# Design of a high-performance tensor-matrix multiplication with BLAS

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#### Abstract

The tensor-matrix multiplication is a basic tensor operation required by various tensor methods such as the HOSVD. This paper presents flexible high-performance algorithms that compute the tensor-matrix product according to the Loopsover-GEMM (LOG) approach. Our algorithms can process dense tensors with any linear tensor layout, arbitrary tensor order and dimensions all of which can be runtime variable. The paper discusses two slicing methods with orthogonal parallelization strategies and propose four algorithms that call BLAS with subtensors or tensor slices. It also provides a simple heuristic which selects one of the four proposed algorithms at runtime. All algorithms have been evaluated on a large set of tensors with various tensor shapes and linear tensor layouts. In case of large tensor slices, our bestperforming algorithm achieves a median performance of 2.47 TFLOPS on an Intel Xeon Gold 5318Y and 2.93 TFLOPS an AMD EPYC 9354. Furthermore, it outperforms batched GEMM implementation of Intel MKL by a factor of 2.57 with large tensor slices. Our runtime tests show that our best-performing algorithm is, on average, at least 6.21% and up to 334.31% faster than frameworks implementing state-of-the-art approaches, including actively developed libraries such as Libtorch and Eigen. For the majority of tensor shapes, it is on par with TBLIS which uses optimized kernels for the TTM computation. Our algorithm performs better than all other competing implementations for the majority of real world tensors from the SDRBench, reaching a maximum speedup of 100.80% or more in some tensor instances. This work is an extended version of the article "Fast and Layout-Oblivious Tensor-Matrix Multiplication with BLAS" (Bassov, 2024)[1].

#### 1. Introduction

Tensor computations are found in many scientific fields
such as computational neuroscience, pattern recognition,
signal processing and data mining [2, 3, 4, 5, 6]. These
computations use basic tensor operations as building blocks
for decomposing and analyzing multidimensional data which
are represented by tensors [7, 8]. Tensor contractions are
an important subset of basic operations that need to be
fast for efficiently solving tensor methods.

There are three main approaches for implementing ten11 sor contractions. The Transpose Transpose GEMM Trans12 pose (TGGT) approach reorganizes tensors in order to
13 perform a tensor contraction using optimized implemen14 tations of the general matrix multiplication (GEMM) [9,
15 10]. GEMM-like Tensor-Tensor multiplication (GETT)
16 method implement macro-kernels that are similar to the
17 ones used in fast GEMM implementations [11, 12]. The
18 third method is the Loops-over-GEMM (LOG) or the BLAS19 based approach in which Basic Linear Algebra Subpro20 grams (BLAS) are utilized with multiple tensor slices or
21 subtensors if possible [13, 14, 15, 16]. The BLAS are
22 considered the de facto standard for writing efficient and
23 portable linear algebra software, which is why nearly all

In this work, we present high-performance algorithms 31 for the tensor-matrix multiplication (TTM) which is used 32 in important numerical methods such as the higher-order  $_{33}$  singular value decomposition and higher-order orthogonal 34 iteration [17, 8, 7]. TTM is a compute-bound tensor op-35 eration and has the same arithmetic intensity as a matrix-36 matrix multiplication which can almost reach the practical 37 peak performance of a computing machine. To our best 38 knowledge, we are the first to combine the LOG approach 39 described in [16, 18] for tensor-vector multiplications with 40 the findings on tensor slicing for the tensor-matrix mul-41 tiplication in [14]. Our algorithms support dense tensors 42 with any order, dimensions and any linear tensor layout 43 including the first- and the last-order storage formats for 44 any contraction mode all of which can be runtime variable. 45 Supporting arbitrary tensor layouts enables other frame-46 works non-column-major storage formats to easily inte-47 grate our library without tensor reformatting and unneces-48 sary copy operations<sup>1</sup>. Our implementation compute the

<sup>&</sup>lt;sup>24</sup> processor vendors provide highly optimized BLAS imple-<sup>25</sup> mentations. LOG-based and TTGT-based implementa-<sup>26</sup> tion are in general easier to maintain and faster to port <sup>27</sup> than GETT solutions. The latter might need to adapt <sup>28</sup> vector instructions or blocking parameters according to a <sup>29</sup> processor's microarchitecture.

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<sup>&</sup>lt;sup>1</sup>For example, Tensorly [19] requires tensors to be stored in the last-order storage format (row-major).

49 tensor-matrix product in parallel using efficient GEMM 102 column-major matrix storage format and benchmarked our 51 their high performance, all algorithms are layout-oblivious  $_{53}$  tensor layout and without tuning. We provide a single al-55 on a simple heuristic.

Every proposed algorithm can be implemented with  $_{57}$  less than 150 lines of C++ code where the algorithmic 58 complexity is reduced by the BLAS implementation and 59 the corresponding selection of subtensors or tensor slices. 60 We have provided an open-source C++ implementation of 61 all algorithms and a python interface for convenience.

The analysis in this work quantifies the impact of the 63 tensor layout, the tensor slicing method and parallel ex-64 ecution of slice-matrix multiplications with varying con-65 traction modes. The runtime measurements of our imple-66 mentations are compared with state-of-the-art approaches 67 discussed in [11, 12, 20] including LibTorch and Eigen. 118 68 While our implementation have been benchmarked with 69 the Intel MKL and AMD AOCL libraries, the user is free 70 to select OpenBLAS. In summary, the main findings of our 71 work are:

• Given a row-major or column-major input matrix, the tensor-matrix multiplication with tensors of any linear tensor layout can be implemented by an inplace algorithm with 1 GEMV and 7 GEMM instances, supporting all combinations of contraction mode, tensor order and tensor dimensions.

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- The proposed algorithms show a similar performance characteristic across different tensor layouts, provided that the contraction conditions remain the same.
  - proposed algorithms at runtime, providing a near-
  - Our best-performing algorithm is a factor of 2.57 faster than Intel's batched GEMM implementation for large tensor slices.
  - Our best-performing algorithm has a median speedup between 6.21% and 334.31% compared to other stateand Eigen when asymmetrically shaped tensors are used.

This work is an extended version of the article "Fast 93 and Layout-Oblivious Tensor-Matrix Multiplication with 94 BLAS" [1]. Compared to our previous publication, we 95 have made several significant additions. We provide run-96 time tests on a more recent Intel Xeon Gold 5318Y CPU 97 and expanded our study to include AMD's AOCL, running 98 additional benchmarks on an AMD EPYC 9354 CPU. We 153 age TuckerMPI for large-scale data compression that is 99 incorporate a newer version of TBLIS and LibTorch while 100 also testing the TuckerMPI TTM implementation. Fur-101 thermore, we extend our implementations to support the

50 without transposing or flattening tensors. In addition to 103 algorithms for both row-major and column-major layouts, analyzing the runtime results in detail. We also present a 52 and provide a sustained performance independent of the 105 heuristic that enables the use of a single TTM algorithm,  $_{106}$  ensuring efficiency across different storage formats and a 54 gorithm that selects one of the proposed algorithms based 107 wide range of tensor shapes. Lastly, we evaluate our and 108 other libraries using real-world tensors from SDRBench

> The remainder of the paper is organized as follows. 111 Section 2 presents related work. Section 3 introduces some 112 notation on tensors and defines the tensor-matrix multi-113 plication. Algorithm design and methods for slicing and 114 parallel execution are discussed in Section 4. Section 5 115 describes the test setup. Benchmark results are presented 116 in Section 6. Conclusions are drawn in Section 8.

#### 117 2. Related Work

Springer et al. [11] present a tensor-contraction gen-119 erator TCCG and the GETT approach for dense tensor 120 contractions that is inspired from the design of a high-121 performance GEMM. Their unified code generator selects 122 implementations from generated GETT, LOG and TTGT 123 candidates. Their findings show that among 48 different 124 contractions 15% of LOG-based implementations are the 125 fastest.

Matthews [12] presents a runtime flexible tensor con-127 traction library that uses GETT approach as well. He de-128 scribes block-scatter-matrix algorithm which uses a special 129 layout for the tensor contraction. The proposed algorithm 130 yields results that feature a similar runtime behavior to 131 those presented in [11].

Li et al. [14] introduce InTensLi, a framework that 133 generates in-place tensor-matrix multiplication according A simple heuristic is sufficient to select one of the 134 to the LOG approach. The authors discusses optimization 135 and tuning techniques for slicing and parallelizing the opoptimal performance for a wide range of tensor shapes. 136 eration. With optimized tuning parameters, they report 137 a speedup of up to 4x over the TTGT-based MATLAB 138 tensor toolbox library discussed in [9].

Başsoy [16] presents LoG-based algorithms that com-140 pute the tensor-vector product. They support dense ten-141 sors with linear tensor layouts, arbitrary dimensions and 142 tensor order. The presented approach contains eight cases of-the art library implementations, including LibTorch 143 calling GEMV and DOT. He reports average speedups of 144 6.1x and 4.0x compared to implementations that use the 145 TTGT and GETT approach, respectively.

> Pawlowski et al. [18] propose morton-ordered blocked 147 layout for a mode-oblivious performance of the tensor-148 vector multiplication. Their algorithm iterate over blocked 149 tensors and perform tensor-vector multiplications on blocked 150 tensors. They are able to achieve high performance and 151 mode-oblivious computations.

In [21] the authors present the C++ software pack-152 154 used for the tensor tucker decomposition. The library pro-155 vides a parallel C++ function of the latter containing dis-156 tributed functions with MPI for the Gram computation

159 computing the tensor-matrix product with submatrices ac-161 corresponds to our corresponds to our corresponds version.

#### 162 3. Background

## 163 3.1. Tensor Notation

An order-p tensor is a p-dimensional array where ten-165 sor elements are contiguously stored in memory[22, 7]. 166 We write a, a, A and A in order to denote scalars, vec-167 tors, matrices and tensors. If not otherwise mentioned, 168 we assume **A** to have order p > 2. The p-tuple **n** =  $(n_1, n_2, \ldots, n_p)$  will be referred to as the shape or dimen-170 sion tuple of a tensor where  $n_r > 1$ . We will use round 171 brackets  $\underline{\mathbf{A}}(i_1,i_2,\ldots,i_p)$  or  $\underline{\mathbf{A}}(\mathbf{i})$  to denote a tensor element where  $\mathbf{i}=(i_1,i_2,\ldots,i_p)$  is a multi-index. For con-173 venience, we will also use square brackets to concatenate 174 index tuples such that  $[\mathbf{i}, \mathbf{j}] = (i_1, i_2, \dots, i_r, j_1, j_2, \dots, j_q)$ where **i** and **j** are multi-indices of length r and q, respec-

### 3.2. Tensor-Matrix Multiplication (TTM)

Let  $\underline{\mathbf{A}}$  and  $\underline{\mathbf{C}}$  be order-p tensors with shapes  $\mathbf{n}_a =$  $\mathbf{n}_{c} = ([\mathbf{n}_{1}, n_{q}, \mathbf{n}_{2}]) \text{ and } \mathbf{n}_{c} = ([\mathbf{n}_{1}, m, \mathbf{n}_{2}]) \text{ where } \mathbf{n}_{1} = (n_{1}, n_{2}, n_{2})$  $(180..., n_{q-1})$  and  $\mathbf{n}_2 = (n_{q+1}, n_{q+2}, ..., n_p)$ . Let **B** be a ma-181 trix of shape  $\mathbf{n}_b = (m, n_q)$ . A q-mode tensor-matrix prod-182 uct is denoted by  $\underline{\mathbf{C}} = \underline{\mathbf{A}} \times_q \mathbf{B}$ . An element of  $\underline{\mathbf{C}}$  is defined

$$\underline{\mathbf{C}}([\mathbf{i}_1, j, \mathbf{i}_2]) = \sum_{i_n=1}^{n_q} \underline{\mathbf{A}}([\mathbf{i}_1, i_q, \mathbf{i}_2]) \cdot \mathbf{B}(j, i_q)$$
(1)

with  $\mathbf{i}_1=(i_1,\ldots,i_{q-1})$ ,  $\mathbf{i}_2=(i_{q+1},\ldots,i_p)$  where  $1\leq i_r\leq n_r$  and  $1\leq j\leq m$  [14, 8]. The mode q is called the 186 contraction mode with  $1 \leq q \leq p$ . TTM generalizes the 187 computational aspect of the two-dimensional case  $\mathbf{C}=$ 188  $\mathbf{B} \cdot \mathbf{A}$  if p = 2 and q = 1. Its arithmetic intensity is 189 equal to that of a matrix-matrix multiplication which is 190 compute-bound for large dense matrices.

