



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

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https://mdh-lang.org

Introductory Remarks

- This talk (briefly!) highlights the main contributions of our paper (~20 slides vs. >70 pages)
- Talk focuses on illustrative examples, rather than formal definitions & details (all provided and thoroughly discussed in the paper)
- There is a (full) arXiv version of the paper that contains all formal details [1]
- Paper is long: >70 pages (>130 pages arXiv)
- Many illustrations and discussions you can get the basic idea even when skipping the formal details

The paper attempts to make a general, fundamental contribution to the community (see next slide)

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

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Data-parallel computations, such as linear algebra routines (BLAS) 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*)¹. 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 data sets 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 \rightarrow Parallel computing methodologies; *Machine learning*; • Theory of computation \rightarrow Program semantics; • Software and its engineering \rightarrow 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

1 INTRODUCTION

Data-parallel computations constitute one of the most relevant classes in parallel computing. Important examples of such computations include linear algebra routines (BLAS) [Whaley and Dongarra 1998], various kinds of

*A full version of this paper is provided by Rasch [2024], which presents our novel concepts with all of their formal details. In contrast to the full version, this paper 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.

1 https://mdh-lang.org

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https://doi.org/10.1145/3665643

ACM Trans. Program. Lang. Syst

[1] Rasch, Ari. "Full Version: (De/Re)-Composition of Data-Parallel Computations via Multi-Dimensional Homomorphisms." arXiv preprint arXiv:2405.05118 (2024).

Goal of this Work

Questions addressed by this talk:

How can data parallelism be formally defined?

How can data-parallel computations be uniformly expressed via higher-order functions?

How can optimizations for the memory and core hierarchies of state-of-the-art parallel architectures be formally expressed?

How can data-parallel computations be expressed agonistic from of hardware and optimization details (and still capture all information relevant for generating high-performing code)?

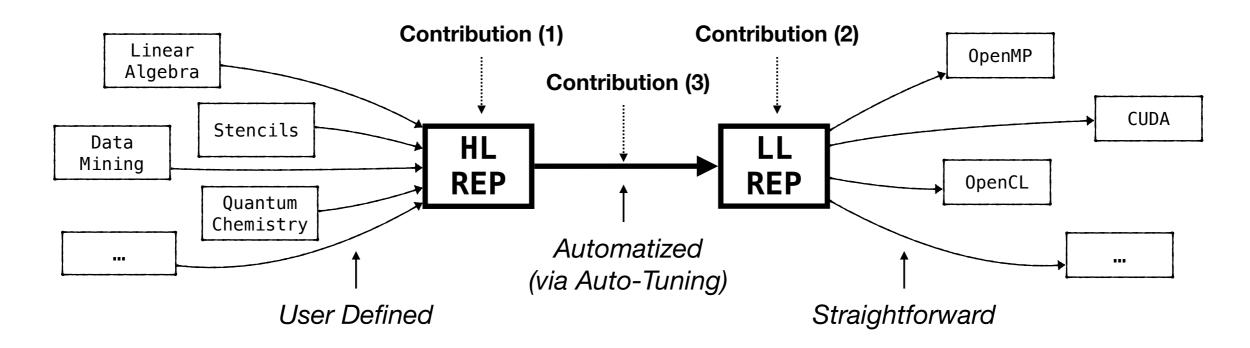
How can such optimizations be generalized to apply to arbitrary data-parallel computations?

How can optimizations for data-parallel computations be expressed and structured so that they can be fully automatically identified (auto-tuned) for a particular target architecture and characteristics of the input and output data?

All questions are answered (fully formally) in the paper!

