Reproducible, Accurately Rounded and Efficient (RARE) BLAS

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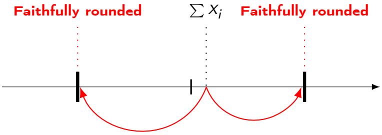
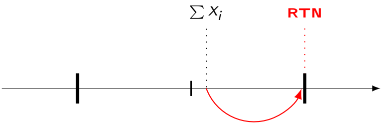
Introduction and Problematic

Limited Machine Precision

- Using floating point numbers as approximation.
- $x \longrightarrow X = fl(x)$ if $x \notin F$ or x if $x \in F$.
- $X + Y \neq X \oplus Y = fl(X + Y)$.
- IEEE-754 standard defines several rounding modes.





Introduction and Problematic

Non-associativity of Addition

- A ⊕ (B ⊕ C) ≠ (A ⊕ B) ⊕ C.
- Catastrophic cancelation : M = 2^{53}; 0 = -M ⊕ (M ⊕ 1) ≠ (-M ⊕ M) ⊕ 1 = 1.

Non-reproducibility of Summation

- For a sum ($\sum_{i=1}^{n} X_i$), the final result depends on the order of the computations.
- Why could operations order be different?
  - Dynamic data scheduling.
  - Non-deterministic reductions.
  - Resources availability.
  - Different instruction sets.

Introduction and Problematic

Is Numerical Reproducibility Really Important ?

- Important for debugging.
- Important for validating results.
- Reproducibility : One of top 10 exascale research challenges (U.S. Department of Energy [DOE], 2014).
    - 10^{18} flop/s.
    - Millions of cores.

"Reproducibility will be expensive if not impossible to achieve on exascale"

Parallel Libraries Solutions

Solutions for Reproducibility Problem

- Static scheduling (OpenMP).
- Deterministic reduction.
- Intel MKL: CNR.

Algorithmic Solutions

- Deterministic error.
  - ReprodSum (Demmel and Nguyen, 2013).
  - FastReprodSum (Demmel and Nguyen, 2013).
  - OneReduction (Demmel and Nguyen, 2014).
  - ReprodBLAS library.
- Higher precision (quadruple precision for instance).
  - SumK and DotK (Ogita and al., 2005).
  - Improve accuracy and consistency (Villa and al., 2009).
  - Reproducibility is not always guaranteed.
- Correctly rounded arithmetic.
  - FP expansions + Super accumulators (Collange and al., 2014).
  - Small and Large Super accumulators (Neal, 2015).

Our Aim

Guarantee the Numerical Reproducibility for BLAS (Basic Linear Algebra Subroutines)

- Level 1 : i_amax, _swap, _copy, _scal, _axpy, _nrm2, _asum, _dot.
- Level 2 : _gemv, _trsv, _ger, _syr, _syr2.
- Level 3 : _gemm, _syrk, _syrk2, _trsm.

In This Talk

- Shared memory parallel implementation.
- Distributed memory parallel implementation.
- Xeon Phi implementation.

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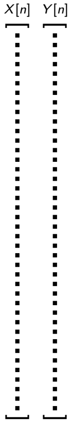

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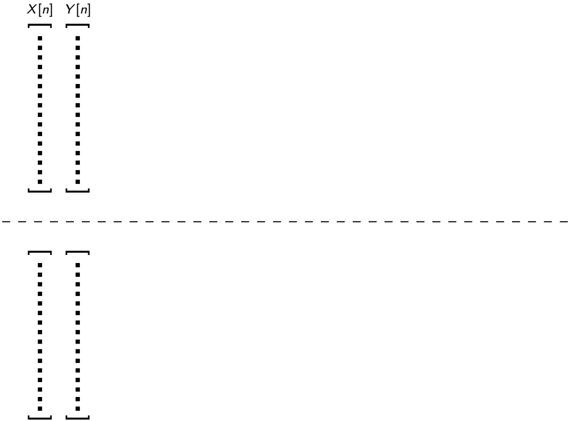