In the following, we assume that the tensors  $\underline{\mathbf{A}}$  and  $\mathbf{C}$ 192 have the same tensor layout  $\pi$ . Elements of matrix **B** can 193 be stored either in the column-major or row-major format. 194 With  $i_q$  iterating over the second mode of **B**, TTM is also 195 referred to as the *q*-mode product which is a building block 196 for tensor methods such as the higher-order orthogonal 197 iteration or the higher-order singular value decomposition 198 [8]. Please note that the following method can be applied, 199 if indices j and  $i_q$  of matrix **B** are swapped.

## 200 3.3. Subtensors

A subtensor references elements of a tensor  $\underline{\mathbf{A}}$  and is 202 denoted by  $\underline{\mathbf{A}}'$ . It is specified by a selection grid that conp sists of p index ranges. In this work, an index range of a  $_{204}$  given mode r shall either contain all indices of the mode

<sub>157</sub> and tensor-matrix multiplication. Th latter invokes a lo-<sub>205</sub> r or a single index  $i_r$  of that mode where  $1 \le r \le p$ . Sub-158 cal version that contains a multi-threaded gemm function, 206 tensor dimensions  $n_r'$  are either  $n_r$  if the full index range  $_{207}$  or 1 if a a single index for mode r is used. Subtensors are 160 cording to the LOG approach. The presented local TTM 208 annotated by their non-unit modes such as  $\underline{\mathbf{A}}'_{u,v,w}$  where 209  $n_u > 1$ ,  $n_v > 1$  and  $n_w > 1$  for  $1 \le u \ne v \ne w \le p$ . The 210 remaining single indices of a selection grid can be inferred 211 by the loop induction variables of an algorithm. The num-212 ber of non-unit modes determine the order p' of subtensor where  $1 \leq p' < p$ . In the above example, the subten-214 sor  $\underline{\mathbf{A}}'_{u,v,w}$  has three non-unit modes and is thus of order 215 3. For convenience, we might also use an dimension tuple 216 **m** of length p' with  $\mathbf{m} = (m_1, m_2, \dots, m_{p'})$  to specify a <sub>217</sub> mode-p' subtensor  $\underline{\mathbf{A}}'_{\mathbf{m}}$ . An order-2 subtensor of  $\underline{\mathbf{A}}'$  is a 218 tensor slice  $\mathbf{A}'_{u,v}$  and an order-1 subtensor of  $\underline{\mathbf{A}}'$  is a fiber

#### 220 3.4. Linear Tensor Layouts

We use a layout tuple  $\pi \in \mathbb{N}^p$  to encode all linear 222 tensor layouts including the first-order or last-order lay-223 out. They contain permuted tensor modes whose priority  $_{224}$  is given by their index. For instance, the general k-order 225 tensor layout for an order-p tensor is given by the layout 226 tuple  $\boldsymbol{\pi}$  with  $\pi_r = k - r + 1$  for  $1 < r \le k$  and r for  $227 k < r \le p$ . The first- and last-order storage formats are 228 given by  $\pi_F = (1, 2, ..., p)$  and  $\pi_L = (p, p - 1, ..., 1)$ . 229 An inverse layout tuple  $\pi^{-1}$  is defined by  $\pi^{-1}(\pi(k)) = k$ . 230 Given the contraction mode q with  $1 \leq q \leq p$ ,  $\hat{q}$  is de-231 fined as  $\hat{q} = \boldsymbol{\pi}^{-1}(q)$ . Given a layout tuple  $\boldsymbol{\pi}$  with p<sup>232</sup> modes, the  $\pi_r$ -th element of a stride tuple **w** is given by <sup>233</sup>  $w_{\pi_r} = \prod_{k=1}^{r-1} n_{\pi_k}$  for  $1 < r \le p$  and  $w_{\pi_1} = 1$ . Tensor ele- $_{234}$  ments of the  $\pi_1$ -th mode are contiguously stored in mem-235 ory. Their location is given by the layout function  $\lambda_{\mathbf{w}}$  $_{236}$  which maps a multi-index i to a scalar index such that  $_{237} \lambda_{\mathbf{w}}(\mathbf{i}) = \sum_{r=1}^{p} w_r(i_r - 1) [23].$ 

## 238 3.5. Reshaping

The reshape operation defines a non-modifying refor-240 matting transformation of dense tensors with contiguously 241 stored elements and linear tensor layouts. It transforms  $_{ ext{242}}$  an order-p tensor  $oldsymbol{\underline{A}}$  with a shape  ${f n}$  and layout  $oldsymbol{\pi}$  tu-<sub>243</sub> ple to an order-p' view  $\underline{\mathbf{B}}$  with a shape  $\mathbf{m}$  and layout <sub>244</sub>  $\boldsymbol{\tau}$  tuple of length p' with p' = p - v + u and  $1 \leq u <$  $v \leq p$ . Given a layout tuple  $\pi$  of  $\underline{\mathbf{A}}$  and contiguous 246 modes  $\hat{\boldsymbol{\pi}} = (\pi_u, \pi_{u+1}, \dots, \pi_v)$  of  $\boldsymbol{\pi}$ , reshape function  $\varphi_{u,v}$ 247 is defined as follows. With  $j_k = 0$  if  $k \leq u$  and  $j_k =$  $_{248} v - u$  if k > u where  $1 \le k \le p'$ , the resulting lay-249 out tuple  $\boldsymbol{\tau}=(\tau_1,\ldots,\tau_{p'})$  of  $\underline{\mathbf{B}}$  is then given by  $\tau_u=$ 250  $\min(\pi_{u,v})$  and  $\tau_k = \pi_{k+j_k} - s_k$  for  $k \neq u$  with  $s_k = 0$  $_{251}$   $|\{\pi_i \mid \pi_{k+j_k} > \pi_i \wedge \pi_i \neq \min(\hat{\boldsymbol{\pi}}) \wedge u \leq i \leq p\}|$ . Elements of 252 the shape tuple **m** are defined by  $m_{\tau_u} = \prod_{k=u}^v n_{\pi_k}$  and <sub>253</sub>  $m_{\tau_k} = n_{\pi_{k+j}}$  for  $k \neq u$ . Note that reshaping is not related 254 to tensor unfolding or the flattening operations which re-<sup>255</sup> arrange tensors by copying tensor elements [8, p.459].

### 256 4. Algorithm Design

257 4.1. Baseline Algorithm with Contiguous Memory Access

The tensor-matrix multiplication (TTM) in equation 1 259 can be implemented with a single algorithm using nested 260 recursion [23]. Such an algorithm consists of two if state-261 ments with recursive calls and an else branch which con-262 stitutes the base case. A naive implementation recursively 263 selects fibers of the input and output tensor for the base 264 case that computes a fiber-matrix product. The outer loop 265 iterates over the dimension m and selects an element of  $\underline{\mathbf{C}}$ 's 266 fiber and a row of  $\mathbf{B}$ . The inner loop then iterates over dimension  $n_q$  and computes the inner product of a fiber of 268  $\underline{\mathbf{A}}$  and the row  $\mathbf{B}$ . In this case, elements of  $\underline{\mathbf{A}}$  and  $\underline{\mathbf{C}}$  are 269 accessed non-contiguously whenever  $\pi_1 \neq q$  and matrix  $\underline{\mathbf{B}}$  270 is accessed only with unit strides if it elements are stored 271 contiguously along its rows.

A better approach is illustrated by Algorithm 1 where  $_{273}$  the loop order is adjusted to the tensor layout  $\pi$  and mem-<sub>274</sub> ory is accessed contiguously for  $\pi_1 \neq q$  and p > 1. The 275 algorithm takes the input order-p tensor  $\underline{\mathbf{A}}$ , input matrix  $_{276}$  B, order-p output tensor C, the shape tuple n of A, the 277 layout tuple  $\pi$  of both tensors, an index tuple  $\pi$  of length  $_{278}$  p, the first dimension m of **B**, the contraction mode q with  $1 \le q \le p$  and  $\hat{q} = \pi^{-1}(q)$ . Initially called with  $\mathbf{i} = \mathbf{0}$ 280 and r = p, the algorithm increments indices with smaller  $_{\text{281}}$  strides as  $w_{\pi_r} \leq w_{\pi_{r+1}}$  with increasing recursion level and  $_{282}$  decreasing r. This is accomplished in line 5 which uses the 283 layout tuple  $\pi$  to select a multi-index element  $i_{\pi_r}$  and to 284 increment it with the corresponding stride  $w_{\pi_r}$ . The two  $_{285}$  if statements in line number 2 and 4 allow the loops over 286 modes q and  $\pi_1$  to be placed into the base case in which a 287 slice-matrix multiplication is performed. The inner-most 288 loop of the base case increments  $i_{\pi_1}$  with a unit stride and 289 contiguously accesses tensor elements of  $\underline{\mathbf{A}}$  and  $\underline{\mathbf{C}}$ . The 290 second loop increments  $i_q$  with which elements of  ${\bf B}$  are  $_{291}$  contiguously accessed if  ${f B}$  is stored in the row-major for- $_{292}$  mat. The third loop increments j and could be placed as  $_{293}$  the second loop if **B** is stored in the column-major format. While spatial data locality is improved by adjusting <sup>295</sup> the loop ordering, slices  $\underline{\mathbf{A}}'_{\pi_1,q}$ , fibers  $\underline{\mathbf{C}}'_{\pi_1}$  and elements  $\underline{\mathbf{B}}(j,i_q)$  are accessed  $m,\ n_q$  and  $n_{\pi_1}$  times, respectively. While the specified fiber of  $\underline{\mathbf{C}}$  might fit into first or second 298 level cache, slice elements of  $\underline{\mathbf{A}}$  are unlikely to fit in the 299 local caches if the slice size  $n_{\pi_1} \times n_q$  is large, leading to 300 higher cache misses and suboptimal performance. Instead 301 of attempting to improve the temporal data locality, we 302 call high-performance BLAS implementations in the base

## 304 4.2. BLAS-based Algorithms with Tensor Slices

 $_{\rm 305}$  BLAS-based algorithms for the TTM call CBLAS gemm  $_{\rm 306}$  function in the base case of Algorithm 1 in order to perform  $_{\rm 307}$  fast slice-matrix multiplications  $^2$ . Function gemm denotes

303 case. The following subsection explains this approach.

**Algorithm 1:** Modified baseline algorithm for TTM with contiguous memory access. The tensor order p must be greater than 1 and the contraction mode q must satisfy  $1 \le q \le p$  and  $\pi_1 \ne q$ . The initial call must happen with r=p where  $\mathbf n$  is the shape tuple of  $\underline{\mathbf A}$  and m is the q-th dimension of  $\underline{\mathbf C}$ . Iteration along mode q with  $\hat q = \pi_q^{-1}$  is moved into the inner-most recursion level

308 a general matrix-matrix multiplication which is defined as 309 C:=a\*op(A)\*op(B)+b\*C where a and b are scalars, A, B and 310 C are matrices, op(A) is an M-by-K matrix, op(B) is a K-by-N 311 matrix and C is an N-by-N matrix. Function op(x) either 312 transposes the corresponding matrix x such that op(x)=x' 313 or not op(x)=x. The CBLAS interface also allows users to 314 specify matrix's leading dimension by providing the LDA, 315 LDB and LDC parameters. A leading dimension specifies 316 the number of elements that is required for iterating over 317 the non-contiguous matrix dimension. The leading dimen-318 sion can be used to perform a matrix multiplication with 319 submatrices or even fibers within submatrices. The lead-320 ing dimension parameter is necessary for the BLAS-based 321 TTM.