Goal of this Work

A (formal) framework for expressing & optimizing data-parallel computations:



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

Agenda

- 1. Contribution 1: High-Level Representation
- 2. Contribution 2: Low-Level Representation
- 3. Contribution 3: Lowering: High-Level Representation → Low-Level Representation
- 4. Experimental Results (Performance & Portability & Productivity)
- 5. Related Work
- 6. Conclusion

Contribution 1
3 slides vs 17p.TOPLAS (26p.arXiv)

Contribution 2
1 slide vs 9p.TOPLAS (20p.arXiv)

Contribution 3
1 slide vs 4p.TOPLAS (2p.arXiv)

Experimentale Results
4 slides vs 23p.TOPLAS (23p.arXiv)

Related Work
1 slide vs 11p.TOPLAS (11p.arXiv)

High-Level Representation

Goals:

1. Uniform:

should be able to express any kind of data-parallel computation, without relying on domain-specific building blocks, extensions, etc.

2. Minimalistic:

should rely on less building blocks to keep language small and simple

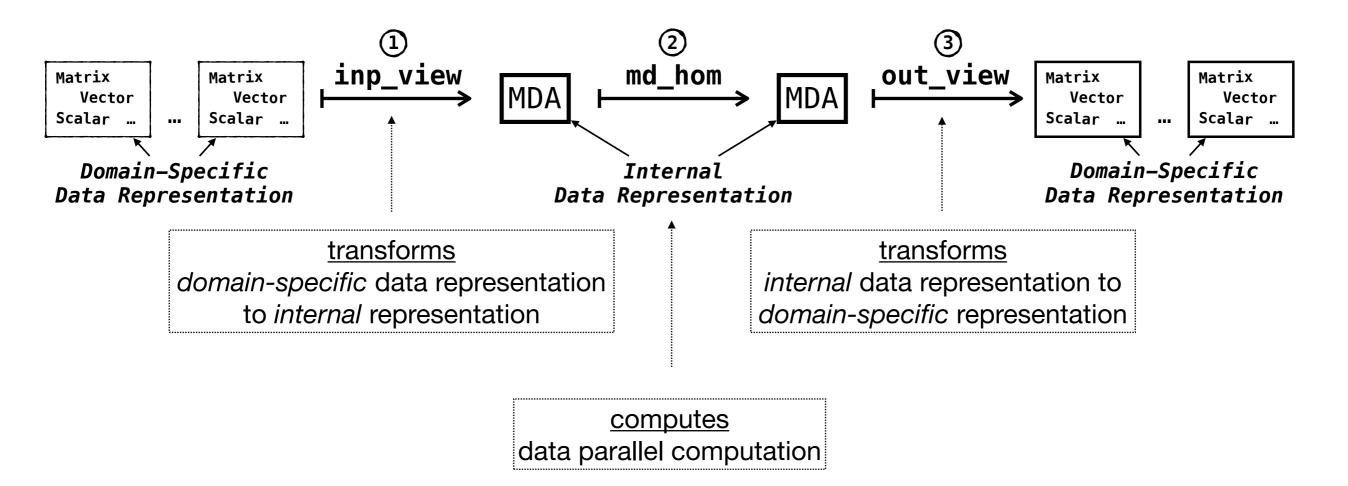
3. Structured:

avoiding compositions and nestings of building blocks as much as possible, thereby further contributing to usability and simplicity of our language

Our High-Level Representation of MatVec

High-Level Representation

Overview:



Our high-level representation defines data-parallel computations as *Multi-Dimensional Homomorphisms (MDH),* and it expresses data-parallel computations using exactly three straightforwardly composed higher-order functions only

High-Level Representation

md_hom	f	⊗1	\otimes_2	⊗3	₩4
Dot	*	+	/	/	/
MatVec	*	++	+	/	/
MatMul	*	++	++	+	/
MatMul ^T	*	++	++	+	/
bMatMul	*	++	++	++	+

	inp_	out_view	
Views	A	В	С
Dot	(k) → (k)	(k) → (k)	(k) → ()
MatVec	(i,k) → (i,k)	(i,k) → (k)	(i,k) → (i)
MatMul	$(i,j,k) \mapsto (i,k)$	$(i,j,k) \mapsto (k,j)$	$(i,j,k) \mapsto (i,j)$
$MatMul^T$	$(i,j,k) \mapsto (k,i)$	$(i,j,k) \mapsto (j,k)$	$(i,j,k) \mapsto (j,i)$
bMatMul	$(b,i,j,k) \mapsto (b,i,k)$	$(b,i,j,k) \mapsto (b,k,j)$	$(b,i,j,k) \mapsto (b,i,j)$

md_hom	f	\otimes_1	\otimes_2	⊗3	\otimes_4	⊗5	⊗6	⊗ 7	⊗8	⊗ 9	⊗ 10
Conv2D	*	++	++	+	+	/	/	/	/	/	/
MCC	*	++	++	++	++	+	+	+	/	/	/
MCC_Capsule	*	++	++	++	++	+	+	+	++	++	+