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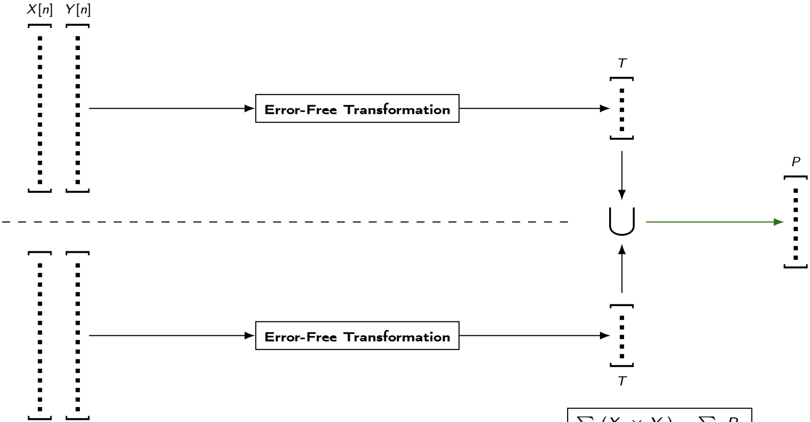
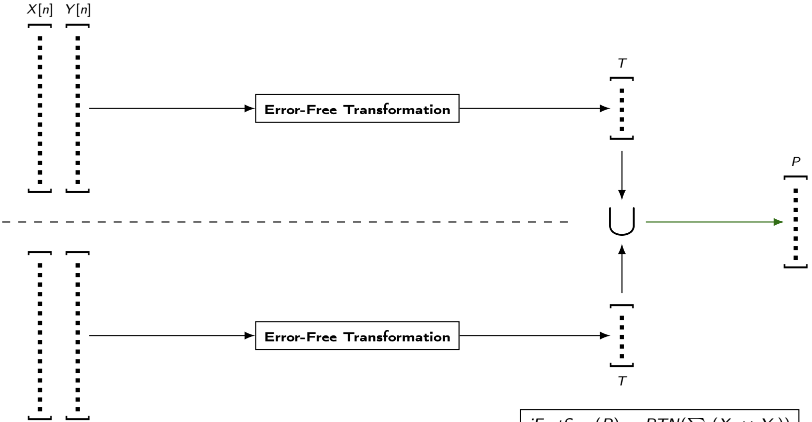


$\sum_i (X_i \times Y_i) = \sum_j P_j$

Parallel Dot Product



$iFastSum(P) = RTN(\sum_i (X_i \times Y_i))$

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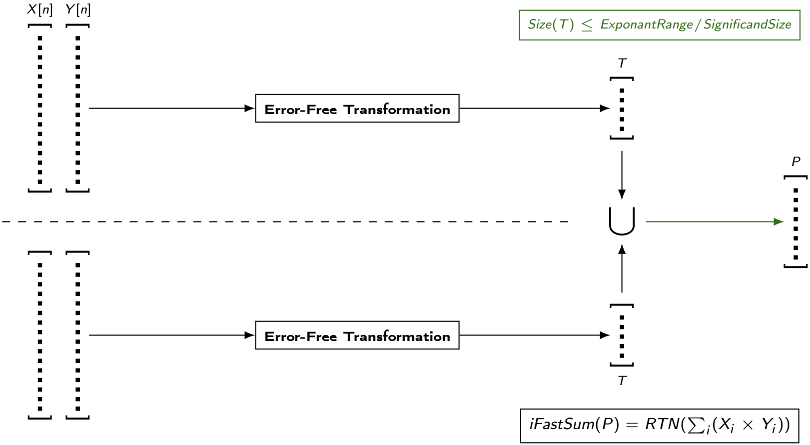

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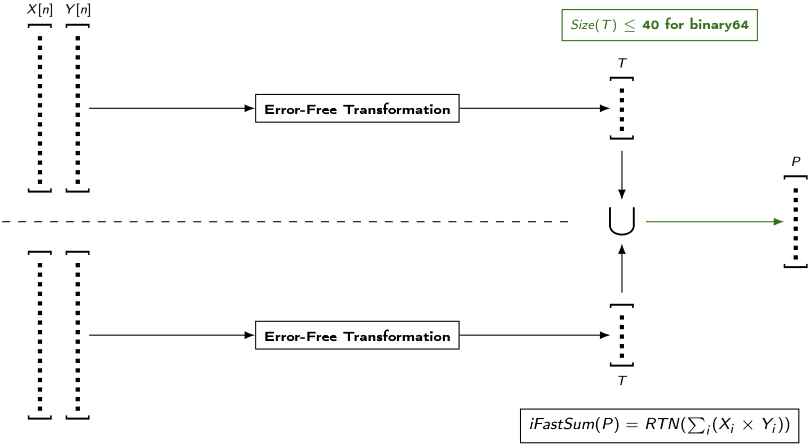

