1.2.C: High performance accurate computing I @ CAB G51, 10:15-10:45 (30min.)

High-Performance Implementation of Reproducible and Accurate Matrix-Multiplication

(Implementation and evaluation of Ozaki-scheme on GPUs)

June 27, 2018, PMAA 18 @ Zurich

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Introduction

- **Background**
  - Numerical computations with floating-point operations suffer from round-off errors, which impact the accuracy & reproducibility of the final result
  - This can be observed not only for ill-conditioned but also for regular problems
- **Accuracy**
  - The accumulation of round-off errors becomes non-negligible in large-scale and long-time computations
  - 64-bit floating-point (double-prec.) may become insufficient in near future
- **Reproducibility**
  - Round-off errors impact reproducibility as well as accuracy because the result of floating-point operations varies depending on the order of computations
    - Factors which may change the order of computations: algorithm, number of threads/processes, use of atomic operations, and so on
  - Loss of reproducibility makes it more difficult to debug a program (e.g. when you port a program to another environment)
  - Scientific experiments should be reproducible by other people

Introduction (cont'd)

- **Examples of linear algebra libraries supporting accurate and/or reproducible computations**
  - Accurate:
    - XBLAS [Li et al.]: for CPU, quadruple-precision (double-double)
    - MBLAS & MLAPACK (MPACK) [Nakata]: for CPU, based on some existing high-precision arithmetic libraries such as MPFR
  - Reproducible:
    - Conditional Numerical Reproducible (CNR) mode in Intel MKL: for CPU
  - Accurate & Reproducible:
    - ReproBLAS [Demmel et al.]: for CPU, accuracy is tunable
    - RARE-BLAS [Chohra et al.]: for CPU, correct rounding
    - ExBLAS [Iakymchuk et al.]: for CPU & GPU (OpenCL), correct rounding
- **Next generation BLAS (BLAS G2)**
  - Accurate and reproducible computations have been discussed as new features of next generation BLAS (at "Workshop on Batched, Reproducible, and Reduced Precision BLAS" in 2016 & 2017)

Introduction (cont'd)

The goal of this study

- To develop a high-performance implementation of accurate & reproducible matrix-multiplication on GPUs and to analyze the performance
- Accurate & reproducible methods: (1) **Ozaki scheme** and (2) ExBLAS scheme
- Ozaki-scheme: an accurate (and reproducible) matrix-multiplication method based on DGEMM [Ozaki et al. 2012]

Motivations

- **GEMM**:
  - Level-3 BLAS, compute-intensive
  - A key kernel in scientific computations
  - Highly-optimized implementation is needed
- **GPU**:
  - A major architecture widely used in HPC systems
  - Huge computational power: suitable for compute-intensive tasks
- **Implementation of Ozaki-scheme**:
  - The first full GPU implementation
  - With some optimization techniques for GPUs

Ozaki scheme [Ozaki et al. 2012]

Overview

- An accurate result is computed as a summation of several multiplications of matrices which are split not to occur rounding-errors during the multiplications:

$$C=AB=(A^{(1)}+A^{(2)}+\ldots+A^{(s)})\cdot(B^{(1)}+B^{(2)}+\ldots+B^{(t)})$$

➢ Matrices are split to be $|A^{(p)}(i,j)| \geq |A^{(q)}(i,j)|$, $|B^{(p)}(i,j)| \geq |B^{(q)}(i,j)|$, $p < q$ and $\mathrm{fl}(A^{(i)}B^{(j)}) = A^{(i)}B^{(j)}$ for any i and j

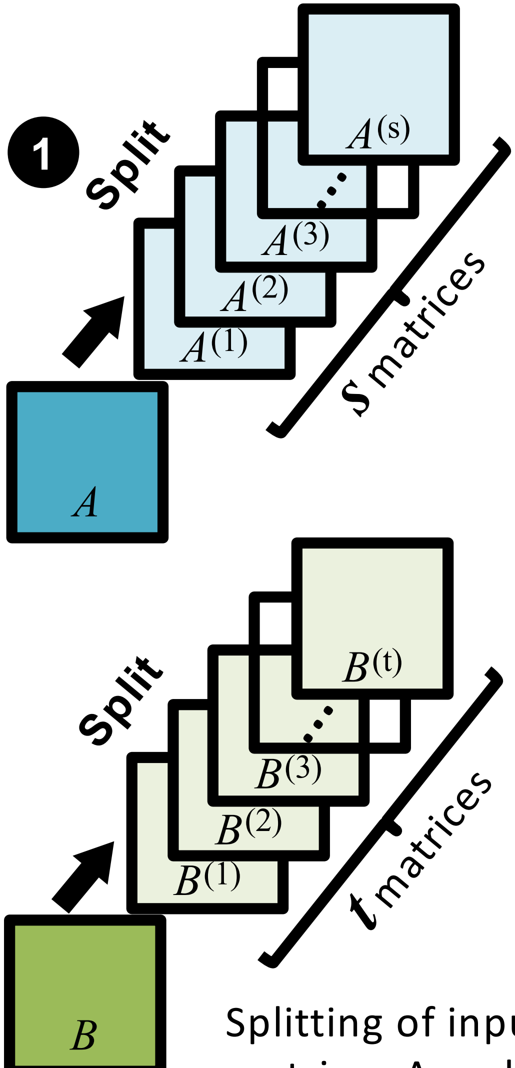
* $\mathrm{fl}(\ldots)$: result of floating-point operations

- If the summation of the multiplications of the split matrices is performed with correct rounding, the final result achieves correct rounding
  - ➢ In this study, we used the *NearSum* algorithm [Rump et al. 2005]
- The multiplications of split matrices can be performed using DGEMM
  - ➢ This is the most time-consuming portion in this method, and highly optimized DGEMM is available on most processors including GPUs
- It consumes a lot of memory
  - ➢ It can be solved using blocking (discussed later)

Ozaki scheme (cont'd)

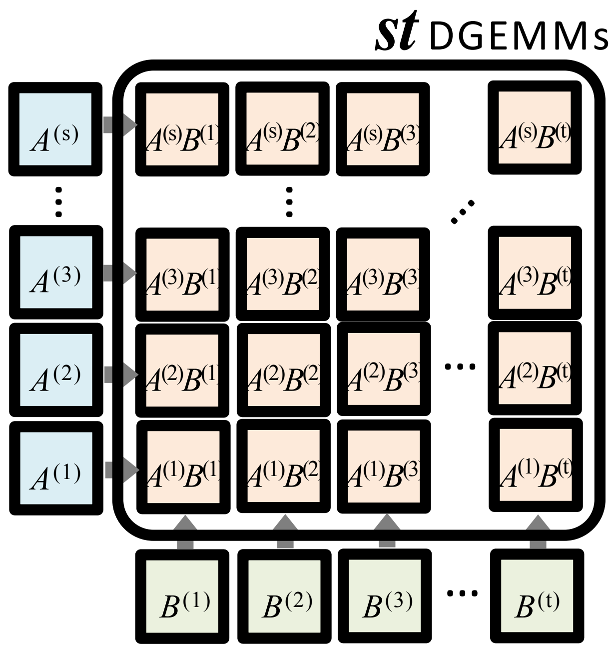
$C = AB = (A^{(1)} + A^{(2)} + \dots + A^{(s)}) \cdot (B^{(1)} + B^{(2)} + \dots + B^{(t)})$

- Matrices are split to be $|A^{(p)}(i,j)| \geq |A^{(q)}(i,j)|$, $|B^{(p)}(i,j)| \geq |B^{(q)}(i,j)|$, $p < q$ and $\mathrm{fl}(A^{(i)}B^{(j)}) = A^{(i)}B^{(j)}$ for any i and j

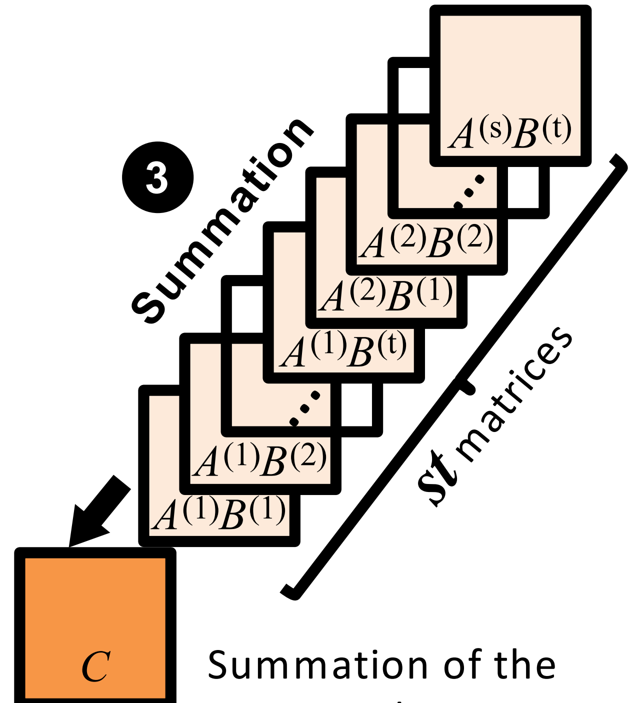


Splitting of input matrices A and B

2 Matrix Multiplications

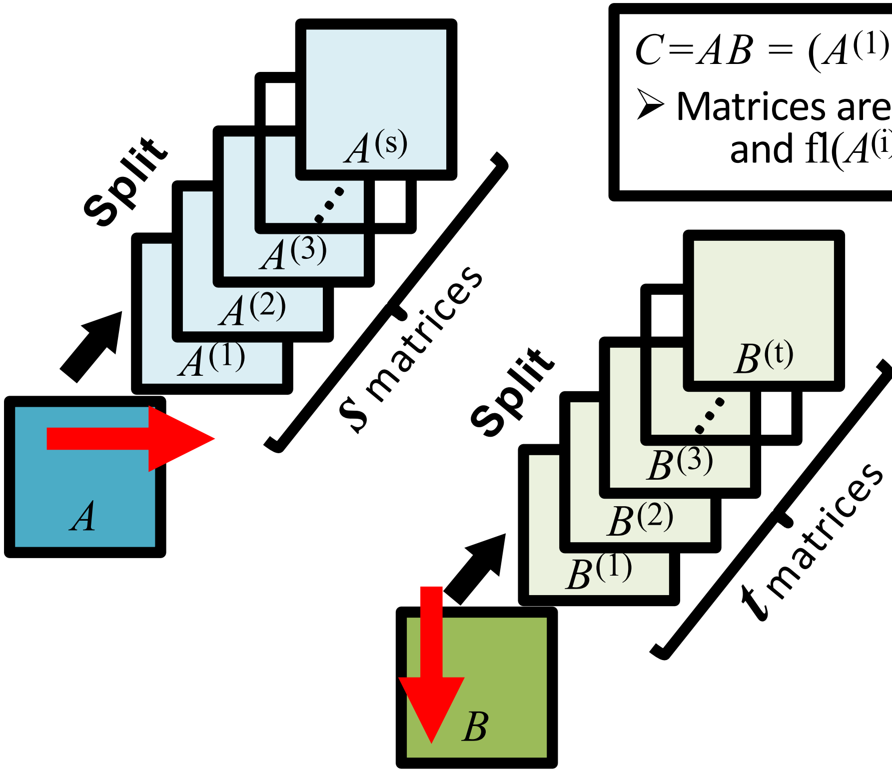


Multiplications of the split matrices by DGEMM



Summation of the computed matrices by NearSum

Ozaki scheme – Matrix splitting



$C = AB = (A^{(1)} + A^{(2)} + \dots + A^{(s)}) \cdot (B^{(1)} + B^{(2)} + \dots + B^{(t)})$

- Matrices are split to be $|A^{(p)}(i,j)| \geq |A^{(q)}(i,j)|$, $|B^{(p)}(i,j)| \geq |B^{(q)}(i,j)|$, $p < q$ and $\mathrm{fl}(A^{(i)}B^{(j)}) = A^{(i)}B^{(j)}$ for any i and j