1) Linear Algebra Routines

md_hom	f	⊗1	\otimes_2
MBBS	id	++prefix-sum(+)	+

	inp_view	out_view
Views	A	Out
MBBS	$(i,j) \mapsto (i,j)$	(i) → (i)

	inp_vi	out_view	
Views	I	F	0
Conv2D	$(p,q,r,s) \mapsto (p+r,q+s)$	$(p,q,r,s) \mapsto (r,s)$	$(p,q,r,s) \mapsto (p,q)$
MCC	$(n,p,) \mapsto (n,p+r,q+s,c)$	$(n,p,) \mapsto (k,r,s,c)$	$(n,p,) \mapsto (n,p,q,k)$
MCC_Capsule	$(n,p,) \mapsto (n,p+r,q+s,c,cm,ck)$	$(n,p,) \mapsto (k,r,s,c,ck,cn)$	$(n,p,) \mapsto (n,p,q,k,cm,cn)$

8) Maximum Bottom Box Sum

2) Convolution Stencils

					inp_view	out_view
md_hom	f	⊗1	\otimes_2	Views	I	0
Jacobi1D	J _{1D}	++	/	Jacobi1D	$(i) \mapsto (i+0)$, $(i) \mapsto (i+1)$, $(i) \mapsto (i+2)$	(i) → (i)
Tacobi 2D	Ion	++	++	Jacobi 2D	$(i i) \mapsto (i i+1) (i i) \mapsto (i+1 i)$	(i i) → (i i)

					inp_	out_view	
md_hom	f	⊗1	⊗2	Views	N	E	М
PRL	wght	++	max _{PRI}	PRL	$(i,j) \mapsto (i)$	$(i,j) \mapsto (j)$	$(i,j) \mapsto (i)$

3) Jacobi Stencils

4) Probabilistic Record Linkage

md_hom	f	⊗1
map(f)	f	++
reduce(⊕)	id	0
$reduce(\oplus, \otimes)$	$(x) \mapsto (x,x)$	(⊕,⊗)

	inp_view	out_view			
Views	I	01	O_2		
map(f)	(i) → (i)	(i) → (i)	/		
reduce(⊕)	(i) → (i)	(i) → ()	/		
$reduce(\oplus, \otimes)$	(i) → (i)	(i) → ()	(i) → ()		

6) Map/Reduce Patterns

				inp_view	out_view
md_hom	f	\otimes_1	Views	I	0
$\mathtt{scan}(\oplus)$	id	$++_{\mathtt{prefix-sum}}(\oplus)$	$\mathtt{scan}(\oplus)$	(i) → (i)	(i) → (i)

7) Scan Pattern

md_hom	f	⊗1	\otimes_2	Views	_
Histo	f _{Histo}	++	+	Histo	

	inp_	out_view			
Views	Bins	Elems	Out		
Histo	(b,e) → (b)	$(b,e) \mapsto (e)$	(b,e) → (b)		