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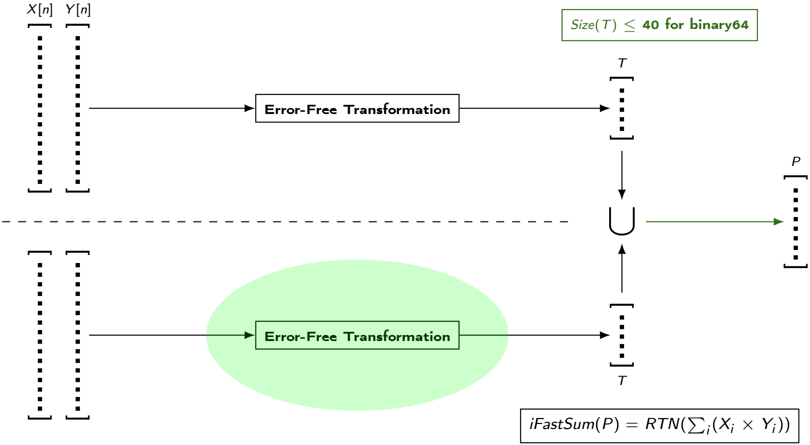

HybridSum (Zhu and Hayes, 2009) and OnlineExact (Zhu and Hayes, 2010)

About Algorithms

- Accumulate together the elements with the same exponent.
- Extra precision is simulated in two ways.
  - Split the input so the standard numbers are considered as accumulators.
  - Use quadruple precision.

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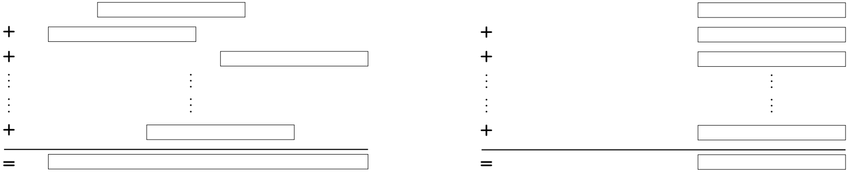

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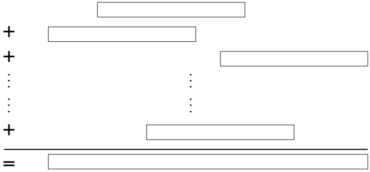
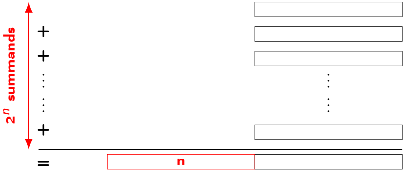
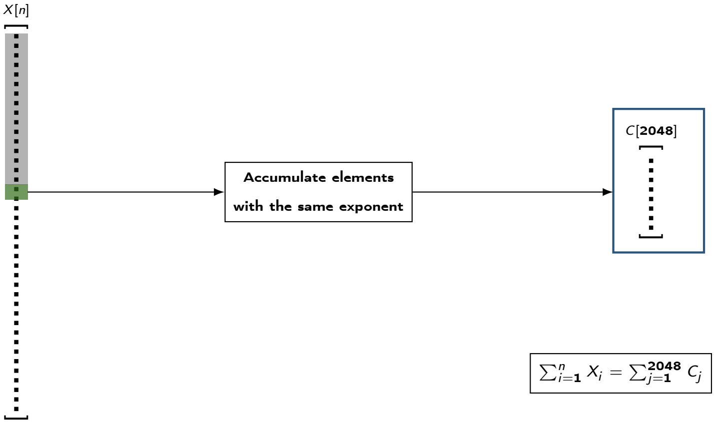


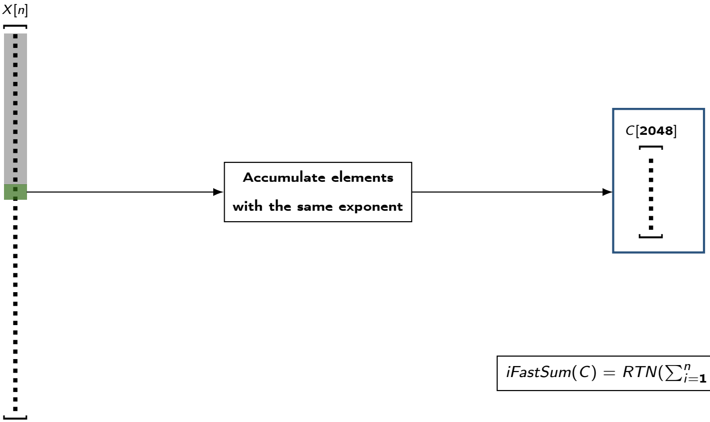


Algorithm OnlineExact (Zhu and Hayes, 2010)



$$\sum_{i=1}^{n} X_i = \sum_{j=1}^{2048} C_j$$

Algorithm OnlineExact (Zhu and Hayes, 2010)