Algorithm 1 Split vector $x = [x_1, x_2, \cdots, x_n]$

function Split(x)
  $i = 1$
  while (norm($x^{(i)}$, inf)! $= 0$) **do**
    $c_1 = \mathtt{ceil}((\log_2 u^{-1} + \log_2(n+1))/2)$
    $c_2 = \mathtt{ceil}(\log_2 \max(|x_i|))$
    $t = 2^{c_1} \cdot 2^{c_2}$
    $\sigma = [t, t, \cdots, t]$
    $x^{(i)} = x' = \mathtt{fl}((x^{(i)} + \sigma) - \sigma)$
    $x^{(i+1)} = \mathtt{fl}(x' - \underline{x}^{(i)})$
    $i = i + 1$
  end while
end function

- Matrices are split not to occur rounding-errors during the multiplications of the split matrices
- This algorithm is the error-free transformation for vector
- Matrix can be split by applying the algorithm to a matrix towards inner-product direction
- # of splits depends on both the length of the vector and the max value

Ozaki scheme – GPU implementation

Overview

- Full CUDA implementation
- Interface compatible with cublasDgemm
  - Computes double-precision matrices located on GPU memory
  - But currently α & β are not supported (just compute C=AB)

Challenges

- To improve performance
- To reduce memory consumption
  - GPUs have limited memory space

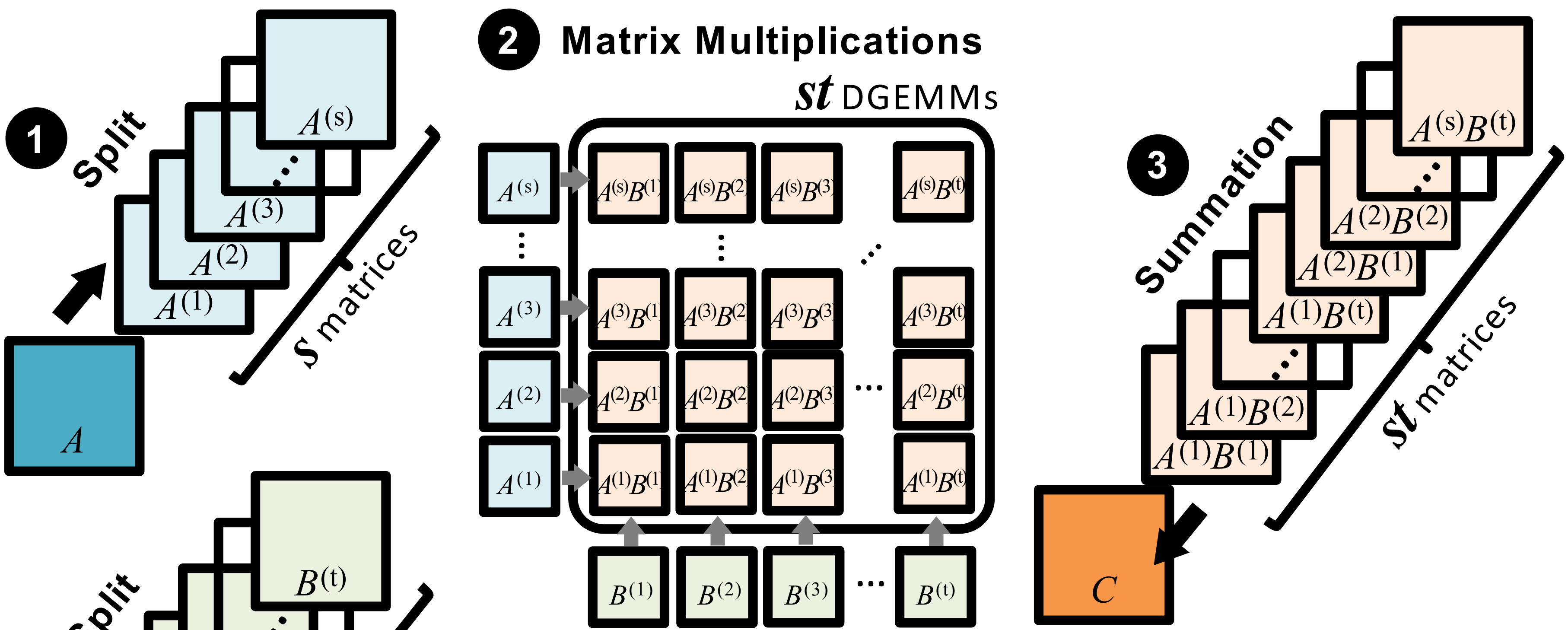
Techniques we applied

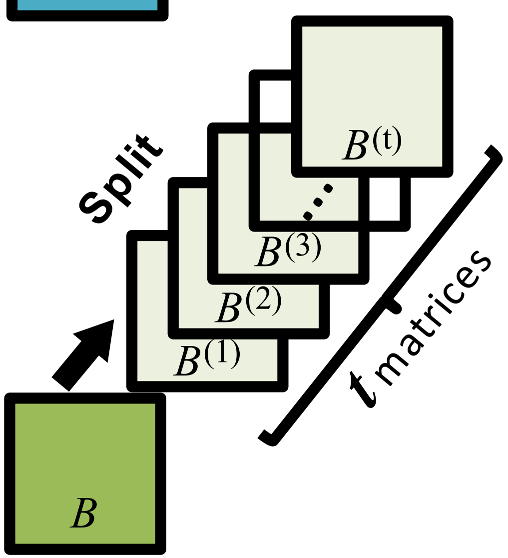
- Blocking (for memory and performance)
- Utilizing batched BLAS (for performance)

```
__host__ int exblasExdgemm (
     cublasHandle_t ch,
     char tranA, char tranB,
     int m, int n, int k,
     double *alpha,
     double *devA, int lda,
     double *devB, int ldb,
     double *beta,
     double *devC, int ldc) {

     …
     Split (devA, devAsplit);
     Split (devB, devBsplit);
     …
     Compute (devAsplit,
                  devBsplit,
                  devCsplit);
     …
     NearSum (devCsplit, devC);
     …
}
```

Ozaki scheme – Blocking

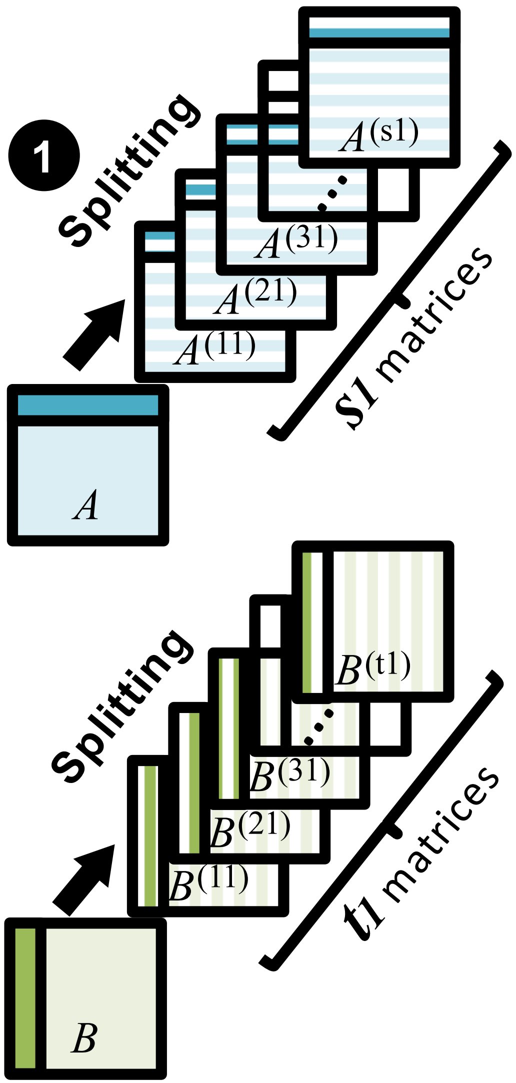


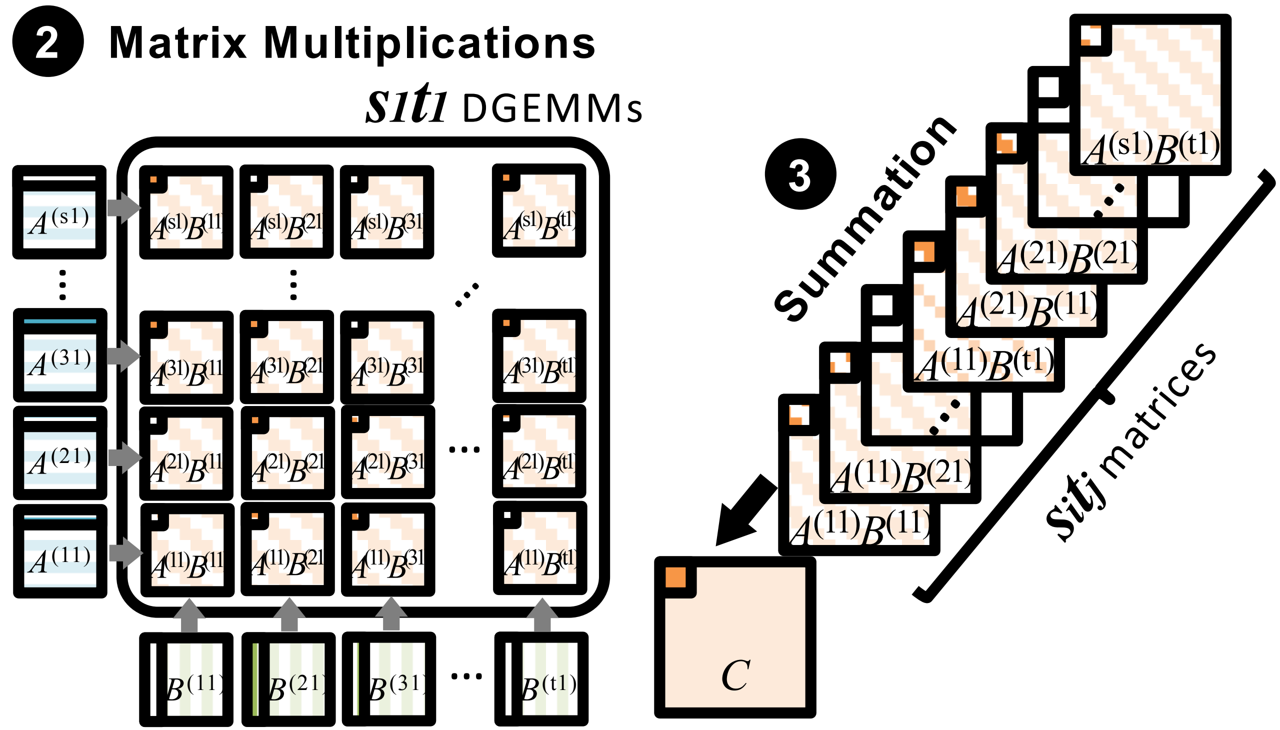


Memory consumption:

When matrices A and B are n x n square matrices, the naïve implementation consumes $(s+t+st)n^2$ extra memory space

Ozaki scheme – Blocking (cont'd)