The eighth TTM case in Table 1 contains all argu-323 ments that are necessary to perform a CBLAS gemm in 324 the base case of Algorithm 1. The arguments of gemm are 325 set according to the tensor order p, tensor layout  $\pi$  and  $_{326}$  contraction mode q. If the input matrix **B** has the row-327 major order, parameter CBLAS\_ORDER of function gemm is 328 set to CblasRowMajor (rm) and CblasColMajor (cm) other- $_{329}$  wise. The eighth case will be denoted as the general case 330 in which function gemm is called multiple times with dif-331 ferent tensor slices. Next to the eighth TTM case, there 332 are seven corner cases where a single gemv or gemm call suf-333 fices to compute the tensor-matrix product. For instance 334 if  $\pi_1 = q$ , the tensor-matrix product can be computed 335 by a matrix-matrix multiplication where the input tensor 336 A can be reshaped and interpreted as a matrix without 337 any copy operation. Note that Table 1 supports all linear  $_{338}$  tensor layouts of A and C with no limitations on tensor 339 order and contraction mode. The following subsection de- $_{340}$  scribes all eight TTM cases when the input matrix  ${f B}$  has 341 the row-major ordering.

 $<sup>\</sup>mathtt{ttm}(\underline{\mathbf{A}},\mathbf{B},\underline{\mathbf{C}},\mathbf{n},\boldsymbol{\pi},\mathbf{i},m,q,\hat{q},r)$ if  $r = \hat{a}$  then 3  $ttm(\underline{\mathbf{A}}, \mathbf{B}, \underline{\mathbf{C}}, \mathbf{n}, \boldsymbol{\pi}, \mathbf{i}, m, q, \hat{q}, r-1)$ 4 else if r > 1 then for  $i_{\pi_r} \leftarrow 1$  to  $n_{\pi_r}$  do 5  $ttm(\underline{\mathbf{A}}, \mathbf{B}, \underline{\mathbf{C}}, \mathbf{n}, \boldsymbol{\pi}, \mathbf{i}, m, q, \hat{q}, r-1)$ 6 for  $j \leftarrow 1$  to m do 8 for  $i_q \leftarrow 1$  to  $n_q$  do 9 10 for  $i_{\pi_1} \leftarrow 1$  to  $n_{\pi_1}$  do 

<sup>&</sup>lt;sup>2</sup>CBLAS denotes the C interface to the BLAS.

Case	Order $p$	Layout $\pi_{\underline{\mathbf{A}},\underline{\mathbf{C}}}$	Layout $\pi_{\mathbf{B}}$	$\mathrm{Mode}\; q$	Routine	T	М	N	K	A	LDA	В	LDB	LDC
1	1	-	rm/cm	1	gemv	-	m	$n_1$	-	В	$n_1$	<u>A</u>	-	-
2	2	cm	rm	1	gemm	В	$n_2$	m	$n_1$	<u>A</u>	$n_1$	В	$n_1$	m
	$^2$	cm	cm	1	gemm	-	m	$n_2$	$n_1$	$\mathbf{B}$	m	$\underline{\mathbf{A}}$	$n_1$	m
3	$^2$	cm	rm	2	gemm	-	m	$n_1$	$n_2$	$\mathbf{B}$	$n_2$	$\underline{\mathbf{A}}$	$n_1$	$n_1$
	$^2$	cm	cm	2	gemm	$\mathbf{B}$	$n_1$	m	$n_2$	$\underline{\mathbf{A}}$	$n_1$	$\mathbf{B}$	m	$n_1$
4	$^2$	rm	rm	1	gemm	-	m	$n_2$	$n_1$	$\mathbf{B}$	$n_1$	$\underline{\mathbf{A}}$	$n_2$	$n_2$
	2	rm	cm	1	gemm	$\mathbf{B}$	$n_2$	m	$n_1$	$\underline{\mathbf{A}}$	$n_2$	$\overline{\mathbf{B}}$	m	$n_2$
5	2	rm	rm	2	gemm	$\mathbf{B}$	$n_1$	m	$n_2$	$\overline{\mathbf{A}}$	$n_2$	$\mathbf{B}$	$n_2$	m
	2	rm	cm	2	gemm	-	m	$n_1$	$n_2$	$\overline{\mathbf{B}}$	m	$\underline{\mathbf{A}}$	$n_2$	m
6	> 2	any	rm	$\pi_1$	gemm	В	$\bar{n}_q$	$\overline{m}$	$n_q$	<u>A</u>	$n_q$	В	$n_q$	$\overline{m}$
	> 2	any	cm	$\pi_1$	gemm	-	m	$\bar{n}_q$	$n_q$	$\mathbf{B}$	m	$\underline{\mathbf{A}}$	$n_q$	m
7	> 2	any	rm	$\pi_p$	gemm	-	m	$\bar{n}_q$	$n_q$	$\mathbf{B}$	$n_q$	$\underline{\mathbf{A}}$	$\bar{n}_q$	$\bar{n}_q$
	> 2	any	cm	$\pi_p$	gemm	$\mathbf{B}$	$\bar{n}_q$	m	$n_q$	$\underline{\mathbf{A}}$	$ar{n}_q$	$\overline{\mathbf{B}}$	m	$\bar{n}_q$
8	> 2	any	rm	$\pi_2,, \pi_{p-1}$	gemm*	-	m	$n_{\pi_1}$	$n_q$	В	$n_q$	<u>A</u>	$w_q$	$w_q$
	> 2	any	cm	$\pi_2,, \pi_{p-1}$	gemm*	$\mathbf{B}$	$n_{\pi_1}$	m	$n_q$	$\underline{\mathbf{A}}$	$w_q$	$\mathbf{B}$	m	$w_q$

Table 1: Eight TTM cases implementing the mode-q TTM with the gemm and gemv CBLAS functions. Arguments of gemv and gemm (T, M, N, dots) are chosen with respect to the tensor order p, layout  $\pi$  of  $\underline{\mathbf{A}}$ ,  $\underline{\mathbf{B}}$ ,  $\underline{\mathbf{C}}$  and contraction mode q where T specifies if  $\underline{\mathbf{B}}$  is transposed. Function gemm\* with a star denotes multiple gemm calls with different tensor slices. Argument  $\bar{n}_q$  for case 6 and 7 is defined as  $\bar{n}_q = (\prod_r^p n_r)/n_q$ . Input matrix **B** is either stored in the column-major or row-major format. The storage format flag set for gemm and gemv is determined by the element ordering of B.

## 342 4.2.1. Row-Major Matrix Multiplication

344 are listed in Table 1.

346 be computed with a gemv operation where  $\underline{\mathbf{A}}$  is an order-1 381 respectively. tensor **a** of length  $n_1$  such that  $\mathbf{a}^T \cdot \mathbf{B}$ .

Case 2-5: If p=2,  $\underline{\mathbf{A}}$  and  $\underline{\mathbf{C}}$  are order-2 tensors with 382 4.2.2. Column-Major Matrix Multiplication 349 dimensions  $n_1$  and  $n_2$ . In this case the tensor-matrix prod-383  $_{350}$  uct can be computed with a single gemm. If  $\bf A$  and  $\bf C$  have  $_{384}$  column-major version of gemm when the input matrix  $\bf B$  is <sub>351</sub> the column-major format with  $\pi = (1,2)$ , gemm either ex- <sub>385</sub> stored in column-major order. Although the number of 352 ecutes  $C = A \cdot B^T$  for q = 1 or  $C = B \cdot A$  for q = 2. 386 gemm cases remains the same, the gemm arguments must be 353 Both matrices can be interpreted C and A as matrices in 387 rearranged. The argument arrangement for the column-354 row-major format although both are stored column-wise. 388 major version can be derived from the row-major version 355 If **A** and **C** have the row-major format with  $\pi = (2,1)$ , 389 that is provided in Table 1. 356 gemm either executes  $\mathbf{C} = \mathbf{B} \cdot \mathbf{A}$  for q = 1 or  $\mathbf{C} = \mathbf{A} \cdot \mathbf{B}^T$  for 390  $_{357}$  q=2. The transposition of **B** is necessary for the TTM  $_{391}$  swapped and the transposition flag for matrix **B** is toggled. 2558 cases 2 and 5 which is independent of the chosen layout. 392 Also, the leading dimension argument of A is adjusted to

360 gemm with the corresponding arguments executes  $\mathbf{C} = \mathbf{A}$ . 394 dimension of B.  $_{361}~\mathbf{B}^T$  and computes a tensor-matrix product  $\mathbf{C} = \mathbf{\underline{A}} imes_{\pi_1} \mathbf{B}$ .  $_{395}$  $\underline{\mathbf{A}}$  Tensors  $\underline{\mathbf{A}}$  and  $\underline{\mathbf{C}}$  are reshaped with  $\varphi_{2,p}$  to row-major  $\underline{\mathbf{A}}$  in Table 1 where tensor  $\underline{\mathbf{A}}$  and matrix  $\mathbf{B}$  are passed to matrices  $\overline{\bf A}$  and  $\overline{\bf C}$ . Matrix  $\overline{\bf A}$  has  $\bar{n}_{\pi_1} = \bar{n}/n_{\pi_1}$  rows and 397 B and A. The corresponding column-major version is at- $_{364}$   $n_{\pi_1}$  columns while matrix C has the same number of rows  $_{398}$  tained when tensor  $\underline{\mathbf{A}}$  and matrix  $\mathbf{B}$  are passed to  $\underline{\mathbf{A}}$  and and m columns. If  $\pi_p = q$  (case 7),  $\underline{\mathbf{A}}$  and  $\underline{\mathbf{C}}$  are reshaped 399 B where the transpose flag for  $\mathbf{B}$  is set and the remaining with  $\varphi_{1,p-1}$  to column-major matrices **A** and **C**. Matrix 400 dimensions are adjusted accordingly.  $n_{\pi_p}$  rows and  $\bar{n}_{\pi_p} = \bar{n}/n_{\pi_p}$  columns while C has 368 m rows and the same number of columns. In this case, a 401 4.2.3. Matrix Multiplication Variations 369 single gemm executes  $\mathbf{C} = \mathbf{B} \cdot \mathbf{A}$  and computes  $\mathbf{C} = \mathbf{A} \times_{\pi_n} \mathbf{B}$ . 402 370 Noticeably, the desired contraction are performed without 403 be used interchangeably by adapting the storage format. 371 copy operations, see also Section 3.5.

<sup>373</sup> 2 with  $\pi_1 \neq q$  and  $\pi_p \neq q$ , the modified baseline Algo- <sup>406</sup> row-major matrices, provided that the arguments are re- $_{374}$  rithm 1 is used to successively call  $\bar{n}/(n_q \cdot n_{\pi_1})$  times gemm  $_{407}$  arranged accordingly. While the argument rearrangement 375 with different tensor slices of  $\underline{C}$  and  $\underline{A}$ . Each gemm com-408 is similar, the arguments associated with the matrices  $\underline{A}$ 

1.1. Row-Major Matrix Multiplication 377 the corresponding tensor slices  $\underline{\mathbf{A}}'_{\pi_1,q}$  and the matrix  $\mathbf{B}$ . The following paragraphs introduce all TTM cases that 378 The matrix-matrix product  $\mathbf{C} = \mathbf{B} \cdot \mathbf{A}$  is performed by  $_{379}$  interpreting both tensor slices as row-major matrices  ${f A}$ Case 1: If p=1, The tensor-vector product  $\underline{\mathbf{A}} \times_1 \mathbf{B}$  can 300 and  $\mathbf{C}$  which have the dimensions  $(n_q, n_{\pi_1})$  and  $(m, n_{\pi_1})$ ,

The tensor-matrix multiplication is performed with the

The CBLAS arguments of M and N, as well as A and B is Case 6-7: If p>2 and if  $q=\pi_1(\text{case 6})$ , a single 393 LDB or LDA. The only new argument is the new leading

Given case 4 with the row-major matrix multiplication

The column-major and row-major versions of gemm can 404 This means that a gemm operation for column-major ma-Case 8 (p > 2): If the tensor order is greater than 405 trices can compute the same matrix product as one for <sub>376</sub> putes one slice  $\underline{\mathbf{C}}'_{\pi_1,q}$  of the tensor-matrix product  $\underline{\mathbf{C}}$  using <sub>409</sub> and B must be interchanged. Specifically, LDA and LDB as  $_{410}$  well as M and N are swapped along with the corresponding  $_{411}$  matrix pointers. In addition, the transposition flag must  $_{412}$  be set for A or B in the new format if B or A is transposed  $_{413}$  in the original version.