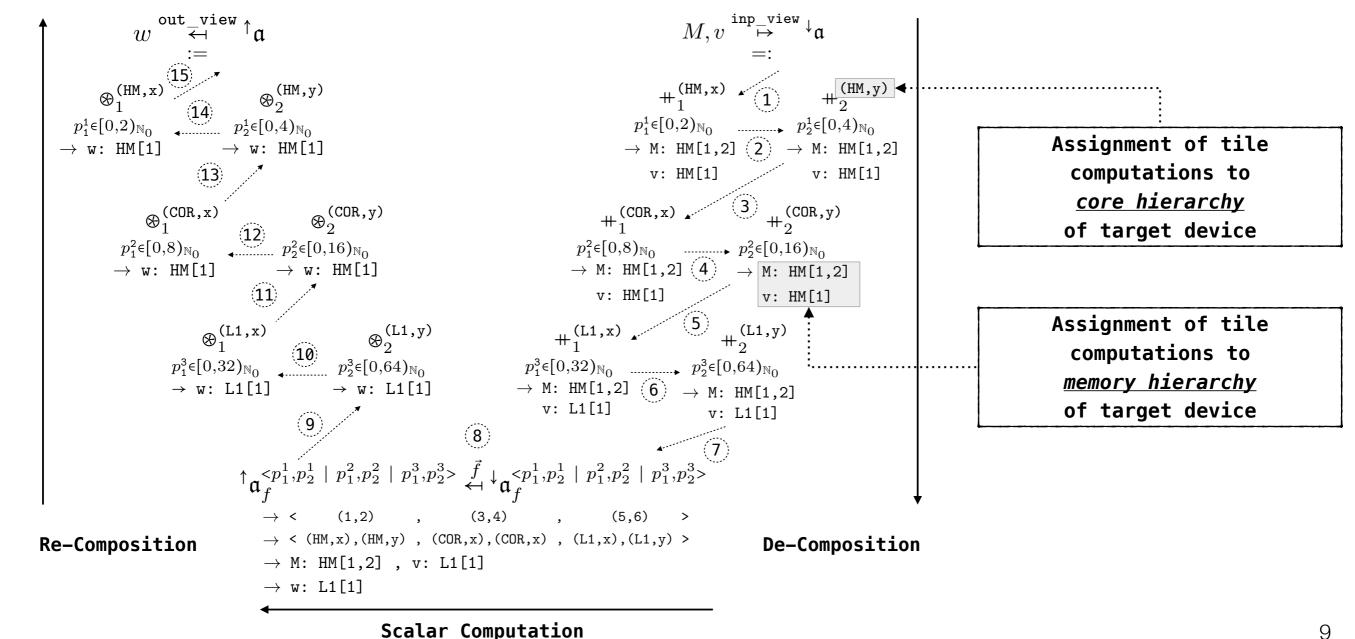
5) Histogram

Our high-level representation is capable of expressing the various kinds of data-parallel computations which often differ in major characteristics