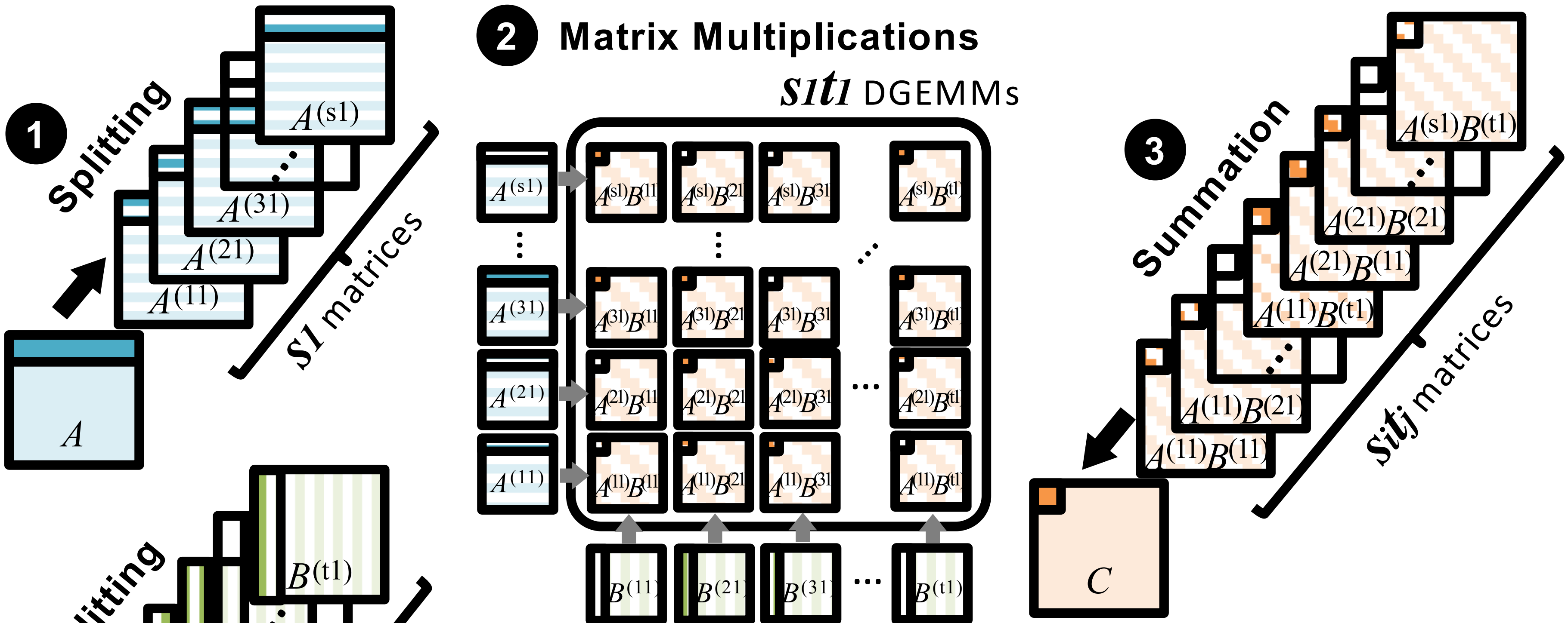


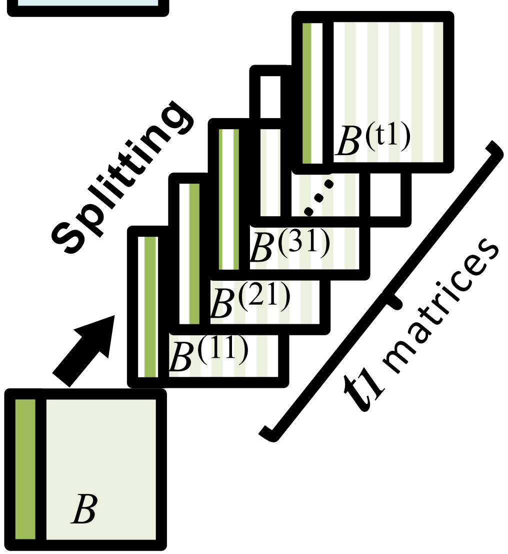
Memory consumption (with blocking):

When block-size=b, # of splits of mat-A $=s_i=s$ $(1< i \leq m/b)$, and # of splits of mat-B $=t_j=t$ $(1< j \leq n/b)$, the required memory space decreases from $(s+t+st)n^2$ to $(s+t)nb+stb^2$

*Note: s_i and t_j may vary depending on the max value in each block, thus there is a possibility to reduce # of splits compared to the non-blocking case

Ozaki scheme – Blocking (cont'd)





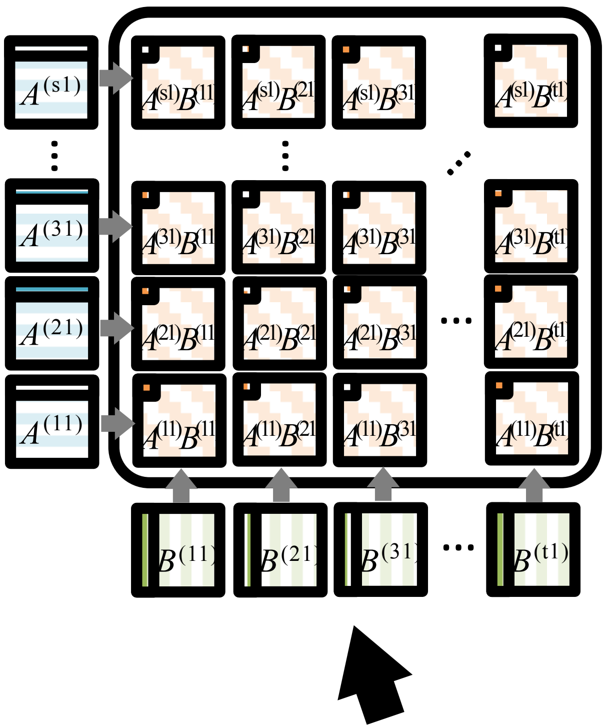
A negative side-effect:

If the block-size is quite small, the throughput of GEMM may decrease as problem size becomes too small to utilize all the cores on a GPU

Ozaki scheme – Batched BLAS

A negative side-effect:

If the block-size is quite small, the throughput of GEMM may decrease as problem size becomes too small to utilize all the cores on a GPU



$$C = AB = (A^{(1)} + A^{(2)} + \ldots + A^{(s)}) \cdot (B^{(1)} + B^{(2)} + \ldots + B^{(t)})$$

A solution: Batched BLAS

- A new BLAS interface that computes multiple independent BLAS operations as a single task
- cuBLAS (intel MKL as well) provides a batched DGEMM routine, which computes multiple small DGEMMs concurrently at a high speed

```
cublasDgemmBatched (cublasHandle_t handle,
        cublasOperation_t transa, cublasOperation_t transb,
        int m, int n, int k, const double *alpha,
        const double *Aarray[], int lda,
        const double *Barray[], int ldb,
        const double *beta, double *Carray[], int ldc,
        int batchCount)
```

$C=Sum(C^{(0)}+C^{(1)}+C^{(2)}+C^{(3)})$

Evaluation

Evaluation

- Performance (effectiveness of blocking & batched BLAS)
- Demonstrations of accuracy

Environment

- GPU: NVIDIA Titan V (Volta architecture)
  - 7449.6 GFlops on double-precision, 16GB memory
- CUDA 9.1, driver version: 390.67

Problem setting

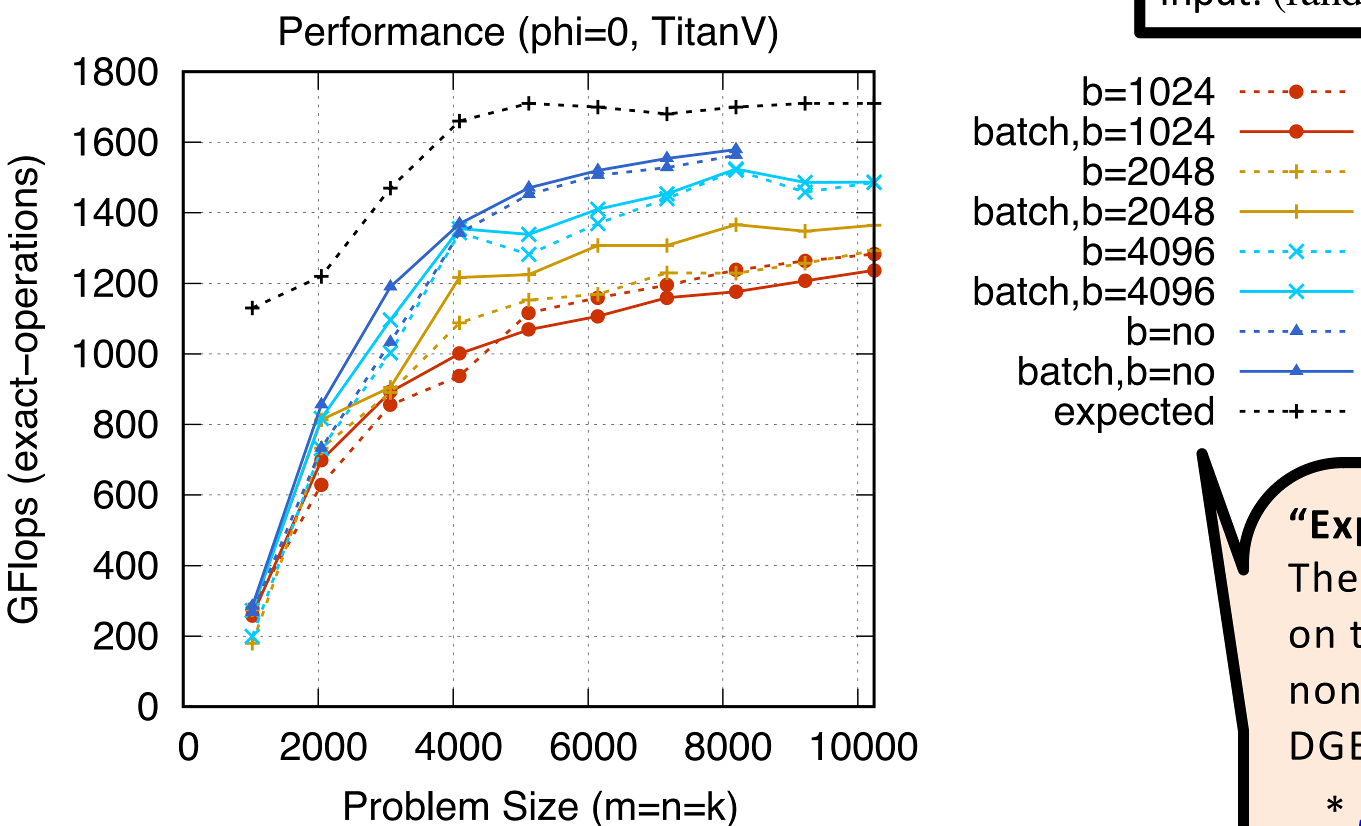
- Matrices are square & initialized as $(\mathrm{rand}(n)\text{-}0.5) * \exp(\phi * \mathrm{randn}(n))$
  - The larger ϕ is, the wider the range of the absolute values in the matrix becomes (and thus, # of splits and DGEMMs also increase)

Theoretical / expected performance

- Cost: the computation by DGEMM is $O(n^3)$, the other parts are $O(n^2)$
- We assume that the expected performance is the performance based on the cost for st times of non-block & non-batched DGEMM (where # of splits for mat A & B are s & t, respectively)

Performance (ϕ=0)

Input: (rand(n)-0.5) * exp(ϕ * randn(n))



* b:block-size

"Expected" performance: The performance based on the cost for ***st*** times of non-block & non-batched DGEMM