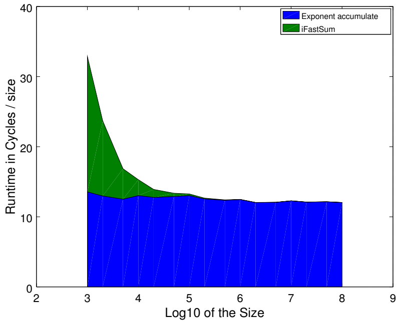


$$iFastSum(C) = RTN(\sum_{i=1}^{n} X_i)$$

Efficiency of the Algorithm OnlineExact

Implementation

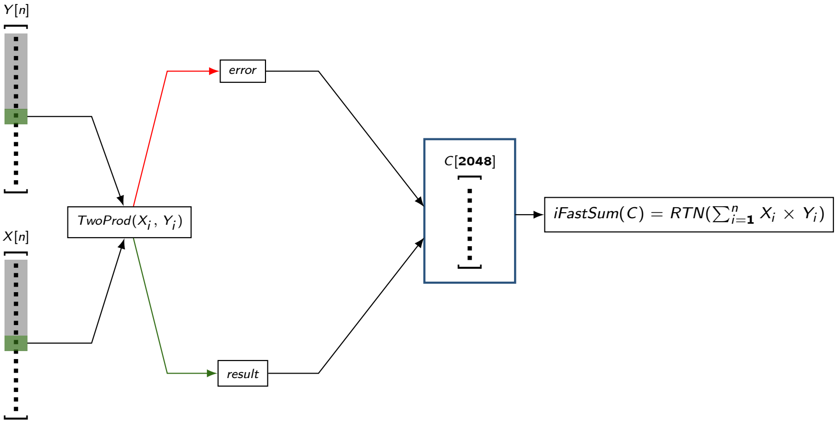
- Entry vector condition number $= 10^{16}$.



Note

- The transformation cost is linear to vector size.
- Post-transformation process cost is negligible for large vectors.
- It is better to use an iterative algorithm on small datasets.

Error-Free Transformation



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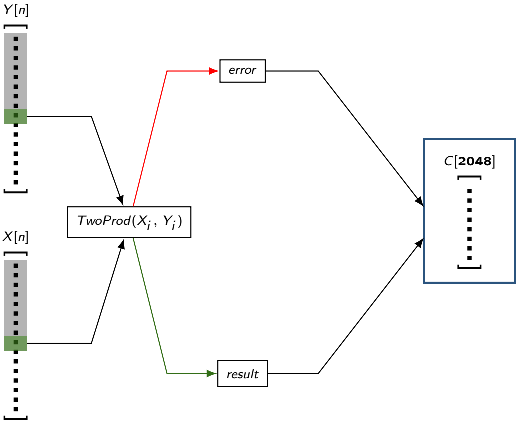

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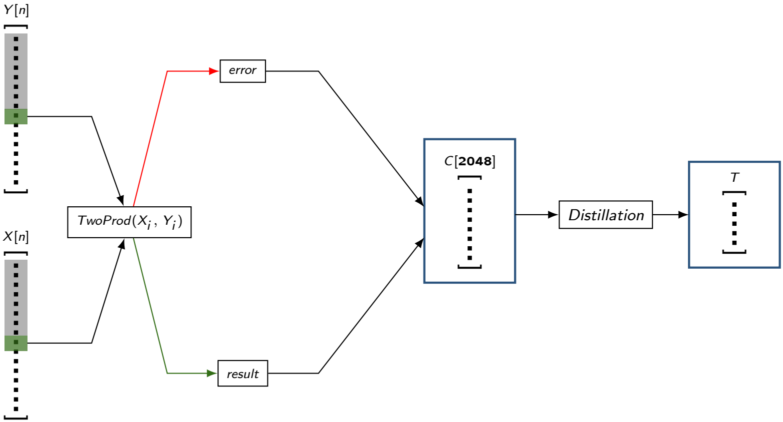


Euclidean Norm

How to Get a Reproducible Euclidean Norm

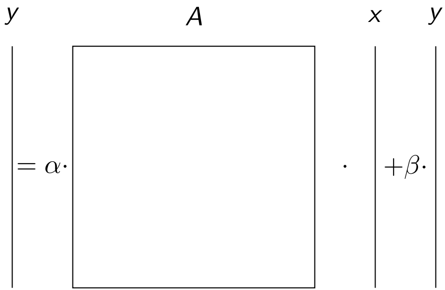
- Nrm2(X) $= \sqrt{\sum_{i=1}^{n} X_i^2}$.
- If $\sum_{i=1}^{n} X_i^2$ is correctly rounded, $\sqrt{\sum_{i=1}^{n} X_i^2}$ is faithfully rounded (Graillat and al., 2014).
- Dot(X,X) $= \sum_{i=1}^{n} X_i^2$ is correctly rounded.
- Nrm2(X) $= \sqrt{Dot(X, X)}$ is faithfully rounded and reproducible.