Low-Level Representation

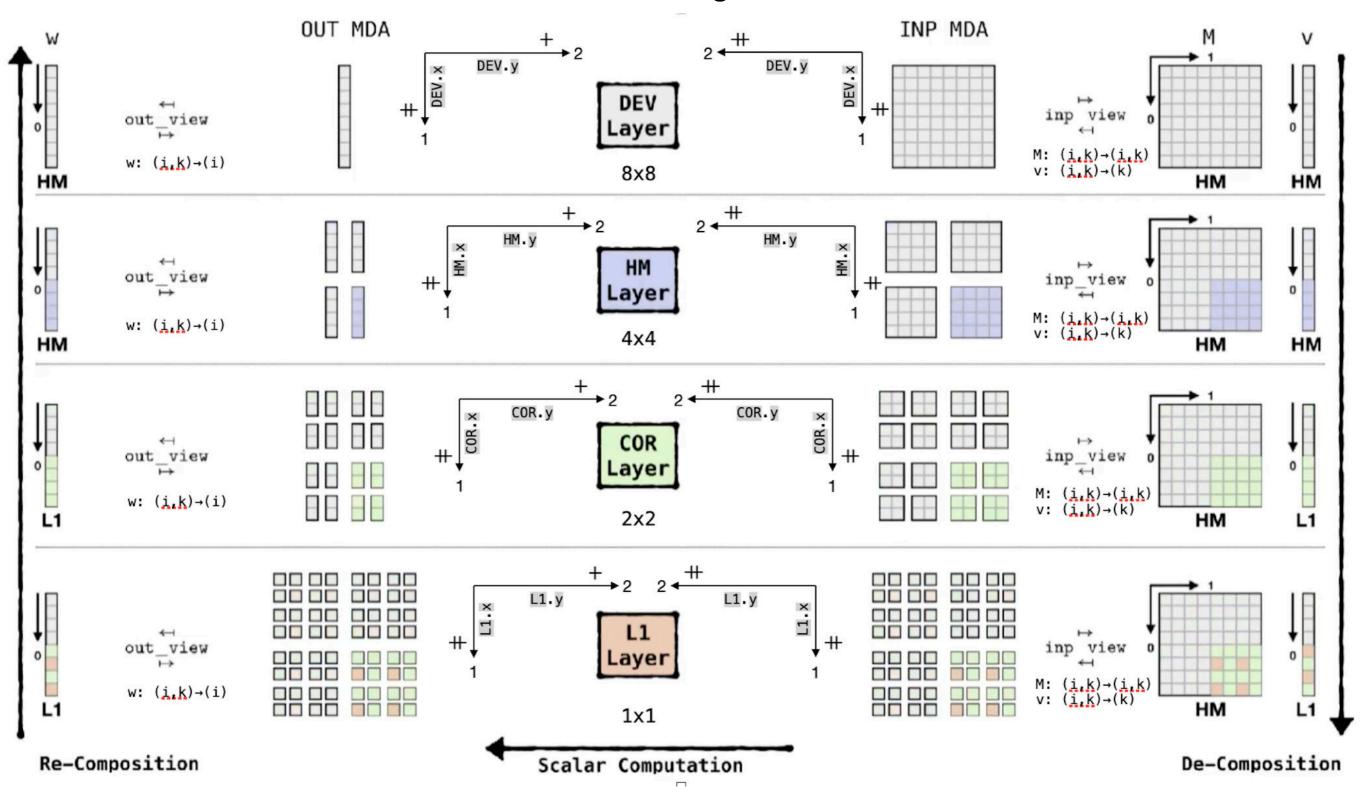
Goals:

- Expressing a hardware- & data-optimized de-composition and re-composition of data-parallel computations, based on an Abstract System Model (ASM)
- Being straightforwardly transformable to executable program code (e.g., in OpenMP, CUDA, and OpenCL) — major optimization decisions explicitly expressed in low-level representation



Low-Level Representation

Excursion: Visualization of MDH Low-Level Programs



Low-Level Representation

Code generation:

```
// 0.1.2. combine operators
                                       // pre-implemented combine operators
                                       // inverse concatenation
                                       \texttt{cc\_inv} << d >> < I_1, ..., I_{d-1}, I_{d+1}, ..., I_D \in \texttt{MDA-IDX-SETs}, \ (P,Q) \in \texttt{MDA-IDX-SETs} \ \dot{\times} \ \texttt{MDA-IDX-SETs} > (P,Q) \in \texttt{MDA-IDX-SETS} + (P,Q) \in \texttt{MDA-IDX
                                                     T^{\text{INP}}[I_1,...,I_{d-1},id(P \cup Q),I_{d+1},...,I_D] \text{ res }) \rightarrow (T^{\text{INP}}[I_1,...,I_{d-1},id(P),I_{d+1},...,I_D] \text{ lhs } I_{d+1},...,I_D]
                                                                                                                                                                                                                                                                                                                                                              T^{\text{INP}}[I_1, ..., I_{d-1}, id(Q), I_{d+1}, ..., I_D] rhs)
10
11
                                                     int i_1 \in I_1
12
                                                                                  int i_{-}\{d-1\} \in I_{d-1}
                                                                                                int i_{-}\{d+1\} \in I_{d+1}
                                                                                                                              int i_D \in I_D
                                                                                                                                                     res[ i_1, ..., i_d, ..., i_D] =: lhs[ i_1, ..., i_d, ..., i_D];
20
21
                                                                                                                                                         res[ i_1, ..., i_d, ..., i_D] =: rhs[ i_1, ..., i_d, ..., i_D];
22
```