* ***s***: # of splits of mat A

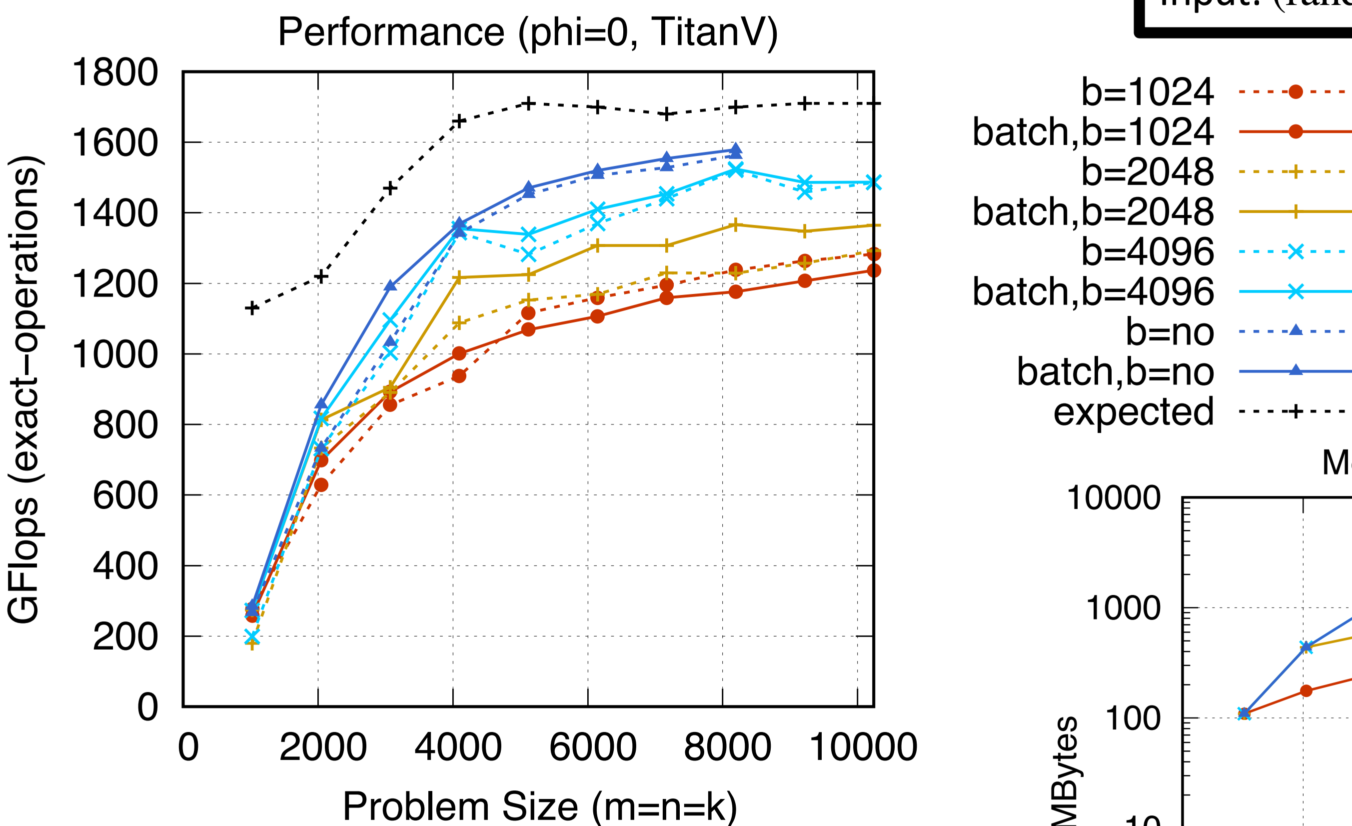
* ***t***: # of splits of mat B

In this case, ***s*** = 2 & ***t*** = 2: the expected overhead is 4x of DGEMM

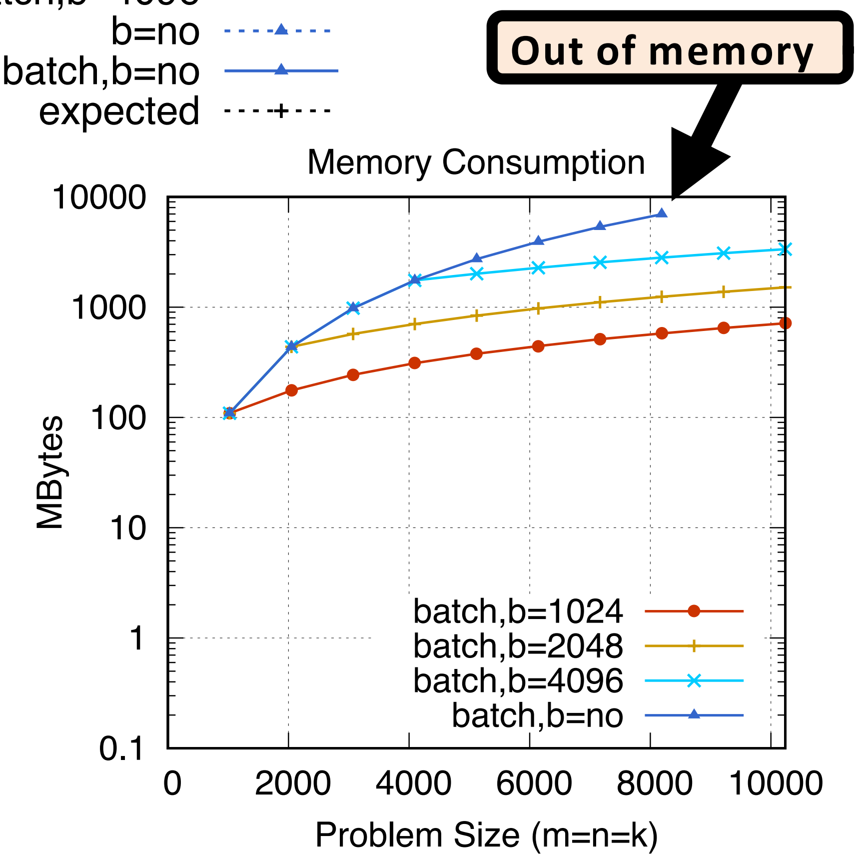
- In this case (ϕ=0, # of splits = 2), the effectiveness of batched BLAS is a little (# of batched tasks is too few)

Performance (ϕ=0)

Input: (rand(n)-0.5) * exp(ϕ * randn(n))

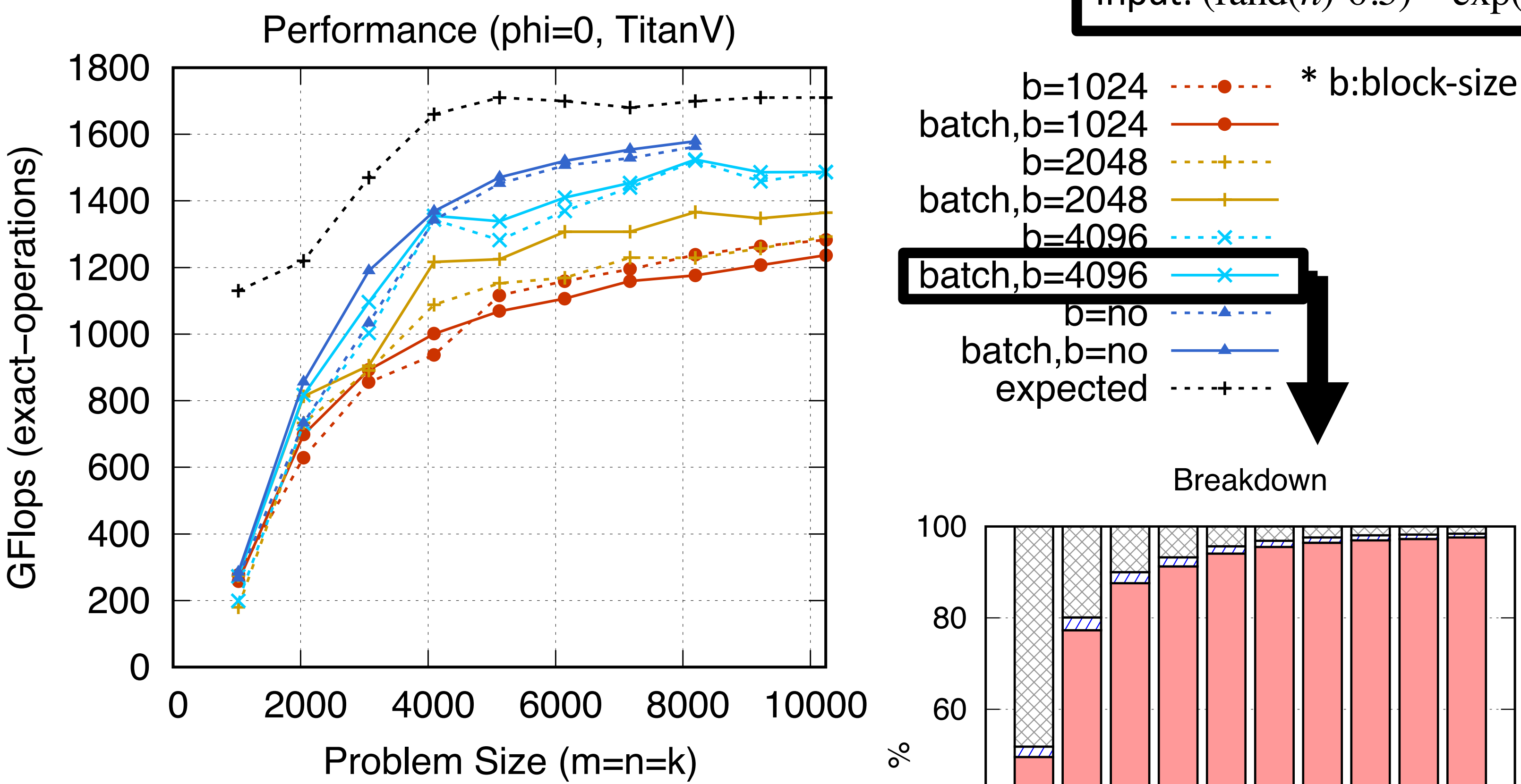


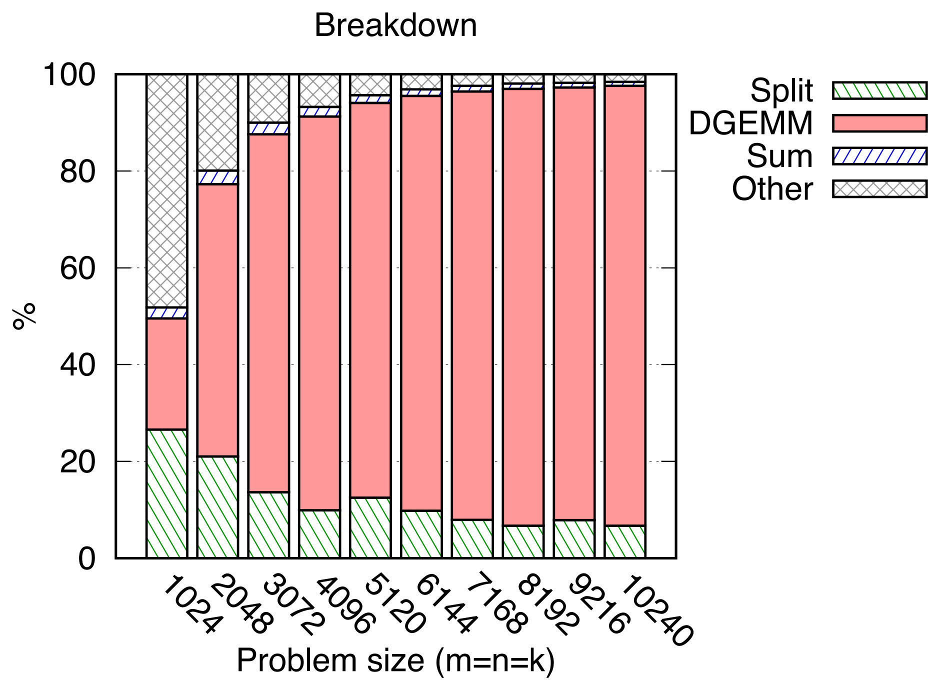
* b:block-size



Performance (ϕ=0)

Input: (rand(n)-0.5) * exp(ϕ * randn(n))