For instance, the column-major matrix multiplication  $_{415}$  in case 4 of Table 1 requires the arguments of A and B to  $_{416}$  be tensor  $\underline{\mathbf{A}}$  and matrix  $\mathbf{B}$  with  $\mathbf{B}$  being transposed. The  $_{417}$  arguments of an equivalent row-major multiplication for A,  $_{418}$  B, M, N, LDA, LDB and T are then initialized with  $\mathbf{B}$ ,  $\underline{\mathbf{A}}$ , m,  $_{419}$   $n_2$ , m,  $n_2$  and  $\mathbf{B}$ .

Another possible matrix multiplication variant with  $_{421}$  the same product is computed when, instead of  $\bf B$ , ten-  $_{422}$  sors  $\bf \underline{A}$  and  $\bf \underline{C}$  with adjusted arguments are transposed. We assume that such reformulations of the matrix multi-  $_{424}$  plication do not outperform the variants shown in Table 1,  $_{425}$  as we expect BLAS libraries to have optimal blocking and  $_{426}$  multiplication strategies.

#### 427 4.3. Matrix Multiplication with Subtensors

Algorithm 1 can be slightly modified in order to call gemm with reshaped order- $\hat{q}$  subtensors that correspond to larger tensor slices. Given the contraction mode q with 1 < q < p, the maximum number of additionally fusible modes is  $\hat{q} - 1$  with  $\hat{q} = \pi^{-1}(q)$  where  $\pi^{-1}$  is the inverse layout tuple. The corresponding fusible modes are there-

The non-base case of the modified algorithm only iterates ates over dimensions that have indices larger than  $\hat{q}$  and thus omitting the first  $\hat{q}$  modes. The conditions in line 2 and 4 are changed to  $1 < r \le \hat{q}$  and  $\hat{q} < r$ , respectively. Thus, loop indices belonging to the outer  $\pi_r$ -th 40 loop with  $\hat{q}+1 \le r \le p$  define the order- $\hat{q}$  subtensors  $\underline{\mathbf{A}}'_{\pi'}$  and  $\underline{\mathbf{C}}'_{\pi'}$  of  $\underline{\mathbf{A}}$  and  $\underline{\mathbf{C}}$  with  $\pi' = (\pi_1, \dots, \pi_{\hat{q}-1}, q)$ . Reshaping the subtensors  $\underline{\mathbf{A}}'_{\pi'}$  and  $\underline{\mathbf{C}}'_{\pi'}$  with  $\varphi_{1,\hat{q}-1}$  for the modes 443  $\pi_1, \dots, \pi_{\hat{q}-1}$  yields two tensor slices with dimension  $n_q$  or 444 m with the fused dimension  $\bar{n}_q = \prod_{r=1}^{\hat{q}-1} n_{\pi_r}$  and  $\bar{n}_q = w_q$ . 445 Both tensor slices can be interpreted either as row-major 446 or column-major matrices with shapes  $(n_q, \bar{n}_q)$  or  $(w_q, \bar{n}_q)$  477 in case of  $\underline{\mathbf{A}}$  and  $(m, \bar{n}_q)$  or  $(\bar{n}_q, m)$  in case of  $\underline{\mathbf{C}}$ , respectable tively.

The gemm function in the base case is called with al- most identical arguments except for the parameter M or solution which is set to  $\bar{n}_q$  for a column-major or row-major multiplication, respectively. Note that neither the selection of the subtensor nor the reshaping operation copy tensor elements. This description supports all linear tensor layouts and generalizes lemma 4.2 in [14] without copying tensor elements, see section 3.5. The division in large subtensors has also been described in [21] for tensors with a first-order layout.

## 459 4.4. Parallel BLAS-based Algorithms

Most BLAS libraries provide an option to change the humber of threads. Hence, functions such as gemm and gemv can be run either using a single or multiple threads. The TTM cases one to seven contain a single BLAS call which

Algorithm 2: Function ttm<par-loop><slice> is an optimized version of Algorithm 1. The reshape function transforms the order-p tensors  $\underline{\mathbf{A}}$  and  $\underline{\mathbf{C}}$  with layout tuple  $\pi$  and their respective dimension tuples  $\mathbf{n}$  and  $\mathbf{m}$  into order-4 tensors  $\underline{\mathbf{A}}'$  and  $\underline{\mathbf{C}}'$  with layout tuple  $\pi'$  and their respective dimension tuples  $\mathbf{n}'$  and  $\mathbf{m}'$  where  $\mathbf{n}' = (n_{\pi_1}, \hat{n}_{\pi_2}, n_q, \hat{n}_{\pi_4})$  and  $m_3' = m$  and  $n_k' = m_k'$  for  $k \neq 3$ . Each thread calls multiple single-threaded gemm functions each of which executes a slice-matrix multiplication with the order-2 tensor slices  $\underline{\mathbf{A}}'_{ij}$  and  $\underline{\mathbf{C}}'_{ij}$ . Matrix  $\underline{\mathbf{B}}$  has the row-major storage format.

<sup>464</sup> is why we set the number of threads to the number of des available cores. The following subsections discuss parallel des versions for the eighth case in which the outer loops of Algorithm 1 and the gemm function inside the base case can des be run in parallel. Note that the parallelization strategies des can be combined with the aforementioned slicing methods.

470 4.4.1. Sequential Loops and Parallel Matrix Multiplication Algorithm 1 is run for the eighth case and does not 472 need to be modified except for enabling gemm to run multi-473 threaded in the base case. This type of parallelization 474 strategy might be beneficial with order- $\hat{q}$  subtensors where 475 the contraction mode satisfies  $q = \pi_{p-1}$ , the inner dimen-476 sions  $n_{\pi_1},\dots,n_{\hat{q}}$  are large and the outer-most dimension  $n_{\pi_p}$  is smaller than the available processor cores. For  $_{478}$  instance, given a first-order storage format and the con-479 traction mode q with q=p-1 and  $n_p=2$ , the di-480 mensions of reshaped order-q subtensors are  $\prod_{r=1}^{p-2} n_r$  and  $n_{p-1}$ . This allows gemm to perform with large dimensions  $_{482}$  using multiple threads increasing the likelihood to reach 483 a high throughput. However, if the above conditions are 484 not met, a multi-threaded gemm operates on small tensor 485 slices which might lead to an suboptimal utilization of the 486 available cores. This algorithm version will be referred to 487 as <par-gemm>. Depending on the subtensor shape, we will 488 either add <slice> for order-2 subtensors or <subtensor> 489 for order- $\hat{q}$  subtensors with  $\hat{q} = \pi_q^{-1}$ .

490 4.4.2. Parallel Loops and Sequential Matrix Multiplication
491 Instead of sequentially calling multi-threaded gemm, it is
492 also possible to call single-threaded gemms in parallel. Sim493 ilar to the previous approach, the matrix multiplication
494 can be performed with tensor slices or order- $\hat{q}$  subtensors.

<sup>495</sup> Matrix Multiplication with Tensor Slices. Algorithm 2 with <sup>496</sup> function ttm<par-loop><slice> executes a single-threaded <sup>497</sup> gemm with tensor slices in parallel using all modes except <sup>498</sup>  $\pi_1$  and  $\pi_{\hat{q}}$ . The first statement of the algorithm calls <sup>499</sup> the reshape function which transforms tensors  $\underline{\mathbf{A}}$  and  $\underline{\mathbf{C}}$  without copying elements by calling the reshaping oper<sup>500</sup> ation  $\varphi_{\pi_{\hat{q}+1},\pi_p}$  and  $\varphi_{\pi_2,\pi_{\hat{q}-1}}$ . The resulting tensors  $\underline{\mathbf{A}}'$ 

 $\underline{\mathbf{C}}'$  are of order 4. Tensor  $\underline{\mathbf{A}}'$  has the shape  $\underline{\mathbf{n}}' = \sum_{r=1}^{p} n_{\pi_r}/n_q$ , respectively. Given the number of physical  $\underline{\mathbf{A}}'$  with dimensions  $m'_r = n'_r$  except for the third dimensions and call  $\operatorname{\mathsf{par-loop}}$  with  $\operatorname{\mathsf{slice}}$  if neores is greater than 506 sion which is given by  $m_3 = m$ .

 $_{508}$  free modes. The outer loop iterates over  $n_4'=\hat{n}_{\pi_4}$  while  $_{562}$  sor slices is not used here. The presented strategy is differ-509 the inner one loops over  $n_2'=\hat{n}_{\pi_2}$  calling  ${\tt gemm}$  with tensor slices  $\underline{\mathbf{A}}_{2,4}'$  and  $\underline{\mathbf{C}}_{2,4}'$ . Here, we assume that matrix  $_{511}$  **B** has the row-major format which is why both tensor 512 slices are also treated as row-major matrices. Notice that 513 gemm in Algorithm 2 will be called with exact same argu-514 ments as displayed in the eighth case in Table 1 where 515  $n_1' = n_{\pi_1}, n_3' = n_q$  and  $w_q = w_3'$ . For the sake of simplic-516 ity, we omitted the first three arguments of gemm which are 569 sion calls in the eighth case a single gemm\_batch function set to CblasRowMajor and CblasNoTrans for A and B. With 518 the help of the reshaping operation, the tree-recursion has 519 been transformed into two loops which iterate over all free

521 Matrix Multiplication with Subtensors. An alternative al- $_{522}$  gorithm is given by combining Algorithm 2 with order- $\hat{q}$  $_{523}$  subtensors that have been discussed in 4.3. With order- $\hat{q}$ 524 subtensors, only the outer modes  $\pi_{\hat{q}+1},\ldots,\pi_p$  are free for 525 parallel execution while the inner modes  $\pi_1, \ldots, \pi_{\hat{q}-1}, q$  are 526 used for the slice-matrix multiplication. Therefore, both 527 tensors are reshaped twice using  $\varphi_{\pi_1,\pi_{\hat{q}-1}}$  and  $\varphi_{\pi_{\hat{q}+1},\pi_p}$ . 528 Note that in contrast to tensor slices, the first reshaping  $n_{\pi_1}$ . The reshaped tensors are 530 of order 3 where  $\underline{\mathbf{A}}'$  has the shape  $\mathbf{n}'=(\hat{n}_{\pi_1},n_q,\hat{n}_{\pi_3})$  with  $\hat{n}_{\pi_1} = \prod_{r=1}^{\hat{q}-1} n_{\pi_r}$  and  $\hat{n}_{\pi_3} = \prod_{r=\hat{q}+1}^p n_{\pi_r}$ . Tensor  $\underline{\mathbf{C}}'$  has 532 the same dimensions as  $\underline{\mathbf{A}}'$  except for  $m_2 = m$ .

Algorithm 2 needs a minor modification for support- $_{534}$  ing order- $\hat{q}$  subtensors. Instead of two loops, the modified 535 algorithm consists of a single loop which iterates over di-536 mension  $\hat{n}_{\pi_3}$  calling a single-threaded gemm with subtensors 537  $\underline{\mathbf{A}}'$  and  $\underline{\mathbf{C}}'$ . The shape and strides of both subtensors as 538 well as the function arguments of gemm have already been 539 provided by the previous Section 4.3. This ttm version will referred to as <par-loop><subtensor>.

