \mapsto (i)$

3) Jacobi Stencils

4) Probabilistic Record Linkage

 $\otimes_2$ 

++

 $\otimes_3 \otimes_4 \otimes_5$ 

+

++

+

+

++

f

\*

\*

⊗1

++

++

				inp_view	out_view		
md_hom	f	$\otimes_1$	Views	I	01	02	
map(f)	f	++	<pre>map(f)</pre>	(i) → (i)	(i) → (i)	/	
$reduce(\oplus)$	id	Ð	$reduce(\oplus)$	(i) → (i)	(i) → ()	/	
$reduce(\oplus,\otimes)$	$(x) \mapsto (x,x)$	(⊕,⊗)	$reduce(\oplus,\otimes)$	(i) → (i)	(i) → ()	(i) → ()	

6) Map/Reduce Patterns



7) Scan Pattern



5) Histogram

MDH is capable of expressing a wide range of data-parallel computations from popular domains

### **Performance Evaluation:** (via runtime comparison)

	NVIDIA Ampere GPU												
Deep		ResNe	et-50			VGG	-16		MobileNet				
Learning	Trai	ning	Inference		Training		Inference		Training	Inference			
	MCC	MatMul	МСС	MatMul	MCC	MatMul	MCC	MatMul	MCC	MCC			
TVM+Ansor	1.00	1.26	1.05	2.22	0.93	1.42	0.88	1.14	0.94	1.00			
PPCG	3456.16	8.26	-	7.89	1661.14	7.06	5.77	5.08	2254.67	7.55			
PPCG+ATF	3.28	2.58	13.76	5.44	4.26	3.92	9.46	3.73	3.31	10.71			
cuDNN	0.92	-	1.85	-	1.22	-	1.94	-	1.81	2.14			
cuBLAS	-	1.58	-	2.67	-	0.93	-	1.04	-	-			
cuBLASEx	-	1.47	-	2.56	-	0.92	-	1.02	-	-			
cuBLASLt	-	1.26	-	1.22	-	0.91	-	1.01	-	-			





MDH speedup over

- TVM: 0.88x 2.22x
- PPCG: 2.58x 13.76x
- (cuBLAS/cuDNN: 0.91x 2.67x)

	Intel Skylake CPU													
Deep		ResNe	et-50			VGG	-16		MobileNet					
Learning	Trai	ning	Inference		Training		Inference		Training	Inference				
	MCC	MatMul	MCC	MatMul	MCC	MatMul	MCC	MatMul	MCC	MCC				
TVM+Ansor	1.53	1.05	1.14	1.20	1.97	1.14	2.38	1.27	3.01	1.40				
Pluto	355.81	49.57	364.43	13.93	130.80	93.21	186.25	36.30	152.14	75.37				
Pluto+ATF	13.08	19.70	170.69	6.57	3.11	6.29	53.61	8.29	3.50	25.41				
oneDNN	0.39	-	5.07	-	1.22	-	9.01	-	1.05	4.20				
oneMKL	-	0.44	-	1.09	-	0.88	-	0.53	-	-				
oneMKL(JIT)	-	6.43	-	8.33	-	27.09	-	9.78	-					
									-					



MDH speedup over

- TVM: 1.05 3.01x
- Pluto: 6.29x 364.43x
- (oneMKL/oneDNN: 0.39x 9.01x)

Case Study "Deep Learning" for which most competitors are highly optimized (most challenging for us!)

Беер	L	Resne	- שכ	1			G-10			renet
Learning,	, Trai	ning	Infer	rence	NVHDIA	Annere	GPU Infe	erence	Training	Inference
SIGNERIOZZAWA	<b>ng</b> ner	Speeg	NIQSJO	r otner	case s	<i>thates</i>	, MCC	MatMuMC	bileMet	MCC
e.a. (cahzaxe	71	// /				iohtfo	ri	1-1	1	
TVM+Ansor	1.53	1.60	1.29	1.53	1.32		1.27	1.02	2.42	1.92

# Code Optimization via ATF



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#### Auto-Tuning Framework (ATF)

Efficient Auto-Tuning of Parallel Programs with Constrained Tuning Parameters

#### Overview

The Auto-Tuning Framework (ATF) is a general-purpose auto-tuning approach: given a program that is implemented as generic in performance-critical program parameters (a.k.a. *tuning parameters*), such as sizes of tiles and numbers of threads, ATF fully automatically determines a hardware- and data-optimized configuration of such parameters.