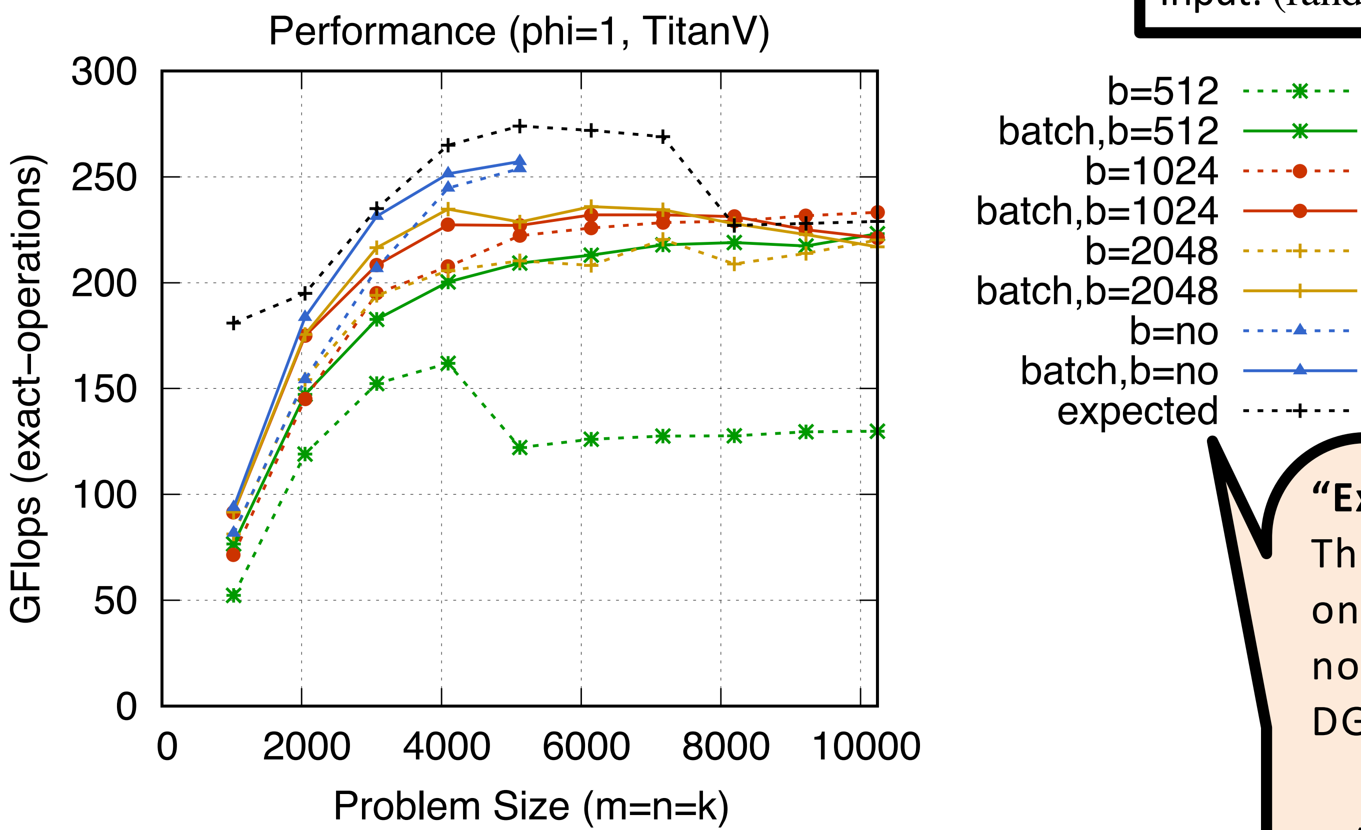




- “Other” is mainly cost for allocating the memory for storing split matrices
- This cost can be ignored as you can use the allocated memory repeatedly in the case you use the routine multiple times

Performance (ϕ=1)

Input: (rand(n)-0.5) * exp(ϕ * randn(n))



* b:block-size

"Expected" performance:
The performance based on the cost for st times of non-block & non-batched DGEMM

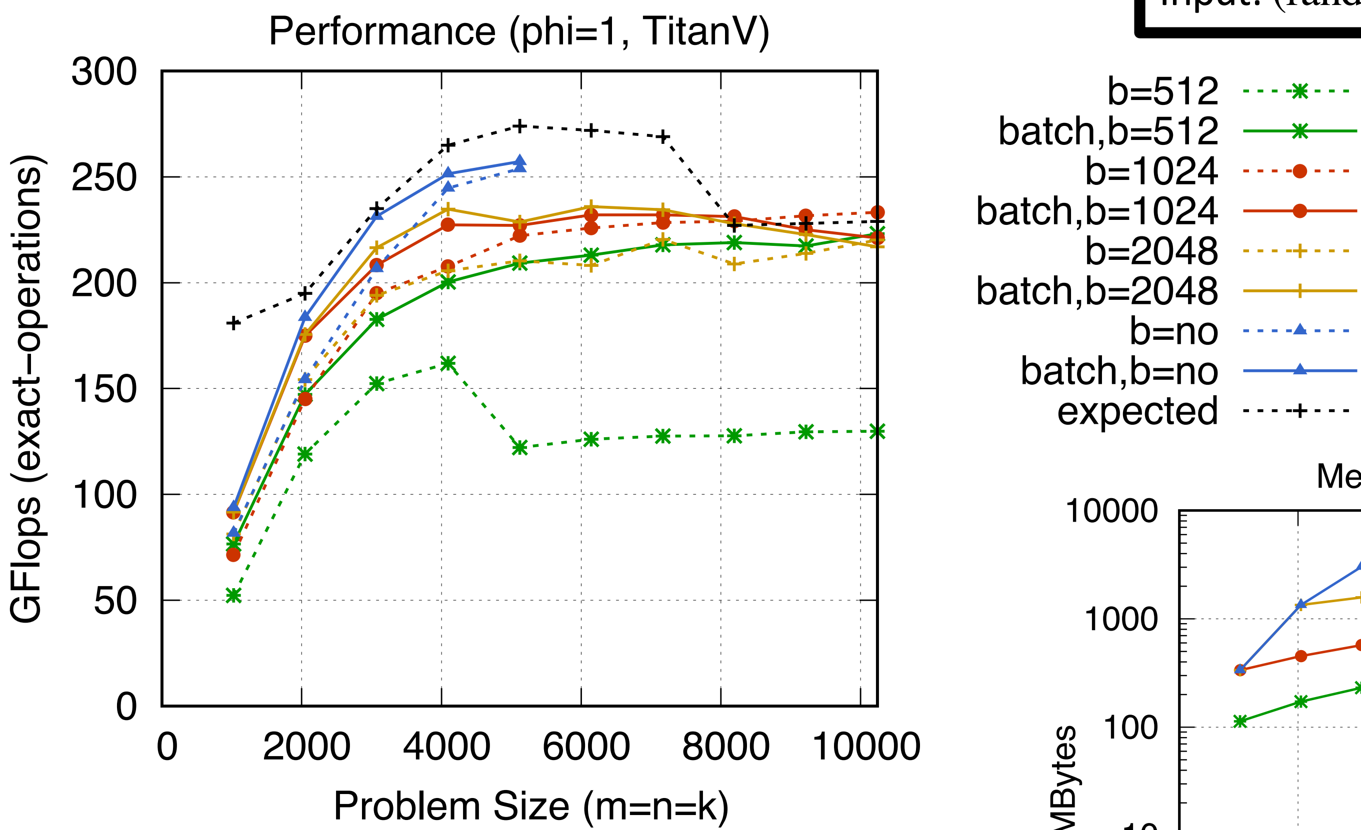
* s: # of splits of mat A
* t: # of splits of mat B

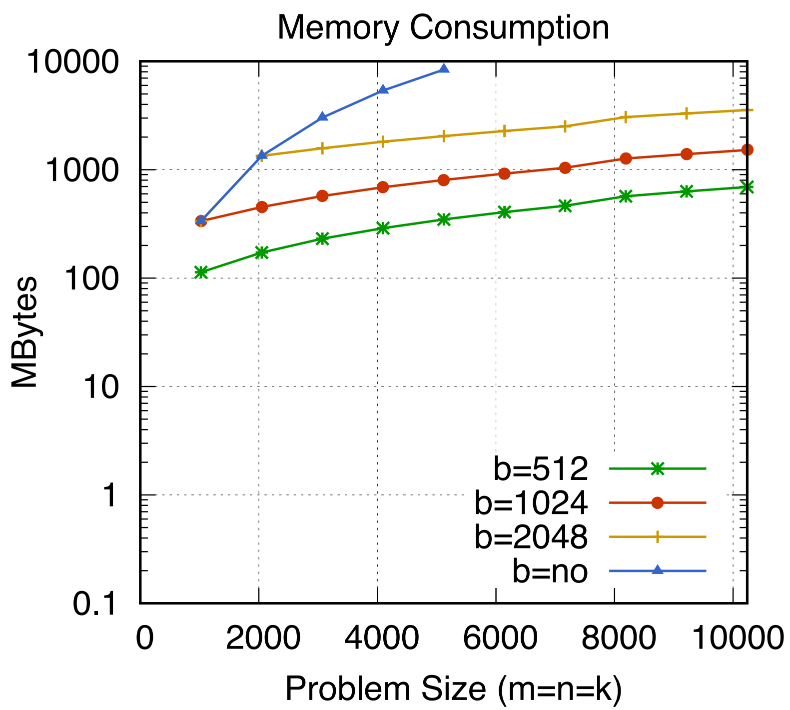
In this case, s = 5 & t = 5 and 6 ($n \geq 8192$): the expected overhead is 25-30x of DGEMM

- In this case (# of splits = 5~6, # of batch tasks = 25-30), even block-size b=512 can achieve a competitive performance when batched BLAS is used

Performance (ϕ=1)

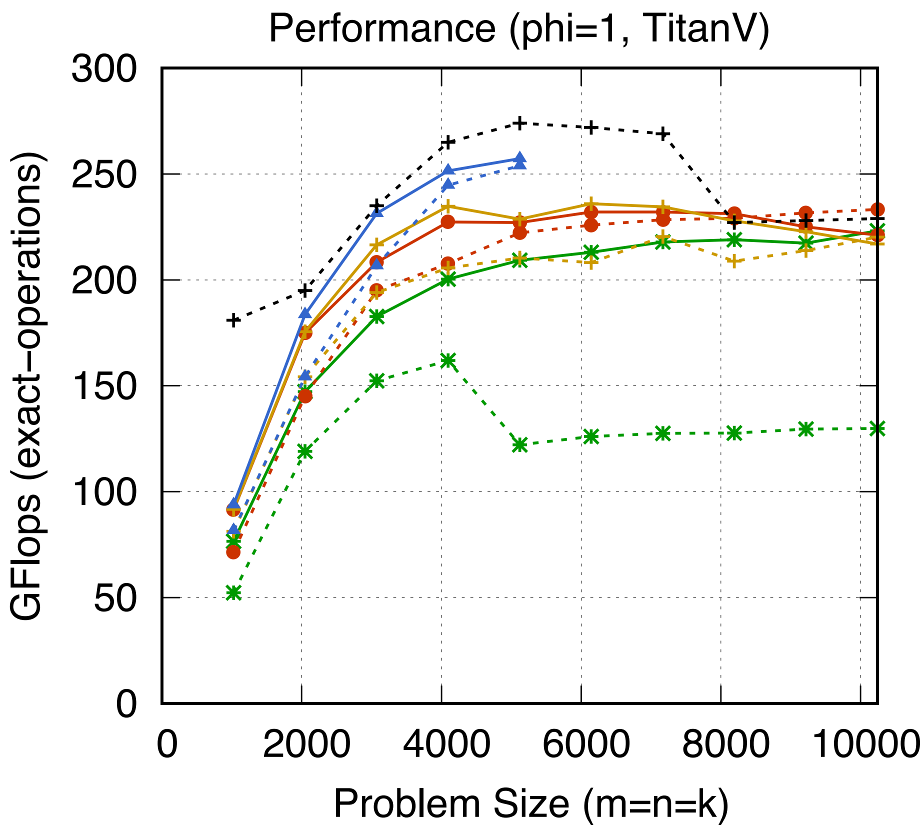
Input: (rand(n)-0.5) * exp(ϕ * randn(n))