Sum of Absolute Values

How to Get a Faithfully Rounded Sum of Absolute Values

- The condition number is always 1.
- Error bounds depend only on size of vector.
- Algorithm SumK can be used.
- K is defined according to vector size.

Matrix Vector Multiplication



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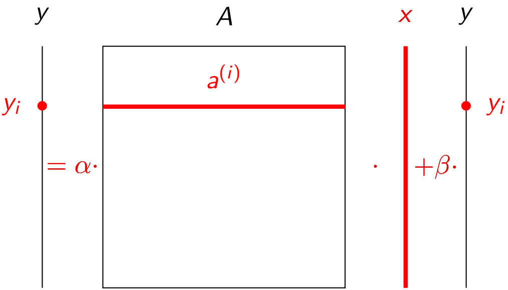

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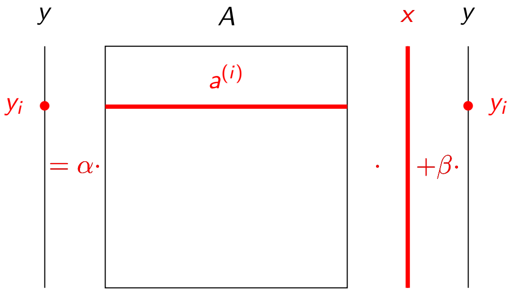
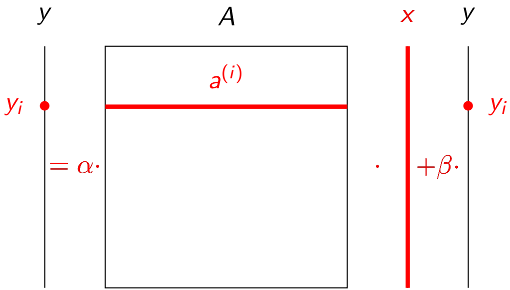


Algorithm Steps

- $y_i = \alpha \cdot (a^{(i)} \cdot x) + \beta \cdot y_i$
- $EFT(a^{(i)} \cdot x) = T \Rightarrow \sum_j (a_j^{(i)} \cdot x_j) = \sum_k T_k$
- $y_i = \alpha \cdot (\sum_k T_k) + \beta \cdot y_i$

Matrix Vector Multiplication



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- $y_i = \alpha \cdot (\sum_k T_k) + \beta \cdot y_i$
- $y_i = RTN(\sum_k (\alpha \cdot T_k) + \beta \cdot y_i)$

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Experimental Framework

Shared Memory

- dual Xeon E5-2650 v2 16 cores (8 per socket).

Distributed Memory

- OCCIGEN (26^{th} supercomputer in top500 list).
- 4212 Xeon E5-2690 v3 socket (12 cores per socket).

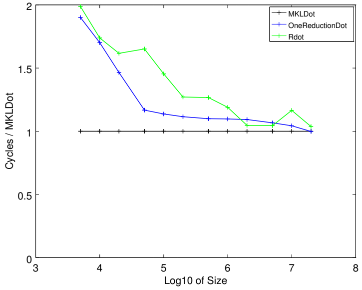
Accelerator

- Intel Xeon Phi 7120 accelerator, 60 cores.

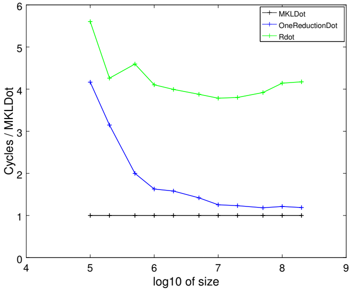
Results for Dot Product

Implementation

- Manually optimized version for all algorithms.
- Entry vectors condition number = 10^8.