#### Key Feature of ATF

A key feature of ATF is its support for *Tuning Parameter Constraints*. Parameter constraints allow auto-tuning programs whose tuning parameters have so-called *interdependencies* among them, e.g., the value of one tuning parameter has to evenly divide the value of another tuning parameter.

ATF's support for parameter constraints is important: modern parallel programs target novel parallel architectures, and such architectures typically have deep memory and core hierarchies thus requiring constraints on tuning parameters, e.g., the value of a tile size tuning parameter on an upper memory layer has to be a multiple of a tile size value on a lower memory layer.

For such parameters, ATF introduces novel concepts for *Generating* & *Storing* & *Exploring* the search spaces of constrained tuning parameters, thereby contributing to a substantially more efficient overall auto-tuning process for such parameters, as confirmed in our *Experiments*.

#### Generality of ATF

For wide applicability, ATF is designed as generic in:

 The target program's Programming Language, e.g., C/C++, CUDA, OpenMP, or OpenCL. ATF offers pre-implemented cost functions for conveniently auto-tuning C/C++ programs, as well as CUDA and OpenCL kernels which require host code for their execution which is automatically generated and executed by ATF's pre-implemented CUDA and OpenCL cost functions. ATF also offers a pre-implemented generic cost function that can be used for conveniently auto-tuning programs in any other programming language different from C/C++, CUDA, and OpenCL.

### https://atf-tuner.org

#### ACM TACO 2021

Efficient Auto-Tuning of Parallel Programs with Interdependent Tuning Parameters via Auto-Tuning Framework (ATF)

ARI RASCH and RICHARD SCHULZE, University of Muenster, Germany MICHEL STEUWER, University of Edinburgh, United Kingdom SERGEI GORLATCH, University of Muenster, Germany

Auto-tuning is a popular approach to program optimization: it automatically finds good configurations of a program's so-called tuning parameters whose values are crucial for achieving high performance for a particular parallel architecture and characteristics of input/output data. We present three new contributions of the Auto-Tuning Framework (ATF), which enable a key advantage in *general-purpose auto-tuning*: efficiently optimizing programs whose tuning parameters have *interdependencies* among them. We make the following contributions to the three main phases of general-purpose auto-tuning: (1) ATF *generates* the search space of interdependent tuning parameters with high performance by efficiently exploiting parameter constraints; (2) ATF *stores* such search spaces efficiently in memory, based on a novel chain-of-trees search space structure; (3) ATF *explores* these search spaces faster, by employing a multi-dimensional search strategy on its chain-of-trees search space representation. Our experiments demonstrate that, compared to the state-of-the-art, general-purpose auto-tuning frameworks, ATF substantially improves generating, storing, and exploring the search space of interdependent tuning parameters, thereby enabling an efficient overall auto-tuning process for important applications from popular domains, including stencil computations, linear algebra routines, quantum chemistry computations, and data mining algorithms.

 $\label{eq:CCS Concepts: General and reference} \rightarrow \mbox{Performance; } \bullet \mbox{Computer systems organization} \rightarrow \mbox{Parallel architectures; } \bullet \mbox{Software and its engineering} \rightarrow \mbox{Parallel programming languages;}$ 

Additional Key Words and Phrases: Auto-tuning, parallel programs, interdependent tuning parameters

#### ACM Reference format:

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This is a new paper, not an extension of a conference paper.