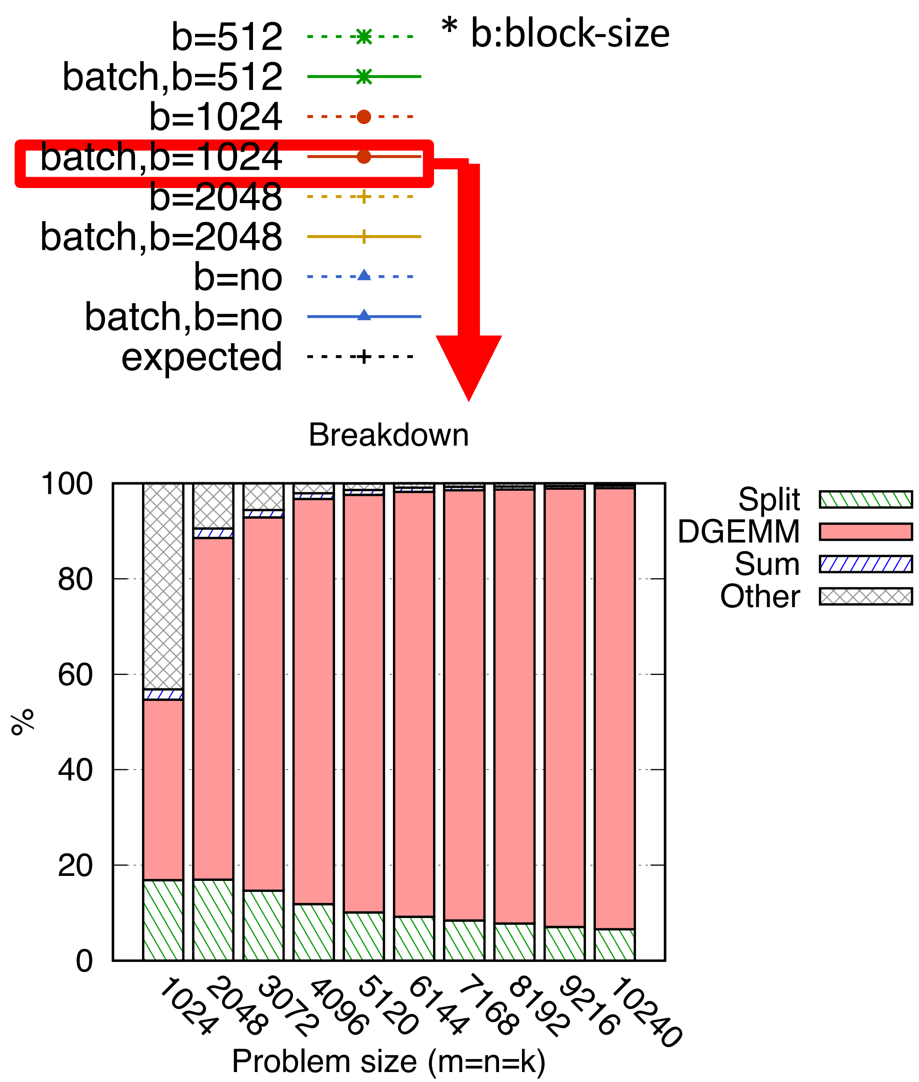




Performance (ϕ=1)

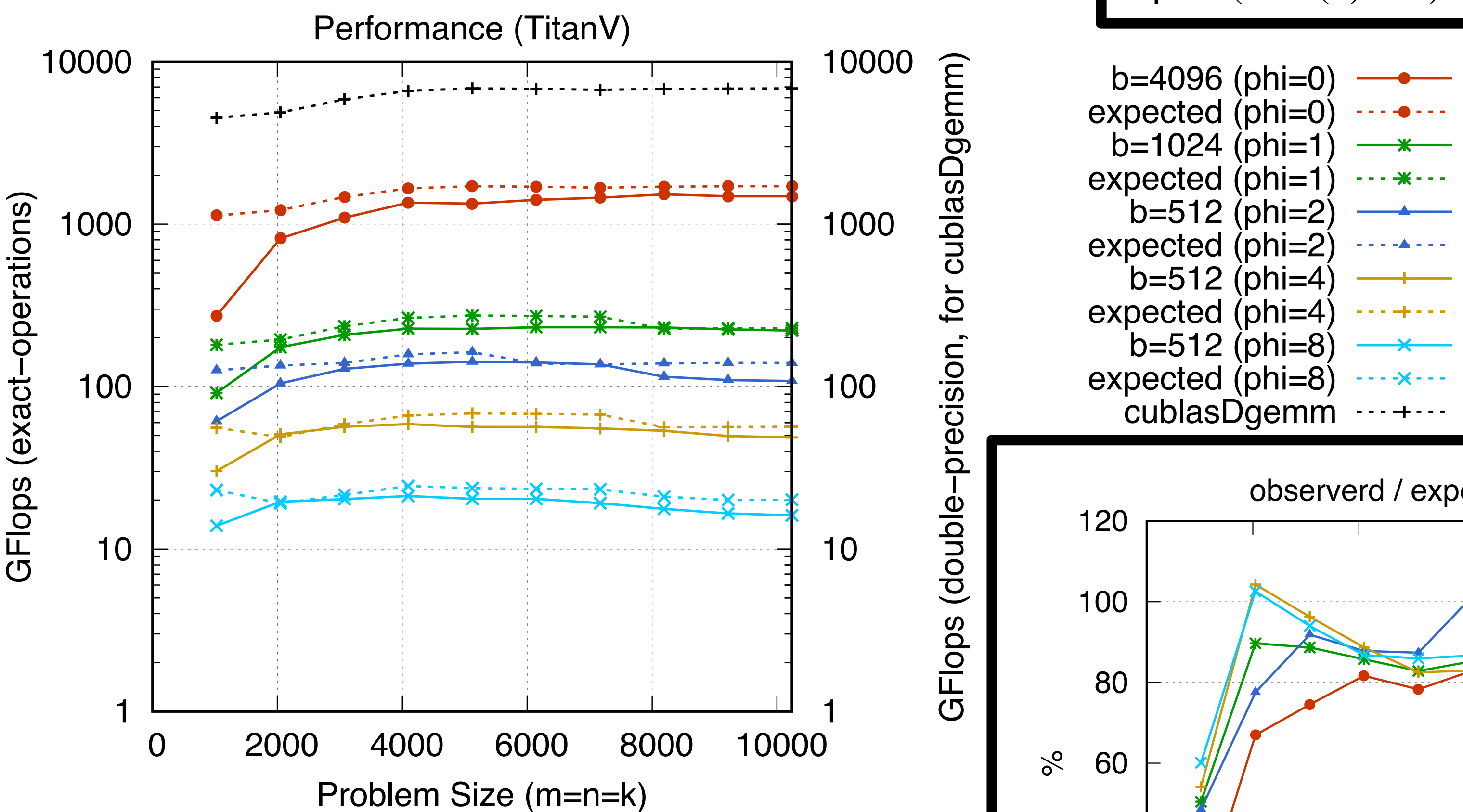
Input: (rand(n)-0.5) * exp(ϕ * randn(n))



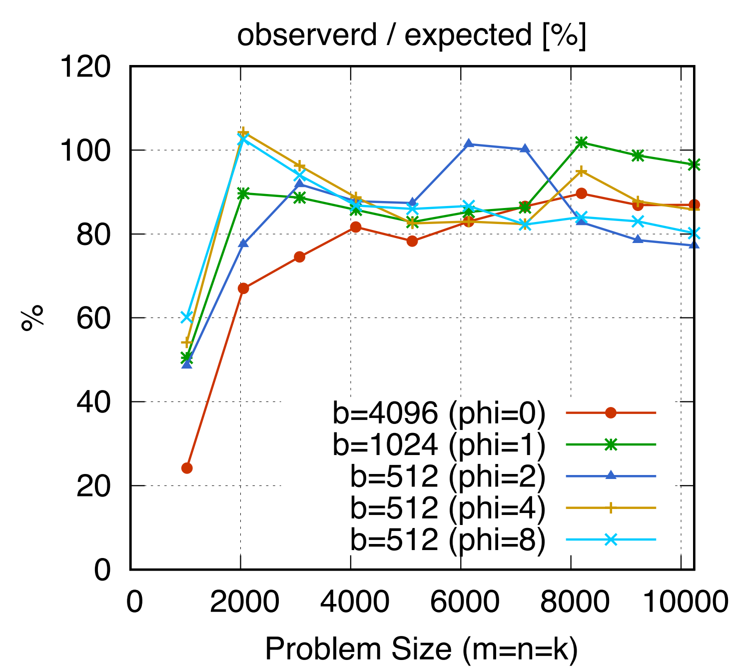


Performance (ϕ=0~8)

Input: (rand(n)-0.5) * exp(ϕ * randn(n))