Note that functions <par-gemm> and <par-loop> imple-542 ment opposing versions of the ttm where either gemm or the 543 fused loop is performed in parallel. Version <par-loop-gemm 544 executes available loops in parallel where each loop thread 545 executes a multi-threaded gemm with either subtensors or 546 tensor slices.

## 547 4.4.3. Combined Matrix Multiplication

The combined matrix multiplication calls one of the 549 previously discussed functions depending on the number 550 of available cores. The heuristic assumes that function 551 cpar-gemm> is not able to efficiently utilize the processor 552 cores if subtensors or tensor slices are too small. The 553 corresponding algorithm switches between <par-loop> and 554 <par-gemm> with subtensors by first calculating the par-555 allel and combined loop count  $\hat{n} = \prod_{r=1}^{q-1} n_{\pi_r}$  and  $\hat{n}' =$ 

 $\hat{n}_{\pi_1}$   $\hat{n}_{\pi_2}$ ,  $n_q$ ,  $\hat{n}_{\pi_4}$ ) with the dimensions  $\hat{n}_{\pi_2} = \prod_{r=2}^{\hat{q}-1} n_{\pi_r}$  so processor cores as noores, the algorithm executes  $\langle par-loop \rangle$  and  $\hat{n}_{\pi_4} = \prod_{r=\hat{q}+1}^p n_{\pi_r}$ . Tensor  $\underline{\mathbf{C}}'$  has the same shape as  $\hat{n}_{\pi_5}$  with  $\langle par_{\pi_7}, q, q, q, q \rangle$  for  $\hat{n}_{\pi_7}$  is a function of  $\hat{n}_{\pi_7}$  and  $\hat{n}_{\pi_4} = \prod_{r=\hat{q}+1}^p n_{\pi_r}$ . Tensor  $\underline{\mathbf{C}}'$  has the same shape as  $\hat{n}_{\pi_5}$  with  $\langle par_{\pi_7}, q, q, q, q \rangle$  for  $\hat{n}_{\pi_7}$  is a function of  $\hat{n}_{\pi_7}$  and  $\hat{n}_{\pi_8}$  is greater than or equal to  $\hat{n}_{\pi_8}$ 560 or equal to  $\hat{n}'$ . Otherwise, the algorithm will default to The following two parallel for loops iterate over all 561 par-gemm> with <subtensor>. Function par-gemm with ten-563 ent to the one presented in [14] that maximizes the number 564 of modes involved in the matrix multiply. We will refer to 565 this version as <combined> to denote a selected combination 566 of <par-loop> and <par-gemm> functions.

#### 567 4.4.4. Multithreaded Batched Matrix Multiplication

The multithreaded batched matrix multiplication ver-570 that is provided by Intel MKL's BLAS-like extension. With 571 an interface that is similar to the one of cblas\_gemm, func-572 tion gemm\_batch performs a series of matrix-matrix op-573 erations with general matrices. All parameters except 574 CBLAS\_LAYOUT requires an array as an argument which is 575 why different subtensors of the same corresponding ten-576 sors are passed to gemm\_batch. The subtensor dimensions 577 and remaining gemm arguments are replicated within the 578 corresponding arrays. Note that the MKL is responsible 579 of how subtensor-matrix multiplications are executed and 580 whether subtensors are further divided into smaller sub-581 tensors or tensor slices. This algorithm will be referred to  $_{582}~\mathrm{as}$  <batched-gemm>.

## 583 5. Experimental Setup

## 584 5.1. Computing System

The runtime benchmark have been executed on a dual 586 socket Intel Xeon Gold 5318Y CPU with an Ice Lake ar-587 chitecture and a dual socket AMD EPYC 9354 CPU with 588 a Zen4 architecture. With two NUMA domains, the Intel 589 CPU consists of  $2 \times 24$  cores which run at a base frequency 590 of 2.1 GHz. Assuming a peak AVX-512 Turbo frequency 591 of 2.5 GHz, the CPU is able to process 3.84 TFLOPS 592 in double precision. We have measured a peak double-593 precision floating-point performance of 3.8043 TFLOPS 594 (79.25 GFLOPS/core) and a peak memory throughput 595 of 288.68 GB/s using the Likwid performance tool. The 596 AMD EPYC 9354 CPU consists of 2 × 32 cores running at 597 a base frequency of 3.25 GHz. Assuming an all-core boost 598 frequency of 3.75 GHz, the CPU is theoretically capable 599 of performing 3.84 TFLOPS in double precision. We mea-600 sured a peak double-precision floating-point performance 601 of 3.87 TFLOPS (60.5 GFLOPS/core) and a peak memory 602 throughput of 788.71 GB/s.

All libraries have been compiled with the GNU com-604 piler v11.2.0 using the highest optimization level -03 to-605 gether with the -fopenmp and -std=c++17 flags. Loops 606 within the eighth case have been parallelized using GCC's 607 OpenMP v4.5 implementation. In case of the Intel CPU,

Dataset	Tensor Shape Ex.	Matrix Shape Ex.
$N_1$	$65536\times1024\times2$	$65536\times1024$
	$2048 \times 1024 \times 2 \times 2 \times 2$	$2048 \times 1024$
$N_2$	$1024 \times 65536 \times 2$	$65536 \times 1024$
	$1024 \times 2048 \times 2 \times 2 \times 2$	$2048 \times 1024$
$N_3$	$1024 \times 2 \times 65536$	$65536 \times 1024$
	$1024 \times 2 \times 2048 \times 2 \times 2$	$2048 \times 1024$
$N_{10}$	$1024 \times 2 \times 65536$	$65536 \times 1024$
	$1024 \times 2 \times 2 \times 2 \times 2048$	$2048\times1024$
$\overline{M}$	$256 \times 256 \times 256$	$256 \times 256$
	$32\times32\times32\times32\times32$	$32 \times 32$

Dataset $Q$ (orig. Name)	Tensor Shape	Matrix Shape Ex.
CESM ATM	$26 \times 1800 \times 3600$	$1800 \times 26$
ISABEL	$100 \times 500 \times 500 \times 13$	$500 \times 100$
NYX	$512 \times 512 \times 512 \times 6$	$512 \times 512$
SCALE-LETK	$98 \times 1200 \times 1200 \times 13$	$1200 \times 98$
QMCPACK	$69 \times 69 \times 115 \times 288$	$69 \times 69$
Miranda	$256 \times 384 \times 384 \times 7$	$384 \times 256$
SP	$500 \times 500 \times 500 \times 11$	$500 \times 500$
EXAFEL	$986 \times 32 \times 185 \times 388$	$32 \times 986$

Table 2: Tensor shape sets and example dimension tuples that are used in our runtime benchmarking. The first 4 shape sets N<sub>1</sub>, N<sub>2</sub>, N<sub>3</sub> and  $N_{10}$  are used to generate asymmetrically shaped tensors, each consisting of 72 dimension tuples. Shape set M contains 48 tensor shapes that are used to generate symmetrically shaped tensors. Shape set Q contains 8 tensor shapes that are part of SDRBench [24]. Note that all matrix shapes depend on the input tensor shapes and contraction mode.

608 the Intel Math Kernel Library 2022 (MKL) and its thread-609 ing library mkl\_intel\_thread, threading runtime library 610 libiomp5 has been used for the three BLAS functions gemv, 611 gemm and gemm\_batch. For the AMD CPU, the AMD library 612 AOCL v4.2.0 has been compiled with the zen4 flag.

#### 613 5.2. OpenMP Parallelization

The loops in the par-loop algorithms have been par-615 allelized using the OpenMP directive omp parallel for to-616 gether with the schedule(static), num\_threads(ncores) and 617 proc\_bind(spread) clauses. In case of tensor-slices, the 618 collapse(2) clause has been added for transforming both 619 loops into one loop which has an iteration space of the 620 first loop times the second one. We also had to enable 621 nested parallelism using omp\_set\_nested to toggle between 622 single- and multi-threaded gemm calls for different TTM cases when using AMD AOCL.

The num\_threads(ncores) clause specifies the number threads within a team where ncores is equal to the 626 number of processor cores. Hence, each OpenMP thread  $_{\rm 627}$  is responsible for computing  $\bar{n}'/{\rm ncores}$  independent slicematrix products where  $\bar{n}' = n_2' \cdot n_4'$  for tensor slices and 667 shapes all of which generate asymmetrically shaped ten- $\bar{n}' = n'_4$  for mode- $\hat{q}$  subtensors.

The schedule(static) instructs the OpenMP runtime 631 to divide the iteration space into equally sized chunks, ex-632 cept for the last chunk. Each thread sequentially com-<sub>633</sub> putes  $\bar{n}'/\text{ncores}$  slice-matrix products. We have decided 634 to use this scheduling kind as all slice-matrix multiplica-635 tions exhibit the same number of floating-point operations 636 with a regular workload where one can assume negligible 637 load imbalance. Moreover, we wanted to prevent schedul-638 ing overheads for small slice-matrix products were data 639 locality can be an important factor for achieving higher throughput.

The OMP\_PLACES environment variable has not been ex-642 plicitly set and thus defaults to the OpenMP cores setting 681 row of the tensor shape array consists 8 dimension tuples  $_{643}$  which defines an OpenMP place as a single processor core.  $_{682}$  of the same length r+1 where elements of one dimension <sub>644</sub> Together with the clause num\_threads(ncores), the num- <sub>683</sub> tuple are equal such that  $m_{r,c} = \mathbf{m}_{r,c}(i) = \mathbf{m}_{r,c}(j)$  for 645 ber of OpenMP threads is equal to the number of OpenMP

647 not measure any performance improvements for a higher 648 thread count.

The proc\_bind(spread) clause additionally binds each 650 OpenMP thread to one OpenMP place which lowers inter-651 node or inter-socket communication and improves local 652 memory access. Moreover, with the spread thread affin-653 ity policy, consecutive OpenMP threads are spread across 654 OpenMP places which can be beneficial if the user decides 655 to set ncores smaller than the number of processor cores.

### 656 5.3. Data sets

The runtime performance of our algorithms have been 658 executed with asymmetrically and symmetrically shaped 659 tensors to account for a wide range of use cases. The corresponding tensor shapes are divided into 12 sets  $N_1$ ,  $N_2$ ,  $_{661} \ldots, N_{10}, M$  and Q. Table 2 contains example dimension 662 tuples for the input tensor and matrix. The shape of the 663 latter is  $(n_2, n_q)$  if q = 1 and  $(n_1, n_q)$  otherwise where q is 664 the contraction mode with  $1 \leq q \leq p$ . The computation of 665 the output tensor dimensions is described in Section 3.2.

The first ten shape sets  $N_1$  to  $N_{10}$  contain  $9 \times 8$  tensor 668 sors. Within one set  $N_k$ , dimension tuples are arranged 669 within 10 two-dimensional shape arrays  $N_k$  of size  $9 \times 8$ 670 with  $1 \leq k \leq 10$ . A dimension tuple  $\mathbf{n}_{r,c}$  within  $\mathbf{N}_k$  is <sub>671</sub> of length r+1 with  $1 \le r \le 9$  and  $1 \le c \le 8$ . Its *i*-th 672 element is either 1024 for  $i = 1 \land k \neq 1$  or  $i = 2 \land k = 1$ , <sub>673</sub> or  $c \cdot 2^{15-r}$  for  $i = \min(r+1, k)$  or 2 otherwise. A special 674 feature of this test set is that the contraction dimension 675 and the leading dimension are disproportionately large.