Shared Memory Performance



Xeon Phi Performance

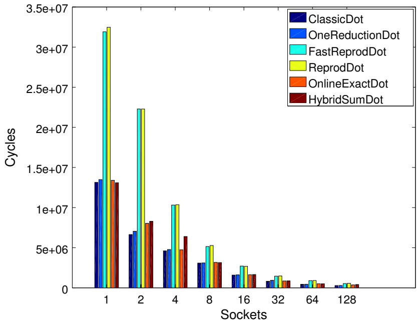
Results for Dot Product

Configurations

- #sockets = 1 .. 128.
- #threads = 12 per socket.

Dataset

- Entry vectors size = 10^7.
- Condition number = 10^{32}.



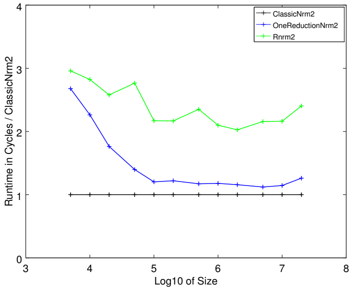
Note

- Good scaling for large datasets.
- Two communications cost limits ReprodDot and FastReprodDot.
- We need only one communication for OneReduction, HybridSum and OnlineExact.

Results for Euclidean Norm

Implementation

- Manually optimized version for all algorithms.



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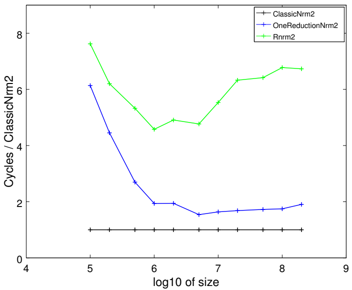

Xeon Phi Performance

Results for Sum of Absolute Values

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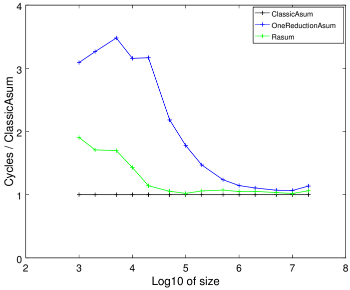
- Manually optimized version for all algorithms.



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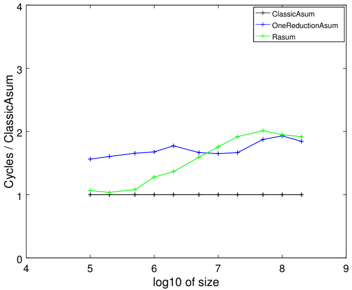

Xeon Phi Performance

Results for Matrix Vector Multiplication

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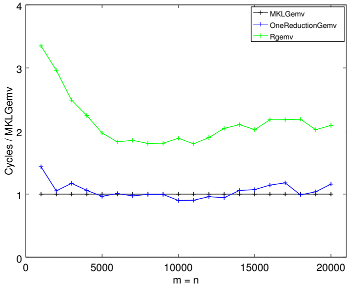

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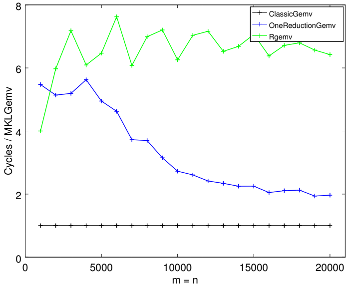
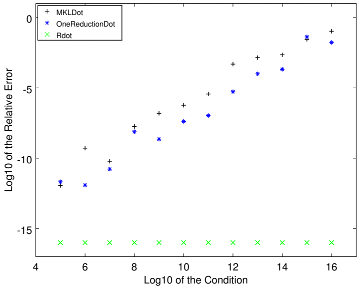
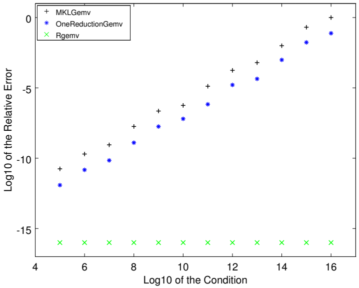


Xeon Phi Performance

Accuracy Results



Accuracy of Dot Product (size = 10^5)



Accuracy of Gemv (m = n = 1000)

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Conclusion

Guarantee the Numerical Reproducibility for BLAS (Basic Linear Algebra Subroutines)

- Level 1 : i_amax, _swap, _copy, _scal, _axpy, _nrm2, _asum, _dot.
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Reproducible Level 1 BLAS

- RTN cost for BLAS is acceptable on CPUs ($1\times - 2\times$).
- Xeon Phi performance are lower but still useful for debugging and validation ($2\times - 6\times$).
- Only one pass through the vector and one communication are required.
- Our solution do not depend on condition.