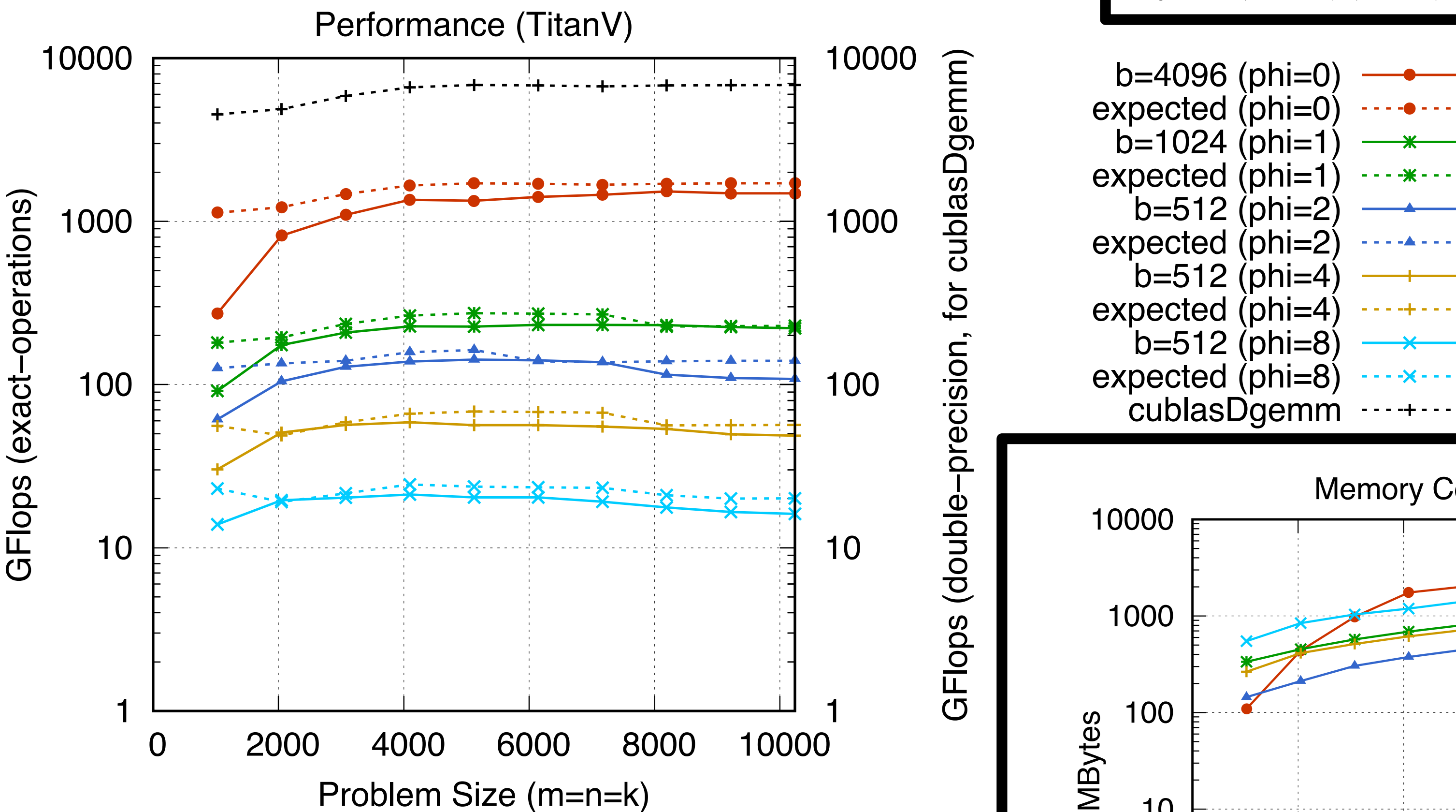
* b:block-size

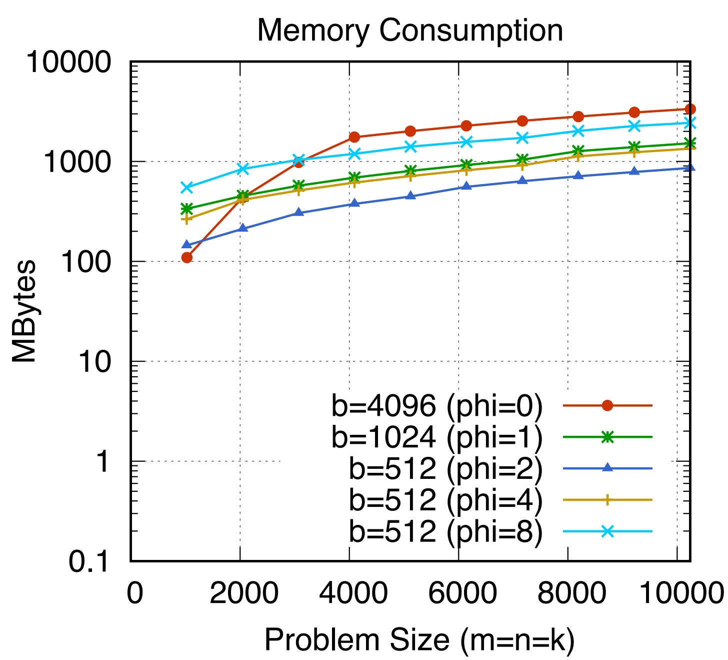


Performance (ϕ=0~8)

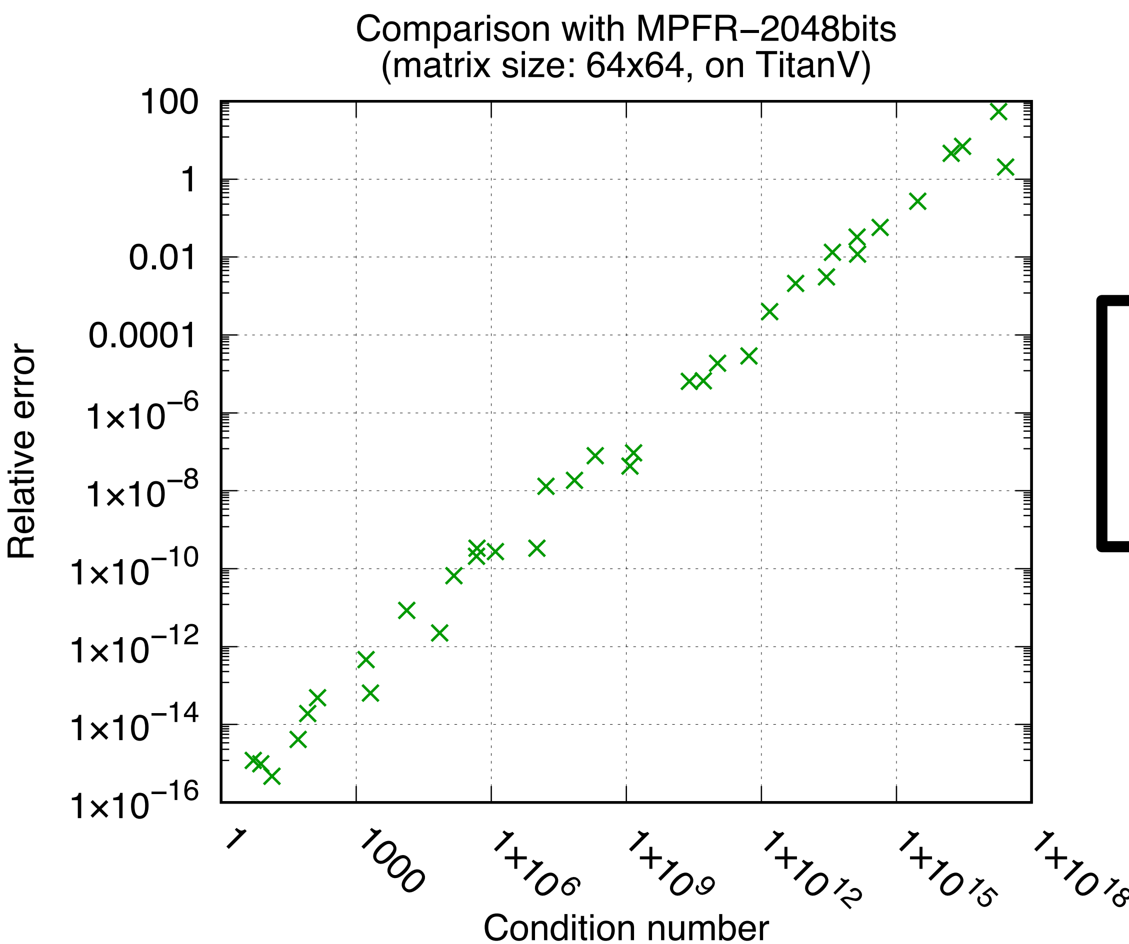
Input: (rand(n)-0.5) * exp(ϕ * randn(n))

* b:block-size





Accuracy test



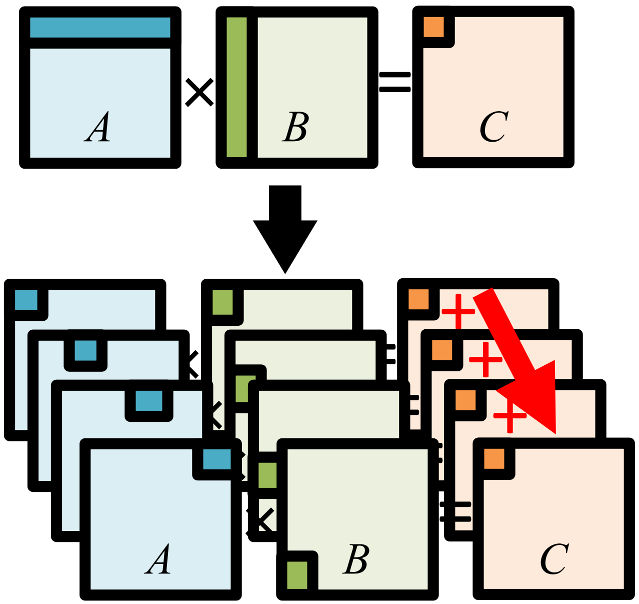
Relative error =

$$\frac{\max(|C_{target}[i]| - |C_{MPFR}[i]|)}{\max(|C_{MPFR}[i]|)}$$

- Compared with MPFR (2048bits), ExDGEMM has no error for any cases (there is nothing to plot)

Further optimization (future work)

- **Blocking towards inner-product direction**
  - It may increase the chance to reduce # of splits since it depends the matrix dimension towards the inner product direction as well as the max value
  - But it increases memory consumption and # of summations to compute the final result
- **Skipping of zero calculations**
  - Split matrices which have lower digits information may include many zero elements (sparse matrix)
  - Sparse GEMM (SpMM) may be used for those computations
- **Auto-tuning**
  - For determining the optimal block-size and use/non-use of batched BLAS
  - For block-size, there is a tradeoff between performance and memory consumption



Conclusion

Summary

- The first full GPU implementation of accurate (correct rounding) and reproducible DGEMM with Ozaki scheme
- Implementation techniques
  - Matrix blocking for reducing memory consumption
  - Use of batched BLAS for improving performance
- More than 90 % of expected performance can be achieved if the optimal block-size is used (the performance is DGEMM-performance-bound)

Future work

- Further optimizations
  - For small matrices
  - Automatic determining of optimal block-size
    - Blocking has a tradeoff between memory-consumption and performance
- Comparison with other methods (ReproBLAS, ExBLAS scheme, etc.)
- Implementation of Full set BLAS

High-Performance Implementation of Reproducible and Accurate Matrix-Multiplication

June 27, 2018

PMAA 18 @ Zurich

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ExBLAS scheme

Overview

- A reproducible + accurate method
  - Reproducibility is achieved by computing with correct-rounding
- Combination of Floating-Point Expansion (FPE) + Super-Accumulator (SuperAcc)

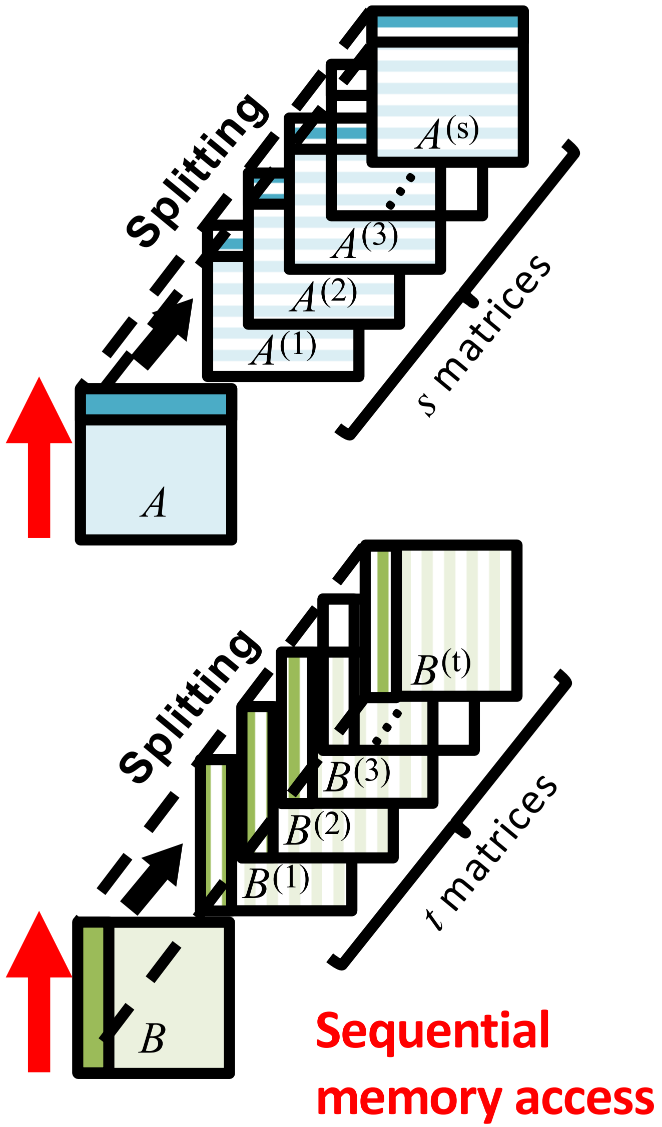
Floating-Point Expansion (FPE)

- Based on error free transformations [Dekker and Knuth]
- Used for avoiding (reducing) the access to SuperAcc (it’s heavy)