Listing 11. Pre-Implemented Combine Operators

```
// 3. re-composition phase
 2
              int p_{-} \sigma_{\uparrow-ord}(1,1) \in \langle \leftrightarrow_{\uparrow-ass} (1,1) \rangle
 5
                   \quad \textbf{int} \quad \textbf{p}\_ \quad \sigma_{\uparrow \text{-ord}}\big(1,2\big) \quad \boldsymbol{\epsilon}^{<} \stackrel{\longleftrightarrow_{\uparrow \text{-ass}}}{\leftarrow} \big(1,2\big)
 8
                            int p_{-} \sigma_{\uparrow-ord}(L, D) \in \langle \leftrightarrow_{\uparrow-ass} (L, D) \rangle
10
11
                                  11\_out\_mda << \sigma_{\uparrow-ord}(L, D) >> :=
12
13
14
15
16
17
18
19
             // 3.2. finalization
             ll\_out\_mda << \bot>> := ll\_out\_mda << \sigma_{\uparrow-ord}(1,1) >>
```

Listing 18. Re-Composition Phase

```
// 2. scalar phase
                                                                                     11_out_mda<<f>>><<
                                                                                                                    p_{-}(1,1) ,..., p_{-}(1,D),
 10
                                                                                                                    p_{L}(L,1) ,..., p_{L}(L,D) >> << b, a>> (
                                                                                                                                                  \mathop{\Longrightarrow}_{\stackrel{\text{MDA}}{\bowtie}}^{1} MDA ( I <<1>>< p_{1}, 1), ..., p_{L}, 1) > (0) ) ,
11
12
                                                                                                                                                 \underset{\Rightarrow}{\overset{D}{\to}} MDA ( I << D >> < p_{1}, D), \dots, p_{L}, D >> (0) )
13
                                                                                     ) _{b\in [1,B^{0\mathrm{B}}]_{\mathbb{N}},a\in [1,A_{L}^{0\mathrm{B}}]_{\mathbb{N}}} := f( ( ll_inp_mda<<f>>>< p_(1,1)
14
  15
 16
                                                                                                                                                                                                                                                                                                                                                                                            p_{L}(L,1) ,..., p_{L}(L,D)>><< b, a>>(
                                                                                                                                                                                                                                                                                                     \stackrel{\text{d}}{=} MDA ( I << 1>>< p_(1,1),...,p_(L,1)>(0) ) ,
17
 18
                                                                                                                                                                                                                                                                                                  \stackrel{d}{\Rightarrow}_{\text{MDA}}^{\text{MDA}}( I << D >> < p_{1}, D), \dots, p_{1}, p_{2}, p_{3}, \dots, p_{n}, 
 19
20
                                                                                                                                                                                                                                                             b \in [1,B^{\mathrm{IB}}]_{\mathbb{N}}, a \in [1,A_h^{\mathrm{IB}}]_{\mathbb{N}}
21
```

Listing 17. Scalar Phase

Our Code Generation Process
is outlined in [1], based on an
imperative-style pseudocode notation
(intended to be described in detail in FW)

<u>Lowering:</u> High Level → Low-Level

Based on (formally defined) performance-critical parameters, for a structured optimization process:

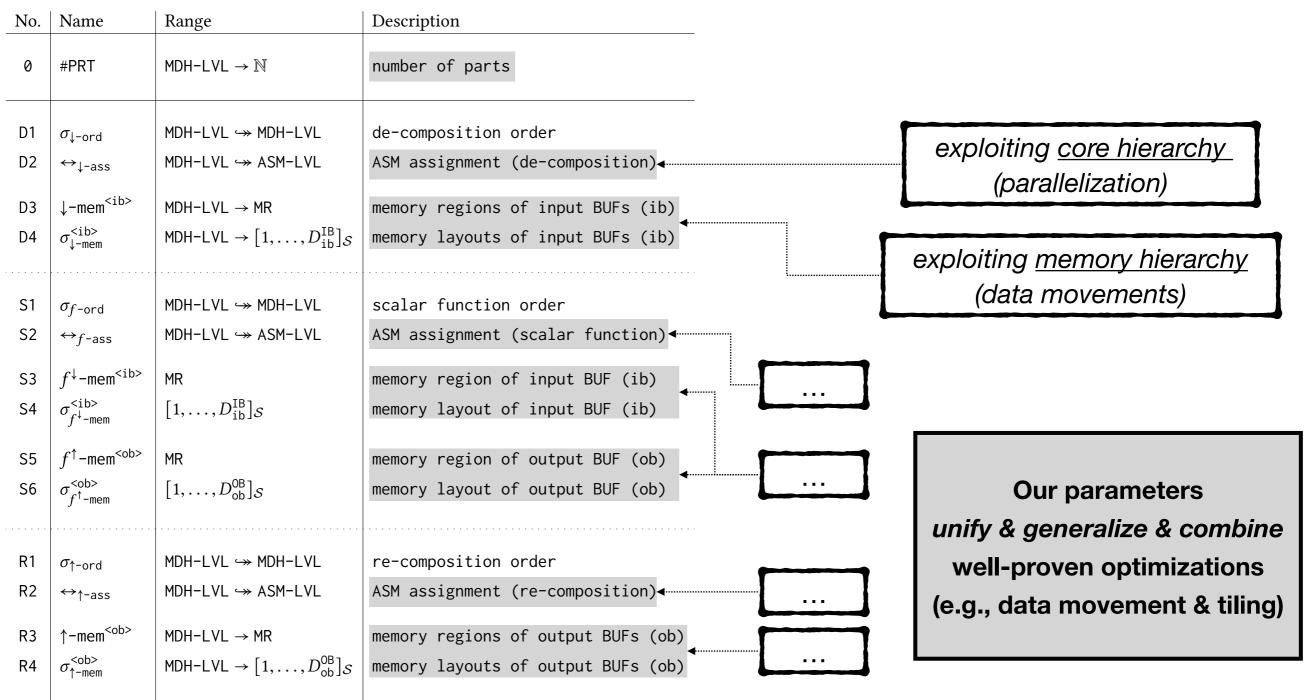


Table 1. Tuning parameters of our low-level expressions

We use our Auto-Tuning Framework (ATF) [1] to fully automatically determine optimized values of parameters

We experimentally evaluate our MDH approach in terms of **Performance** & **Portability** & **Productivity**:

Competitors:

- 1. Scheduling Approach:
 - Apache TVM [2] (GPU & CPU)
- 2. Polyhedral Compilers:
 - PPCG [3] (GPU)
 - Pluto [4] (CPU)
- 3. Functional Approach:
 - Lift [5] (GPU & CPU)
- 4. Domain-Specific Libraries:
 - NVIDIA cuBLAS & cuDNN (GPU)
 - Intel oneMKL & oneDNN (CPU)
- [2] Chen et al., "TVM: An Automated End-to-End Optimizing Compiler for Deep Learning", OSDI'18
- [3] Verdoolaege et al., "Polyhedral Parallel Code Generation for CUDA", TACO'13
- [4] Bondhugula et al., "PLuTo: A Practical and Fully Automatic Polyhedral Program Optimization System", PLDI'08
- [5] Steuwer et al., "Generating Performance Portable Code using Rewrite Rules", ICFP'15

Case Studies:

- 1. Linear Algebra Routines:
 - Matrix Multiplication (MatMul)
 - Matrix-Vector Multiplication (MatVec)
- 2. Stencil Computations:
 - Jacobi Computation (Jacobi1D)
 - Gaussian Convolution (Conv2D)
- 3. Quantum Chemistry:
 - Coupled Cluster (CCSD(T))
- 4. Data Mining:
 - Probabilistic Record Linkage (PRL)
- 5. Deep Learning:
 - Multi-Channel Convolution (MCC)
 - Capsule-Style Convolution (MCC_Capsule)







Performance Evaluation: (via runtime comparison)



		NVIDIA Ampere GPU									
Deep		ResNe	et-50		VGG-16				MobileNet		
Learning	Training		Inference		Training		Inference		Training	Inference	
	MCC	MatMul	MCC	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		ResNo	et-50			VGG	MobileNet				
Learning	Training		Infe	Inference		Training		Inference		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!)