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Future Work

Work in Progress

- Reproducible Triangular Solver.

Future Work

- Level 2 BLAS : _ger.
- Level 3 BLAS : _gemm, _trsm.
- Matrix decompositions.

THANK YOU

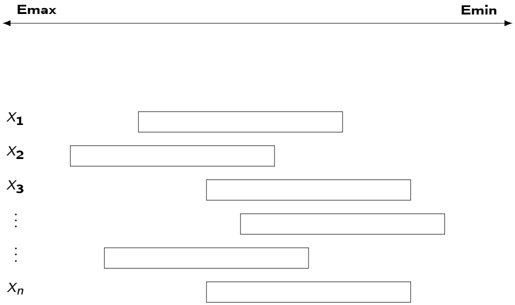
FOR

YOUR ATTENTION

ReprodSum and FastReprodSum (Demmel and Nguyen, 2013)

About Algorithms

- Inspired from AccSum (Rump and al, 2008) and FastAccSum (Rump and al, 2009).



Steps for Sequential

- Compute max.

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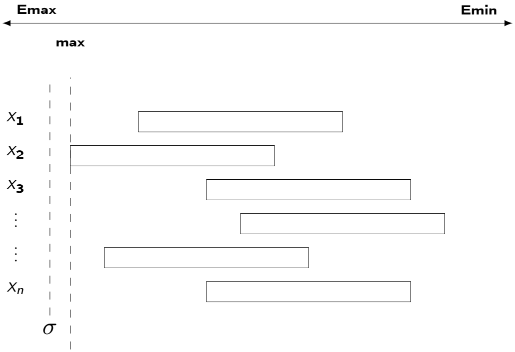

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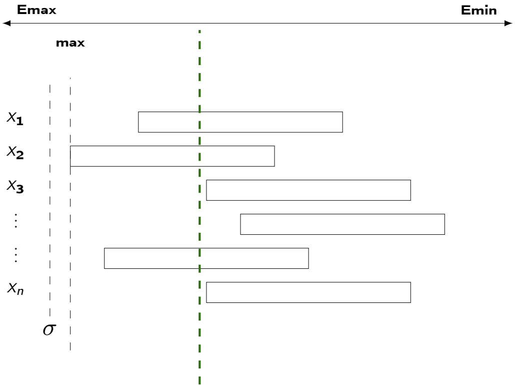

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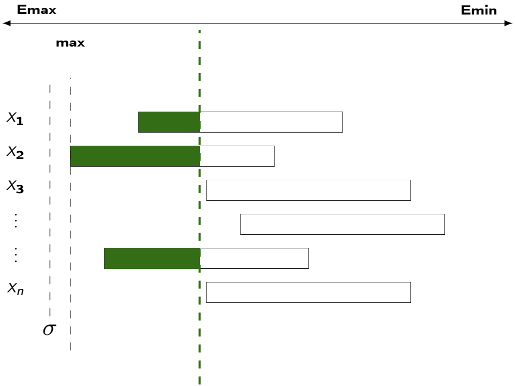

Steps for Sequential

- Compute max.
- Sum each fold.

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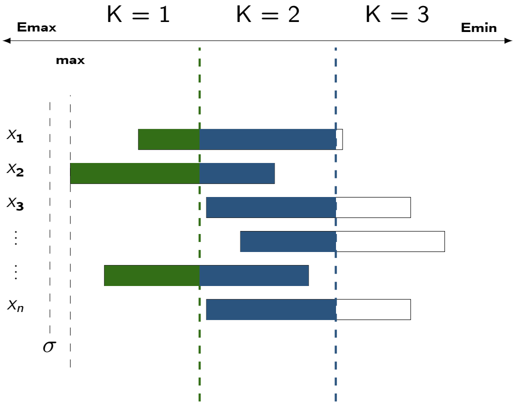

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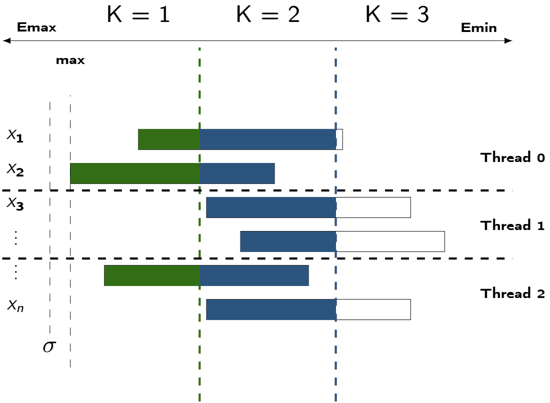


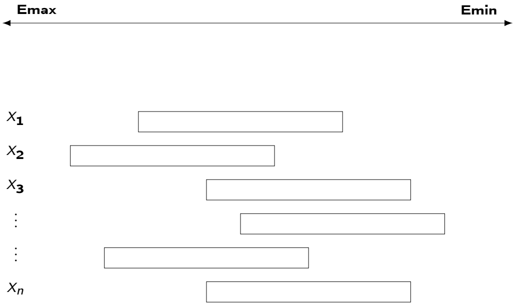
Steps for Sequential

- Compute max.
- Sum each fold.