The second shape set M contains 48 tensor shapes 677 that used to generate symmetrically shaped tensors. The 678 shapes are arranged within one two-dimensional shape ar-<sub>679</sub> ray **M** of size  $6 \times 8$ . Similar to the previous setup, the row 680 number r is equal to the tensor order r+1 with  $1 \le r6$ . A 684  $1 \leq i, j \leq r+1$ . With eight shapes and the step size of  $_{646}$  places, i.e. to the number of processor cores. We did  $_{685}$  each row  $s_r = (m_{r,8} - m_{r,1})/8$ , the respective intermediate dimensions  $m_{r,c}$  are given by  $m_{r,c} = m_{r,1} + (c-1)s_r$  with tensors have also been used in [16, 23].

690 tensors from the scientific data reduction benchmark (SDR-744 in the previous section 5. 691 Bench) [24]. The scientific datasets in SDRBench mainly 692 consist of order-3 tensors with different tensor shapes and 745 6.1. Slicing Methods 693 number of data fields, originating from various real-world 746 694 simulations. Tensors from the SP dataset for instance has 747 posed slicing methods <slice> and <subtensor> that have 695 been used for benchmarking the truncated Tucker decom-696 position in [21] We perform runtime tests with order-4 ten-697 sors that are generated with dimension tuples of the ten- $_{698}$  sor shape set Q. Their first three dimensions correspond 699 to the respective ones mentioned in the original data sets 700 and the last dimension to the number of data fields. All 701 tensor shapes are provided in Table 2.

## 702 5.4. Profiling setup

<sub>704</sub> from one of tensor shape sets for one contraction mode q <sub>758</sub> first element which corresponds to TTM case 2. The first 705 with  $1 \leq q \leq \max_p$  where  $\max_p$  is the maximum ten- 759 row, excluding the first element, is generated by TTM case 706 sor order within the shape set. Tensor and matrix el- 760 6 function. TTM case 7 is covered by the diagonal line of <sub>707</sub> ements are randomly generated single-precision floating- <sub>761</sub> performance values when q=p. Although Fig. 1 suggests <sub>708</sub> point numbers in case of the data set Q. In all other test <sub>762</sub> that q > p is possible, our profiling program ensures that  $_{709}$  cases double-precision is used. The profiler first sweeps  $_{763}$  q=p. TTM case 8 with multiple gemm calls is represented 710 through tensor shapes belonging to one tensor order and 764 by the triangular region which is defined by 1 < q < p. 711 then iteratively selects one larger tensor order for the next 765 712 sweep. Given a dimension tuple, the profiler generates two 713 tensors and a matrix, executes a mode-q TTM implemen-714 tation 20 times and finally computes the median runtime 768 (2.77 TFLOPS), it performs on average 89.64% faster than 715 of the benchmarked TTM implementation. To prevent 769 760  $_{716}$  caching of the output tensor, we invalidate caches which  $_{770}$  q=p-1 or q=p-2 can be explained by the small 717 is excluded from the timing.

719 TTM implementation are stored in a two-dimensional ar- 773 shapes for dimensions p=3 and p=4 as well, its perfor- $_{720}$  ray with shape  $\max_p \times k$  where k is either 8 in case of  $_{774}$  mance improves with increasing order due to the increasing <sub>722</sub> case of the set Q. It should be noted that if q > p, the <sub>776</sub> age 17.34 GFLOPS/core (832.42 GFLOPS) if symmetri-723 contraction mode q is set to p. Hence, our profiler gener- 777 cally shaped tensors are used. If subtensors are used, func-724 ates 10 runtime arrays of shape 9 × 8 with asymmetrically 778 tion 778 tion par-loop, subtensor achieves a mean throughput of <sub>725</sub> shaped tensors for 10 contraction modes using the shape <sub>779</sub> 17.62 GFLOPS/core (846.16 GFLOPS) and is on average 726 sets  $N_1, N_2, \ldots, N_{10}$ . Generating symmetrically shaped 780 9.89% faster than  $\protect$ par-loop,slice>. The performances of 727 tensors with the shape set M, the profiler returns 7 run- 781 both functions are monotonically decreasing with increas- $_{728}$  time arrays of shape  $6 \times 8$  for 7 contraction modes. Using  $_{782}$  ing tensor order, see plots (1.c) and (1.d) in Fig. 1. 729 the shape set Q, 4 one-dimensional runtime arrays for 4 contraction modes are computed.

 $_{732}$  the data sets N and M can be used to create two dimen-  $_{786}$  Using subtensors, function <par-gemm, subtensor> exhibits 733 sional performance maps, as it is done in the following 734 Section 6. Each value in a performance map corresponds 735 to a mean or median value over tensor sizes (i.e. dimen-736 sion tuples with the same length), over tensor orders or 790 tensors and tensor slices achieve a mean throughput 15.98 737 contraction modes.

### 738 6. Experimental Results and Discussion

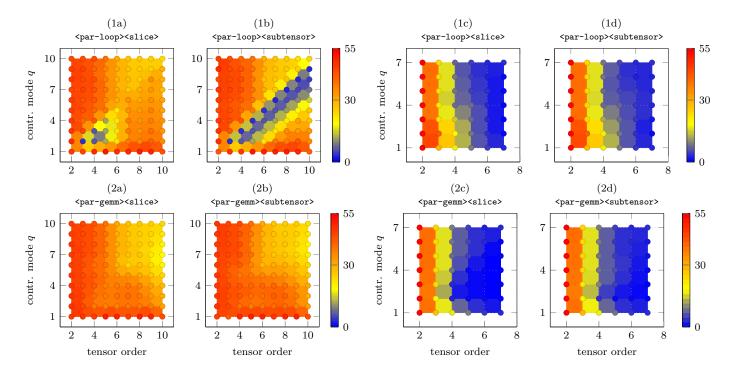
 $_{687}$  1  $\leq c \leq 8$ . Symmetrically and asymmetrically shaped  $_{741}$  tensors. The last subsection also considers tensors with 742 real-world tensor shapes from SDRBench. The correspond-We have also benchmarked our algorithm using eight 743 ing tensor shapes and their shape sets have been described

This section analyzes the performance of the two pro-748 been discussed in section 4.4. Fig. 1 contains eight per-749 formance contour plots of four ttm functions <par-loop> 750 and remm>. Both functions either compute the slice-751 matrix product with subtensors <subtensor> or tensor slices 752 <slice> on the Intel Xeon Gold 5318Y CPU. Each contour 753 level within the plots represents a mean GFLOPS/core 754 value that is averaged across tensor sizes.

Every contour plot contains all applicable TTM cases 756 listed in Table 1. The first column of performance values is Our benchmark suite iterates through dimension tuples 757 generated by gemm belonging to the TTM case 3, except the

With asymmetrically shaped tensors, <par-loop, slice> 766 runs on average with 34.96 GFLOPS/core (1.67 TFLOPS). 767 With a maximum performance of 57.805 GFLOPS/core 771 loop count of the function that are 2 and 4, respectively. 

Function <par-gemm, slice > averages 36.42 GFLOPS/-784 core (1.74 TFLOPS) and achieves up to 57.91 GFLOPS/-The three-dimensional runtime data generated with 785 core (2.77 TFLOPS) with asymmetrically shaped tensors. 787 almost identical performance characteristics and is on av-788 erage 3.42% slower than its counterpart with tensor slices. 789 For symmetrically shaped tensors, <par-gemm> with sub-791 GFLOPS/core (767.31 GFLOPS) and 15.43 GFLOPS/-792 core (740.67 GFLOPS), respectively. However, function 793 <par-gemm, subtensor is on average 87.74% faster than 794 <par-gemm, slice> which is hardly visible due to small per-The runtime results within the following subsections 795 formance values around 5 GFLOPS/core or less whenever  $_{740}$  are executed with asymmetrically and symmetrically shaped  $_{796}$  q < p and the dimensions are smaller than 256. The



varying tensor orders p and contraction modes q. The top row of maps (1x) depict measurements of the <par-loop> versions while the bottom row of maps with number (2x) contain measurements of the cpar-gemm> versions. Tensors are asymmetrically shaped on the left four maps (a,b) and symmetrically shaped on the right four maps (c,d). Tensor A and C have the first-order while matrix B has the row-major ordering. All functions have been measured on an Intel Xeon Gold 5318Y.

<sub>797</sub> speedup of the <subtensor> version can be explained by the <sub>824</sub> respectively. The speedup mostly occurs when 1 < q < p798 smaller loop count and slice-matrix multiplications with 825 where the performance gain is a factor of 2.23. This perlarger tensor slices.

Our findings indicate that, regardless of the paralleliza-804 the contraction mode and leading dimension are large.

## 805 6.2. Parallelization Methods

This subsection compares the performance results of the two parallelization methods, <par-gemm> and <par-loop>, 835 <par-gemm> outperform <par-loop> with any type of slicing. as introduced in Section 4.4 and illustrated in Fig. 1.

With asymmetrically shaped tensors, both par-gemm> 810 functions with subtensors and tensor slices compute the 811 tensor-matrix product on average with ca. 36 GFLOP- $_{812}\,\mathrm{S/core}$  and outperform function <par-loop, subtensor> on 813 average by a factor of 2.31. The speedup can be explained 814 by the performance drop of function <par-loop, subtensor> 815 to 3.49 GFLOPS/core at q = p - 1 while both versions of <par-loop,slice> performs better for reasons explained in 818 the previous subsection. However, it is on average 30.57% 819 slower than function <par-gemm, slice> due to the aforementioned performance drops.

In case of symmetrically shaped tensors, <par-loop> 822 with subtensors and tensor slices outperform their corre-823 sponding sponding counterparts by 23.3% and 32.9%,

826 formance behavior can be expected as the tensor slice sizes 827 decreases for the eighth case with increasing tensor order 801 tion method employed, subtensors are most effective with 828 causing the parallel slice-matrix multiplication to perform 802 symmetrically shaped tensors, whereas tensor slices are 829 on smaller matrices. In contrast, <par-loop> can execute 803 preferable with asymmetrically shaped tensors when both 830 small single-threaded slice-matrix multiplications in par-

> In summary, function <par-loop, subtensor> with sym-833 metrically shaped tensors performs best. If the leading and 834 contraction dimensions are large, both versions of function

### 836 6.3. LoG Variants

The contour plots in Fig. 1 contain performance data 838 that are generated by all applicable TTM cases of each 839 ttm function. Yet, the presented slicing or parallelization 840 methods only affect the eighth case, while all other TTM 841 cases apply a single multi-threaded gemm with the same 842 configuration. The following analysis will consider perfor-843 mance values of the eighth case in order to have a more 844 fine grained visualization and discussion of the loops over 845 gemm implementations. Fig. 2 contains cumulative perfor-846 mance distributions of all the proposed algorithms includ-847 ing the functions <batched-gemm> and <combined> for the 848 eighth TTM case only. Moreover, the experiments have 849 been additionally executed on the AMD EPYC processor 850 and with the column-major ordering of the input matrix 851 as well.

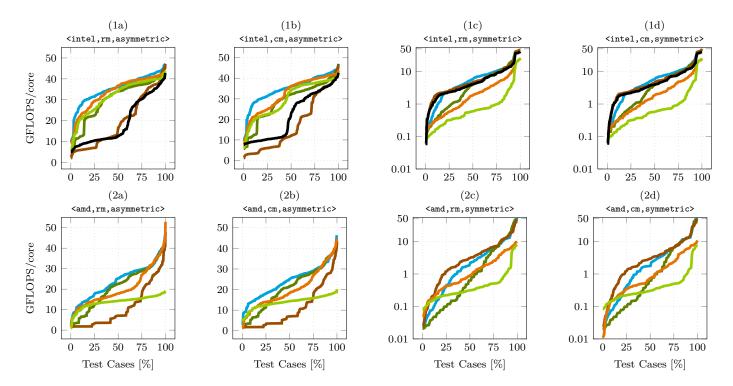


Figure 2: Cumulative performance distributions in double-precision GFLOPS/core of the proposed algorithms for the eighth case. Each distribution belongs to one algorithm: <batched-gemm> ( —), <combined> ( ——), <par-gemm,slice> ( and <par-loop,slice> ( and <par-loop, subtensor> ( ). The top row of maps (1x) depict measurements performed on an Intel Xeon Gold 5318Y with the MKL while the bottom row of maps with number (2x) contain measurements performed on an AMD EPYC 9354 with the AOCL. Tensors are asymmetrically shaped in (a) and (b) and symmetrically shaped in (c) and (d). Input matrix has the row-major ordering (rm) in (a) and (c) and column-major ordering (cm) in (b) and (d).