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# Code Optimization via ATF



Advantage of ATF over state-of-the-art general-purpose AT approaches:

**ATF** finds values of performance-critical parameters with *interdependencies* among them via optimized processes to *generating* & *storing* & *exploring the spaces of interdependent parameters* 

→ We illustrate ATF by comparing it to MIT's *OpenTuner* [PACT'14] & *CLTune* [MCSoC'15] which is the foundation of many related approaches (e.g., KernelTuner & KTT).

<u>Note:</u> BaCO [ASPLOS'23] & KTT recently adopted the ATF techniques to also efficiently handle interdependent tuning parameters.

# Code Optimization via ATF



How does ATF achieve its efficiency for *interdependent tuning parameters*:



**Highlights only** 

# Code Optimization via ATF



## ATF is able to auto-tune modern parallel computations, e.g., for GPUs & CPUs:

**NVIDIA** 

Stencil

ATF is able to auto-tune CONV to:

>40x higher performance >104x higher performance than CONV+CLTune than CONV+CLTune on GPU on CPU

>3x higher performance than Intel MKL-DNN on CPU (intel)

>15x higher performance than NVIDIA cuDNN on GPU

## Linear Algebra

- ATF is able to auto-tune GEMM to: >2x higher performance >120x higher performance than GEMM+CLTune than GEMM+CLTune on CPU on GPU
- >2x higher performance >2x higher performance than Intel MKL than NVIDIA cuBLAS on CPU on GPU (intel)

## Data Mining

ATF is able to auto-tune CCSD(T) to:

Quantum Chemistry

>2x higher performance than Facebook TC on GPU

CLTune fails! (too high search space generation time)

ATF is able to auto-tune PRL to:

>1.6x higher performance >1.07x higher perform. than PRL+**CLTune** than PRL+CLTune on CPU on GPU

OpenTuner fails for all studies

## Code Execution via HCA



#### Overview

The Host Code Abstraction (HCA) is a high-level programming abstraction that simplifies implementing and optimizing socalled host code which is required in modern parallel programming approaches (e.g., CUDA and OpenCL) to execute code on the devices of distributed, heterogeneous systems.

More details will follow soon!

Contact

#### https://hca-project.org

# **Skipped for brevity**

#### Journal of Supercomputing 2019

The Journal of Supercomputing (2020) 76:5117–5138 https://doi.org/10.1007/s11227-019-02829-2

dOCAL: high-level distributed programming with OpenCL and CUDA

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#### Abstract

In the state-of-the-art parallel programming approaches OpenCL and CUDA, socalled host code is required for program's execution. Efficiently implementing host code is often a cumbersome task, especially when executing OpenCL and CUDA programs on systems with multiple nodes, each comprising different devices, e.g., multi-core CPU and graphics processing units; the programmer is responsible for explicitly managing node's and device's memory, synchronizing computations with data transfers between devices of potentially different nodes and for optimizing data transfers between devices' memories and nodes' main memories, e.g., by using pinned main memory for accelerating data transfers and overlapping the transfers with computations. We develop distributed OpenCL/CUDA abstraction layer (dOCAL)—a novel high-level C++ library that simplifies the development of host code. dOCAL combines major advantages over the state-of-the-art high-level approaches: (1) it simplifies implementing both OpenCL and CUDA host code by providing a simple-to-use, high-level abstraction API; (2) it supports executing arbitrary OpenCL and CUDA programs; (3) it allows conveniently targeting the devices of different nodes by automatically managing node-to-node communications; (4) it simplifies implementing data transfer optimizations by providing different, specially allocated memory regions, e.g., pinned main memory for overlapping data transfers with computations; (5) it optimizes memory management by automatically avoiding unnecessary data transfers; (6) it enables interoperability between OpenCL and CUDA host code for systems with devices from different vendors. Our experiments show that dOCAL significantly simplifies the development of host code for heterogeneous and distributed systems, with a low runtime overhead.



Check fo

# Summary

# The MDH+ATF+HCA approach achieves *Performance & Portability & Productivity* for data-parallel computations targeting modern parallel architectures:



MDH

HCA