Super-Accumulator (SuperAcc)

- A long accumulator which can cover the exponent range of double-precision
- It consists of array of 64-bit integer (39 elements)

Further optimization

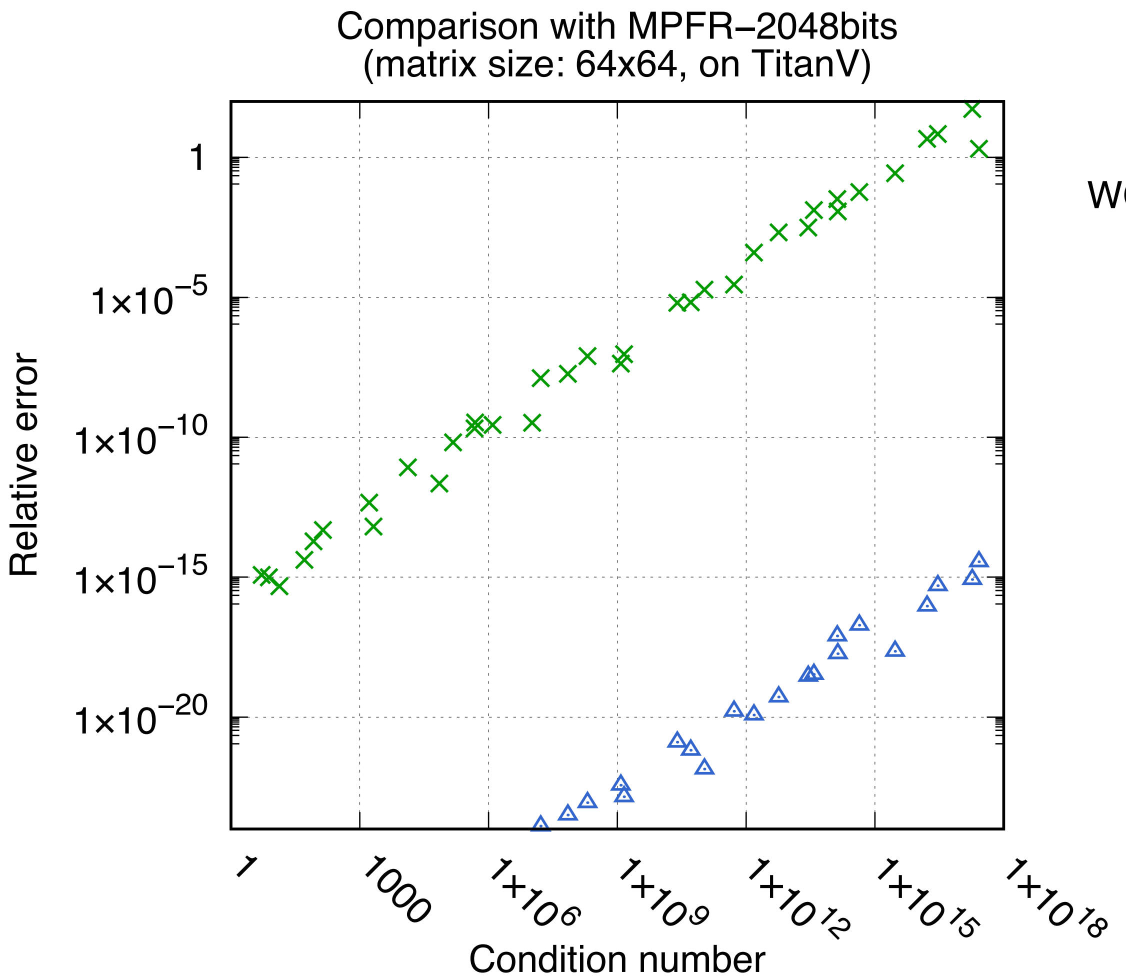


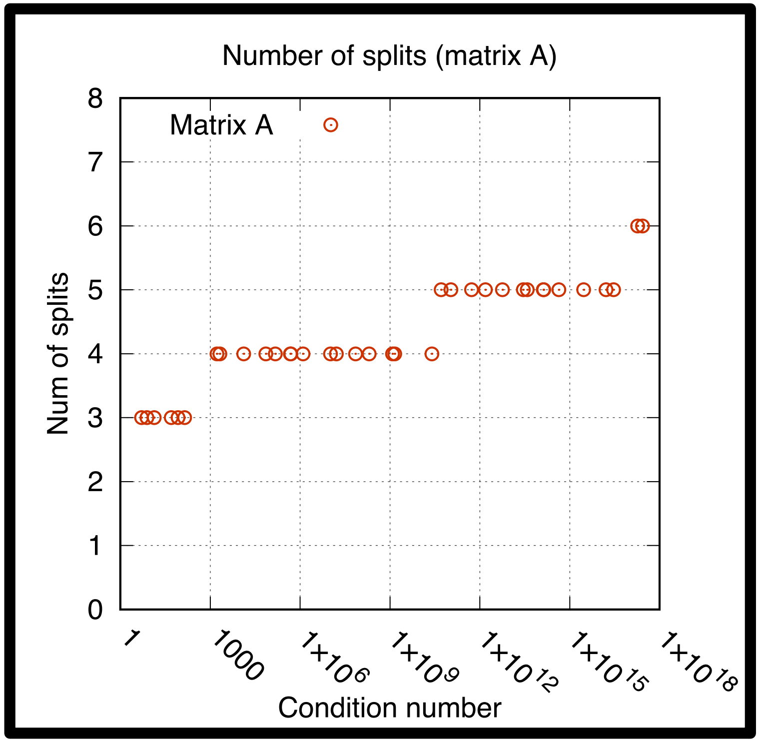
Splitting of matrix A:

- Determining the number of splitting (= finding the max number in row-direction) requires non-sequential memory access
- To avoid the performance degradation, we transposed the matrix A before splitting
- The computations of split matrices are performed using batched DGEMM-TN
- The transposition cost is negligibly small

Note: although this approach is actually effective to improve the performance of splitting of mat A, the performance of cuBLAS DGEMM-TN is unstable when the matrix size is large: the total performance decreases when this approach applies on Titan V (we didn’t apply this in our current implementation)

Accuracy test

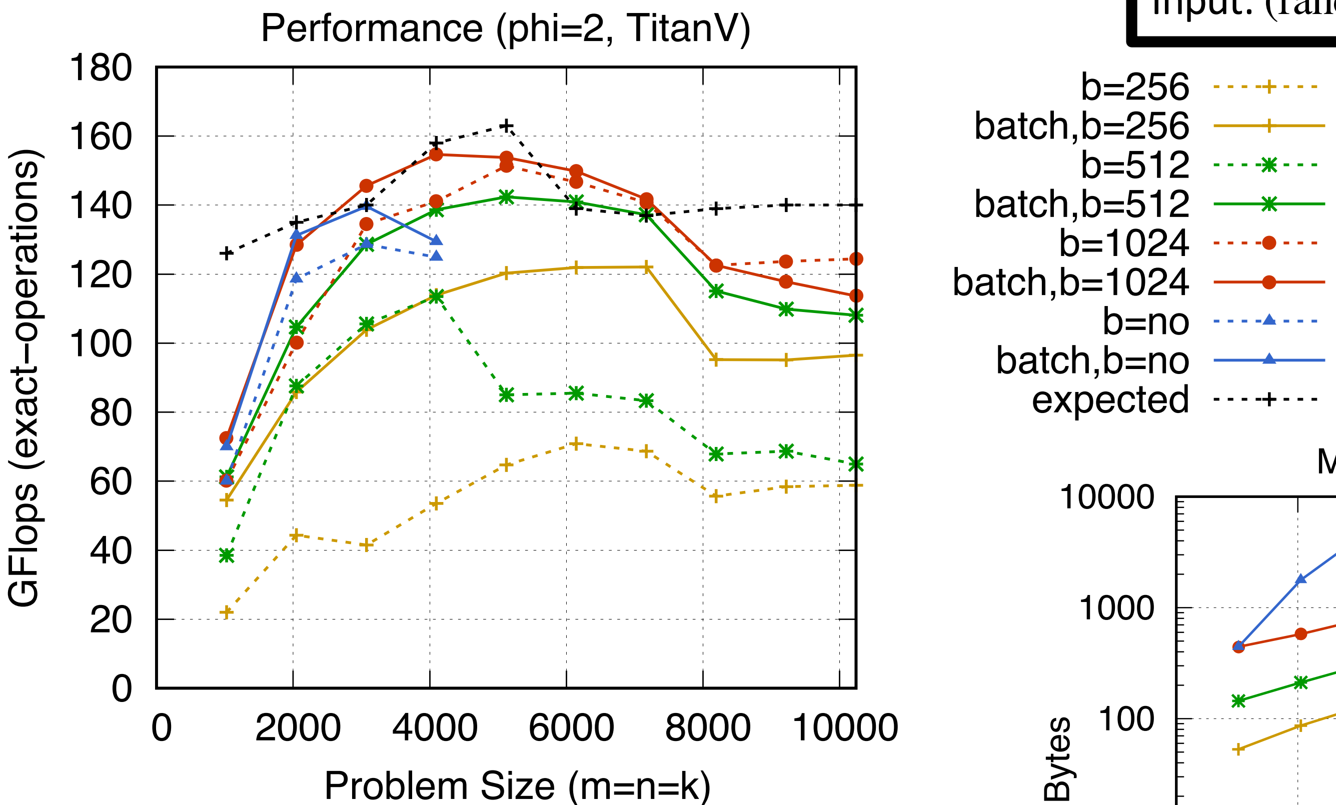




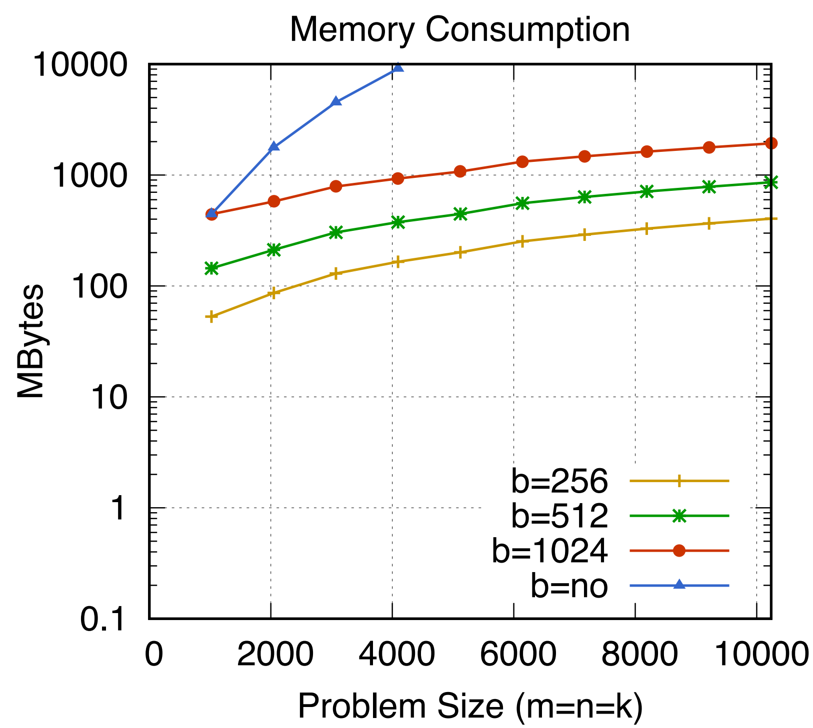
- Compared with MPFR (2048bits), ExDGEMM has no error for any cases (impossible to plot the results with logscale axis)

Performance (ϕ=2)

Input: (rand(n)-0.5) * exp(ϕ * randn(n))



* b:block-size



Memory consumption

Input: (rand(n)-0.5) * exp(ϕ * randn(n))

* b:block-size