The probability x of a point (x,y) of a distribution 878 853 function for a given algorithm corresponds to the number 879 brary has a performance distribution that is akin to the 854 of test instances for which that algorithm that achieves 880 <par-loop, subtensor>. In case of asymmetrically shaped 855 a throughput of either y or less. For instance, function 881 tensors, all functions except <par-loop, subtensor> outper-857 asymmetrically shaped tensors in 25% of the tensor in- 883 to a factor 4 for  $2 \le q \le 5$  with  $q+2 \le p \le q+5$ . In 859 note that the four plots on the right, plots (c) and (d), have 885 a similar performance behavior in the plot (1c) and (1d) 860 a logarithmic y-axis for a better visualization.

## 861 6.3.1. Combined Algorithm and Batched GEMM

This subsection discusses the performance of function 889 <batched-gemm> and <combined> against those of <par-loop> and <par-gemm> for the eighth TTM case.

Given a row-major matrix ordering, the combined func-866 tion <combined> achieves on the Intel processor a median throughput of 36.15 and 4.28 GFLOPS/core with asymmetrically and symmetrically shaped tensors. Reaching 894 6.3.2. Matrix Formats up to 46.96 and 45.68 GFLOPS/core, it is on par with 895 871 forms them for some tensor instances. Note that both 897 the proposed functions. The cumulative performance dis-872 functions run significantly slower either with asymmetri- 898 tributions in Fig. 2 suggest that the storage format of 873 cally or symmetrically shaped tensors. The observable su- 899 the input matrix has only a minor impact on the perfor-874 perior performance distribution of <combined> can be at- 900 mance. The Euclidean distance between normalized row-875 tributed to the heuristic which switches between cpar-loop> 901 major and column-major performance values is around 5 876 and <par-gemm> depending on the inner and outer loop 902 or less with a maximum dissimilarity of 11.61 or 16.97, in-877 count as explained in section 4.4.

Function <batched-gemm> of the BLAS-like extension li-<batched-gemm> computes the tensor-matrix product with 882 form <batched-gemm> on average by a factor of 2.57 and up 886 for symmetrically shaped tensors, running on average 3.55 and 8.38 times faster than par-gemm> with subtensors and 888 tensor slices, respectively.

> In summary, <combined> performs as fast as, or faster 890 than, <par-gemm, subtensor> and <par-loop, slice>, depend-891 ing on the tensor shape. Conversely, <batched-gemm> un-892 derperforms for asymmetrically shaped tensors with large 893 contraction modes and leading dimensions.

This subsection discusses if the input matrix storage <par-gemm,subtensor> and <par-loop,slice> and outper- 896 formats have any affect on the runtime performance of 903 dicating a moderate similarity between the corresponding



Figure 3: Box plots visualizing performance statics in double-precision GFLOPS/core of the function with row-major (left) or column-major matrices (right). Box plot number k denotes the k-order tensor layout of symmetrically shaped tensors with order 7.

905 respective median values with their first and third quar- $_{906}$  tiles differ by less than 5% with three exceptions where the  $_{932}$  $_{907}$  difference of the median values is between 10% and 15%.

## 6.3.3. BLAS Libraries

This subsection compares the performance of functions 910 that use Intel's Math Kernel Library (MKL) on the Intel 911 Xeon Gold 5318Y processor with those that use the AMD Optimizing CPU Libraries (AOCL) on the AMD EPYC 913 9354 processor. Comparing the performance per core and 914 limiting the runtime evaluation to the eighth case, MKLbased functions with asymmetrically shaped tensors run 916 on average between 1.48 and 2.43 times faster than those with the AOCL. For symmetrically shaped tensors, MKL- $_{918}$  based functions are between 1.93 and 5.21 times faster 919 than those with the AOCL. In general, MKL-based func-920 tions on the respective CPU achieve a speedup of at least 921 1.76 and 1.71 compared to their AOCL-based counterpart 922 when asymmetrically and symmetrically shaped tensors 923 are used.

## 924 6.4. Tensor Layouts

Fig. 3 contains four box plots summarizing the perfor-926 mance distribution of the <combined> function using the 927 AOCL and MKL. Every k-th box plot has been computed 928 from benchmark data with symmetrically shaped order-7

904 row-major and column-major data sets. Moreover, their 930 7-order layout, for instance, are the first-order and last-931 order storage formats of an order-7 tensor.

> The reduced performance of around 1 and 2 GFLOPS 933 can be attributed to the fact that contraction and lead-934 ing dimensions of symmetrically shaped subtensors are at 935 most 48 and 8, respectively. When <combined> is used 936 with MKL, the relative standard deviations (RSD) of its 937 median performances are 2.51% and 0.74%, with respect 938 to the row-major and column-major formats. The RSD 939 of its respective interquartile ranges (IQR) are 4.29% and 940 6.9%, indicating a similar performance distributions. Us-941 ing <combined> with AOCL, the RSD of its median per-942 formances for the row-major and column-major formats  $_{943}$  are 25.62% and 20.66%, respectively. The RSD of its re-944 spective IQRs are 10.83% and 4.31%, indicating a similar 945 performance distributions. A similar performance behav-946 ior can be observed also for other ttm variants such as 947 <par-loop, slice>. The runtime results demonstrate that 948 the function performances stay within an acceptable range  $_{949}$  independent for different k-order tensor layouts and show 950 that our proposed algorithms are not designed for a spe-951 cific tensor layout.

## 952 6.5. Comparison with Related Work

This subsection compares our best performing algo-954 rithm with libraries that do not use the LOG approach. 955 **TCL** implements the TTGT approach with a high-perform  $_{929}$  tensors that has a k-order tensor layout. The 1-order and  $_{956}$  tensor-transpose library **HPTT** which is discussed in [11]. 957 TCL has been used with the same BLAS libraries as TLIB

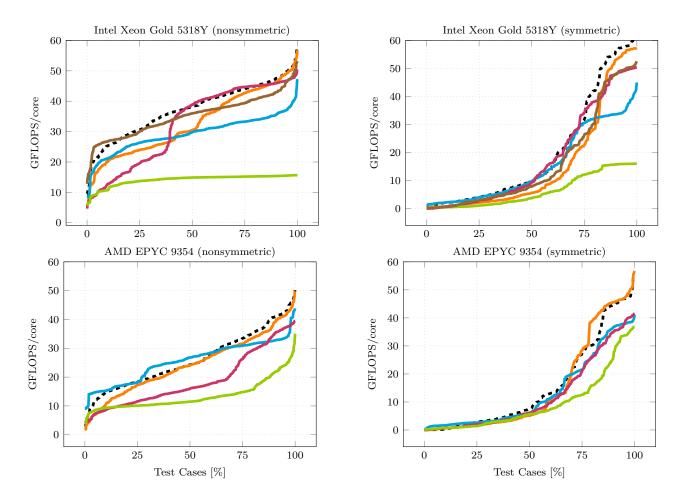


Figure 4: Cumulative performance distributions of TTM implementations in double-precision GFLOPS/core. Each distribution corresponds to a library: TLIB[ours] (---), TCL (--—), TBLIS (——), LibTorch (——), Eigen ( ), TuckerMPI (——). Libraries have been tested with asymmetrically-shaped (left plot) and symmetrically-shaped tensors (right plot).

958 to ensure a fair comparison. TBLIS (v1.2.0) implements 980 benchmark is executed with asymmetrically and symmetr-959 the GETT approach that is akin to BLIS' algorithm de- 961 rically shaped tensors. The corresponding tensor shapes 960 sign for the matrix multiplication [12]. The library has 982 and their shape sets have been described in Section 5. 961 been compiled with the zen4 and skx-2 to enable architec- 983 962 ture specific optimization. The tensor extension of Eigen 984 mance of 38.21 GFLOPS/core (1.83 TFLOPS) and reaches 963 (v3.4.90) is used by the Tensorflow framework. Library 965 with asymmetrically shaped tensors at most 57.68 GFLOPversion implements the LOG approach using a BLAS im-<sub>969</sub> plementation and computes the TTM product similar to <sub>991</sub> S/core, yet only reach a peak performance 50.48 and 53.21 <sub>970</sub> our function <par-gemm, subtensor>. Note that we were use <sub>992</sub> GFLOPS/core. Both are 17.47% and 6.97% slower than the current TuckerMPI version with Intel's MKL, which is 974 discussed <combined> algorithm. If not otherwise stated, 996 a speedup for at least 33% more tensor instances and is 975 all of the following performance and comparisons numbers 997 at least 3.08% faster. Moreover, TLIB achieves a median 976 represent medians across a specified tensor set.

## 977 6.5.1. Artificial Tensor Shapes

979 plementation with the previously mentioned libraries. The 1002

Using MKL on the Intel CPU, TLIB achieves a perfor-**LibTorch** (v2.5.0) is the C++ distribution of PyTorch  $_{986}$  S/core (2.76 TFLOPS), given the shape sets  $N_k$  with [20]. The **TuckerMPI** library is a parallel C++ soft- 987  $1 \le k \le 10$ . TLIB is in at least 2.03x as many tenware package for large-scale data compression which pro- 988 sor instances faster than other libraries and achieves a vides a local and distributed TTM function [21]. The local 989 speedup of at least 6.36%. LibTorch and TuckerMPI have 990 almost the same performance of 38.17 and 35.98 GFLOP-993 TLIB. In case of symmetrically shaped tensors from the 972 why TuckerMPI's TTM has only been executed on the 994 shape set M, TLIB's computes the TTM with 8.99 GFLOP-<sub>973</sub> Intel CPU. **TLIB** denotes our library and the previously <sub>995</sub> S/core (431.52 GFLOPS). Except for TBLIS, TLIB achieves 998 speedup of 12.98% and 6.23% compared to LibTorch and 999 TuckerMPI. With a higher performance of 9.73 GFLOP-1000 S/core, TBLIS is faster than TLIB for about the same Fig. 2 compares the performance distribution of our im- 1001 amount of tensor instances and is 1.38% slower than TLIB. On the AMD CPU, TLIB computes the tensor prod-

Library	Perform	nance [GFL	Speedup [%]		
	Min	Median	Max	Median	
TLIB	9.45	38.27	57.87	-	
TCL	7.14	30.46	56.81	6.36	
TBLIS	8.33	29.85	47.28	23.96	
LibTorch	4.65	38.17	50.48	17.47	
Eigen	5.85	14.89	15.67	170.77	
TuckerMPI	12.79	35.98	53.21	6.97	
TLIB	0.14	8.99	58.14	-	
TCL	0.36	5.64	57.35	3.08	
TBLIS	1.11	9.73	45.03	1.38	
LibTorch	0.02	9.31	50.44	12.98	
Eigen	0.21	3.80	16.06	216.69	
TuckerMPI	0.12	7.91	52.57	6.23	

Library	Perfor	mance [GFI	Speedup [%]		
	Min	Median	Max	Median	
TLIB	2.71	24.28	50.18	-	
TCL	1.67	24.11	49.85	0.57	
TBLIS	9.06	26.81	47.83	0.43	
LibTorch	0.63	16.04	50.84	29.68	
Eigen	4.06	11.49	35.08	117.48	
TLIB	0.02	7.75	54.16	-	
TCL	0.01	5.14	56.75	6.10	
TBLIS	0.06	6.14	41.11	13.64	
LibTorch	0.06	6.04	41.65	12.37	
Eigen	0.07	5.58	36.76	114.22	