Portability Evaluation: (via Pennycook Metric [6])

	Pennycook Metric										
Deep	ResNet-50				VGG-16				MobileNet		
Learning	Training		Inference		Training		Inference		Training	Inference	
	MCC	MatMul	MCC	MatMul	MCC	MatMul	MCC	MatMul	MCC	MCC	
MDH+ATF	0.67	0.76	0.91	1.00	0.98	0.95	0.97	0.68	0.98	1.00	
TVM+Ansor	0.53	0.62	0.89	0.59	0.76	0.81	0.70	0.61	0. 54	0. 75	

The other related approaches achieve lowest portability — of "0.00" — only, because they are designed for particular architectures and/or application classes only



Productivity Evaluation: (via intuitive argumentation)

```
1 cublasSgemv( /* ... */ );
```

Listing 4. cuBLAS program expressing Matrix-Vector Multiplication (MatVec)

```
for( int i = 0 ; i < M ; ++i )
for( int k = 0 ; k < K ; ++k )
w[i] += M[i][k] * v[k];</pre>
```

Listing 2. PPCG/Pluto program expressing Matrix-Vector Multiplication (MatVec)

Listing 1. TVM program expressing Matrix-Vector Multiplication (MatVec)

Listing 3. Lift program expressing Matrix-Vector Multiplication (MatVec)

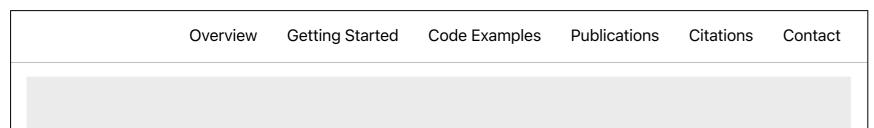
Related Work

MDH often achieves higher *Performance & Portability & Productivity* than state-of-practice approaches:

Class	Popular Examples	Performance	Portability	Productivity	
	MDH	\	✓		
Scheduling	TVM, Halide, Fireiron	✓	often require re-design/extension for new architectures	incorporate user into optimization process	
Polyhedral	TC, PPCG, Pluto	struggle with reductions (e.g., dot in MatMul)	transformations chosen toward particular architectures and data characteristics	✓	
Functional	Lift	✓	transformations designed toward particular architectures and data characteristics	often incorporate user into optimization process	
Domain-Specific	cuBLAS, oneMKL	✓	hand-optimized toward particular architecture and data characteristics	(✓)	
Higher-Level	Futhark, Dex, ATL, Yang et al.[POPL'21],	We consider these appro	paches as greatly combinable	e with our approach 👍	

Conclusion

- MDH is a formalism for expressing and optimizing data-parallel computations.
- MDH achieves higher performance & portability & productivity than related approaches.





Multi-Dimensional Homomorphisms (MDH)

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

Overview

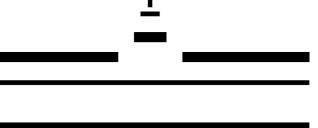
The approach of Multi-Dimensional Homomorphisms (MDH) is an algebraic formalism for systematically reasoning about *decomposition* and *re-composition* strategies of data-parallel computations (such as linear algebra routines and stencil computations) for the memory and core hierarchies of state-of-the-art 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;

We have a Website





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Questions?

Grateful for any kind of feedback



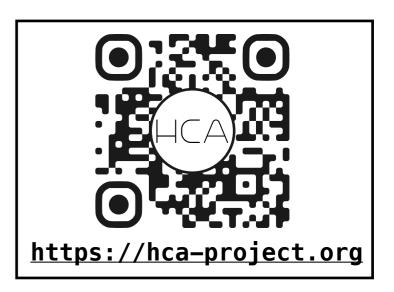
Ari Rasch a.rasch@wwu.de



Code Generation



Code Optimization



Code Execution