Table 3: The table presents the minimum, median, and maximum runtime performances in GFLOPS/core alongside the median speedup of TLIB compared to other libraries. The tests were conducted on an Intel Xeon Gold 5318Y CPU (left) and an AMD EPYC 9354 CPU (right). The performance values on the upper and lower rows of one table were evaluated using asymmetrically and symmetrically shaped tensors,

1003 uct with 24.28 GFLOPS/core (1.55 TFLOPS), reaching 1040 to the sixth and seventh TTM case in Table 1 for which 1004 with asymmetrically shaped tensors a maximum perfor- 1041 TLIB will call a single gemm. The multiplication over the 1005 mance of 50.18 GFLOPS/core (3.21 TFLOPS). TBLIS 1042 second and third mode corresponds to the eighth TTM 1006 and TCL execute the TTM with 26.81 and 24.11 GFLOP- 1043 case where a gemm is called multiple times. 1007 S/core, executing the TTM equally fast as TLIB with a 1044 1008 speedup percentage of 0.57 and 0.43. Moreover, TLIB is 1045 size of each bar is the total running time of the respective 1009 faster than TBLIS and TCL in the same number of ten- 1046 TTM implementation over all modes that is executed on 1010 sor instances as in the opposite case. The three libraries 1047 an Intel Xeon Gold 5318Y CPU and an AMD EPYC 9354 1011 are 29.68% and a factor of 2.17 faster than LibTorch and 1048 CPU. Note that TCL was not able to compute the TTM 1012 Eigen, respectively. In case of symmetrically shaped ten- 1049 for the EXAFEL data set which is why the runtime is set 1013 sors, TLIB has a median performance of 7.52 GFLOPS/- 1050 to zero. 1014 core (481.39 GFLOPS). Compared to the second-fastest 1051 1015 library TCL, TLIB speeds up the computation by 6.10% 1052 most tensor shapes and reaches a maximum speedup of 1016 and is in 43.66% more tensor instances faster than TCL. 1053 137.32% (TCL), 100.80% (TBLIS), 210.71% (LibTorch),

1020 across all TTM cases with few exceptions. On the AMD 1057 13.7% faster than TLIB TuckerMPI and LibTorch com-1021 CPU, TCL achieves a higher throughput of about 9% for 1058 pute the tensor product faster than TLIB in case of fourth 1022 the second and third TTM cases when asymmetrically 1059 contraction mode, independent of tensor shape. 1023 shaped tensors are used. TBLIS is 12.63% faster than 1060  $_{1025}$  On the Intel CPU, LibTorch is in the 7th TTM case 16.94%  $_{1062}$  in some instances. TLIB reaches a maximum speedup 1026 faster than TLIB. The TCL library runs on average as 1063 of 33.36% (TCL), 117.22% (TBLIS), 221.25% (LibTorch), 1027 fast as TLIB in the 6th and 7th TTM cases. The perfor- 1064 205.80% (Eigen). TCL outerperforms TLIB by 16.22% 1028 mances of TLIB, TBLIS and TuckerMPI in the 8th TTM 1065 (NYX) and 71.65% (Miranda). In this case, TCL com-1029 case are almost on par, TLIB executing the TTM about 1066 putes the tensor product over the fourth mode faster than 1030 3.2% faster. In case of symmetrically shaped tensors, TB- 1067 TLIB for almost all tensors. LibTorch outperforms TLIB 1031 LIS and LibTorch outperform TLIB in the 7th TTM case 1068 for the CESM-ATM data set by 42.02%. 1032 by 38.5% and 219.5%.

## 1033 6.5.2. Real-World Tensor Shapes

We have additionally conducted performance tests with 1072 world tensor shapes. 1035 an order-3 and seven order-4 tensors with real-world tensor 1036 shapes that are listed in Table 2. With a maximum tensor 1037 order of 4, every tensor is multiplied with a matrix along  $_{1038}$  every mode using a TTM implementation. Note that the  $_{1074}$ 

Fig. 5 contains bar plots for all tensor shapes. The

On the Intel Xeon Gold 5318Y CPU, TLIB is faster for TBLIS, LibTorch and Eigen are slower than TLIB by at 1054 798.91% (Eigen), 581.73% (TuckerMPI). TCL is on par 1055 with TLIB for the CESM-ATM data set. TuckerMPI is In most instances, TLIB is faster than other libraries 1056 for the CESM-ATM and Miranda data sets 46.8% and

On the AMD EPYC 9354 CPU, TLIB performs better TLIB for the eighth TTM case with the same tensor set. 1061 than most other libraries except for TCL and LibTorch

> The runtime tests with tensors from the SDRBench 1070 demonstrate that TLIB is able to compute the tensor prod-1071 uct faster than other libraries for most tensors with real-

#### 1073 7. Summary

We have presented efficient layout-oblivious algorithms  $_{1039}$  multiplication over the first and fourth mode corresponds  $_{1075}$  for the compute-bound tensor-matrix multiplication that

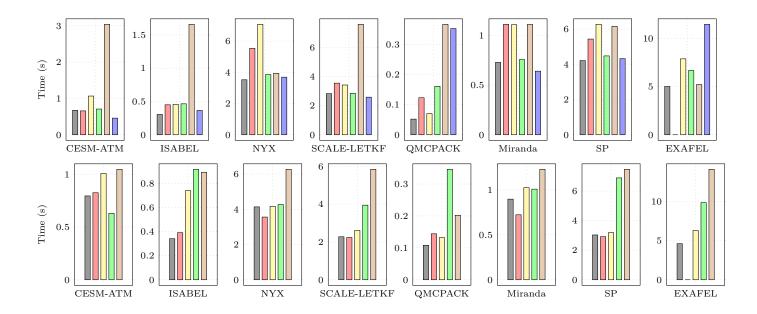


Figure 5: Bar plots contain median running times in seconds of TLIB ( III), TCL ( III), TBLIS ( III), LibTorch ( III), Eigen ( IIII) and TuckerMPI (III). The tests were performed on an Intel Xeon Gold 5318Y CPU (top) and an AMD EPYC 9354 CPU (bottom) using order-3 and order-4 tensors with shapes that are described in Table 2.

1077 use of the LOG method and computes the tensor-matrix 1110 as fast as <par-gemm, subtensor> and <par-loop, slice>, de-1078 product in-place without transposing tensors. It applies 1111 pending on the tensor shape. Function <br/>
<a href="https://doi.org/10.1007/journal.org/">batched-gemm</a> is 1079 the flexible approach described in [16] and generalizes the 1112 less efficient in case of asymmetrically shaped tensors with 1082 tensors with arbitrary tensor order, dimensions and with 1115 formance, runtime measurements show that a TTM using 1083 any linear tensor layout all of which can be runtime vari- 1116 MKL on the Intel Xeon Gold 5318Y CPU achieves higher 1084 able. This degree of flexibility simplifies the integration 1117 per-core performance than a TTM with AOCL on the different requirements and tensor layouts.

1088 eighth TTM case which either calls a single- or multi- 1121 and do not depend on a specific tensor format. 1089 threaded cblas\_gemm with small or large tensor slices in 1122 1090 parallel or sequentially. Additionally, a simple heuristic 1123 <combined> version of TTM is either performs equally well 1091 has been proposed, selecting one of the variants based on 1124 or faster than other libraries for the majority of tensor in-1092 the performance evaluation in the original work [1]. We 1125 stances. In case of tensors with artificial tensor shapes, 1093 have evaluated all algorithms using a large set of tensor in- 1126 TLIB computes the tensor product at least 12.37% faster 1094 stances with artificial and real-world tensor shapes on an 1127 than LibTorch and Eigen, independent of the processor. 1098 ings indicate that, subtensors are most effective with sym-1131 eighth TTM case across the majority of tensor instances, 1099 metrically shaped tensors, irrespective of the paralleliza- 1132 indicating that our proposed heuristic is efficient. In case 1101 geous when dealing with asymmetrically shaped tensors, 1134 better than all libraries for the majority of tensor shapes, 1102 particularly when both the contraction mode and leading 1135 reaching a maximum speedup of at least 100.80% in some 1103 dimension are large. Our runtime results demonstrate that 1136 tensor instances. Exceptions are the CESM-ATM and Mi- $_{1104}$  parallel executed single-threaded gemm performs best with  $_{1137}$  randa data sets where TuckerMPI is 46.8% and 13.7%1105 symmetrically shaped tensors. If the leading and contrac- 1138 faster than TLIB on the Intel CPU. Also TCL is 16.22% 1106 tion dimensions are large, functions with a multi-threaded 1139 and 71.65% faster than TLIB when using the NYX and 1107 gemm outperforms those with a single-threaded gemm for 1140 Miranda data sets on the AMD CPU, respectively. any type of slicing. It can also be observed that function

1076 is essential for many tensor methods. Our approach makes 1109 <combined> with a simple heuristic performs in most cases findings on tensor slicing in [14] for linear tensor layouts. 1113 large contraction and leading dimensions. While matrix The resulting algorithms are capable of processing dense 1114 storage formats have only a minor impact on TTM perand application of our library in existing frameworks with 1118 AMD EPYC 9354 processor. We have also demonstrated that our algorithms perform consistently well for k-order We have presented multiple algorithm variations of the 1120 tensor layouts, indicating that they are layout-oblivious

Our runtime tests with other libraries show that TLIB's Intel Xeon Gold 5318Y and an AMD EPYC 9354 CPUs. 1128 TBLIS and TCL achieve a median throughput that is com-More precisely, we analyzed the impact of performing the 1129 parable with TLIB when run on the AMD CPU. We obgemm function with subtensors and tensor slices. Our find-1130 served that most libraries are slower than TLIB for the tion method. Conversely, tensor slices are more advanta- 1133 of tensors with real-world tensor shapes, TLIB performs

#### 1141 8. Conclusion and Future Work

The performance tests show that our algorithms are 1201  $_{1143}$  layout-oblivious and do not need layout-specific optimiza-  $^{1202}$ 1144 tions, even for different storage ordering of the input ma-1145 trix. Despite the flexible design, our best-performing algo-1146 rithm is able to outperform Intel's BLAS-like extension 1206  $_{\rm 1147}\,{\rm function}$  cblas\_gemm\_batch by a factor of up to 2.57 in  $^{\rm 1207}$  $_{1148}$  case of asymmetrically shaped tensors. Furthermore, the  $_{1209}^{110}\,[11]$ 1149 performance results demonstrate that TLIB computes the 1210 1150 tensor-matrix product with asymmetrically shaped tensors 1211  $_{1151}$  on average at least 6.21% and up to 334.31% faster than  $_{1212}^{1212}\,[12]$ 1152 TuckerMPI, LibTorch and Eigen. Our findings leads us to 1214 1153 the conclusion that the LOG-based approach is a viable 1215 [13]  $_{\rm 1154}$  solution for the general tensor-matrix multiplication, ca-  $^{\rm 1216}$ pable of matching efficient GETT-based and TGGT-based  $^{1211}_{1218}$ 1156 implementations. Hence, other actively developed libraries 1219 [14] 1157 such as LibTorch and Eigen might benefit from our algo- 1220 1158 rithm design. Our header-only library provides C++ in-1159 terfaces and a python module which allows frameworks to 1160 easily integrate our library.

In the near future, we intend to incorporate our im1225
1162 plementations in TensorLy, a widely-used framework for
1163 tensor computations [25, 19]. We also would like to in1164 tegrate our solution to the TuckerMPI library [21] and 1229
1165 investigate the performance of HOSVD algorithms using 1230 [17]
1166 our approach. Insights provided in [14] could help to fur1167 ther increase the performance. Additionally, we want to 1231 [18]
1168 explore to what extend our approach can be applied for 1234
1169 the general tensor contractions.

## 1170 8.0.1. Source Code Availability

Project description and source code can be found at ht 1172 tps://github.com/bassoy/ttm. The sequential tensor-matrix multiplication of TLIB is part of Boost's uBLAS library.

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1200