Steps for Parallel

- Max (Compute).
- Max (Reduce).
- Sum (Compute).
- Sum (Reduce).

OneReduction (Demmel and Nguyen, 2013)



Steps for Parallel

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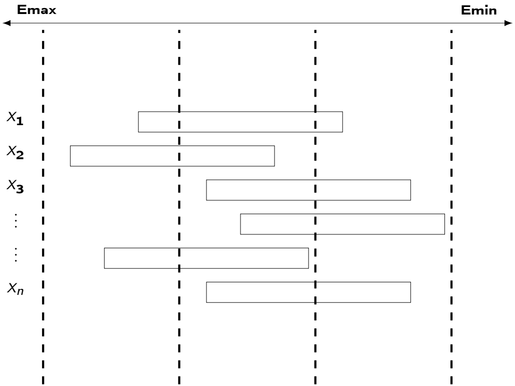

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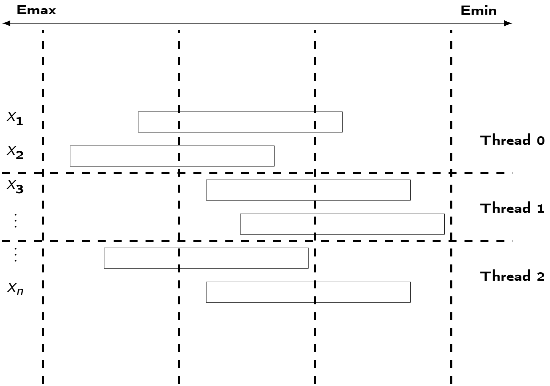

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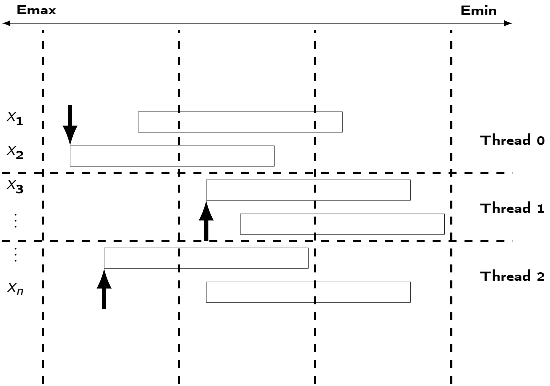
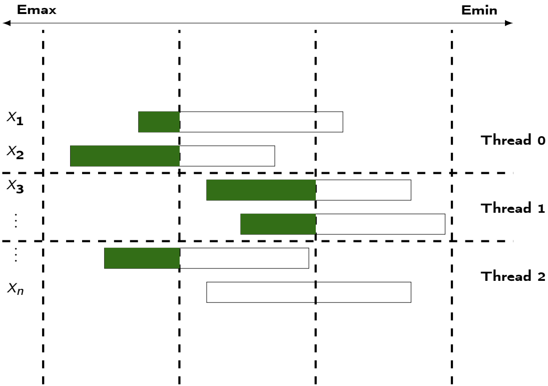


Steps for Parallel

- Max (Compute).

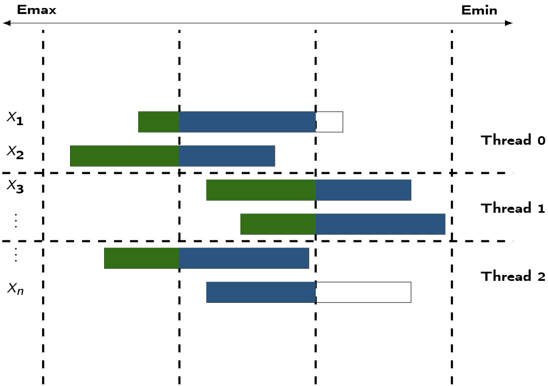
OneReduction (Demmel and Nguyen, 2013)



Steps for Parallel

- Max (Compute).
- Sum (Compute).

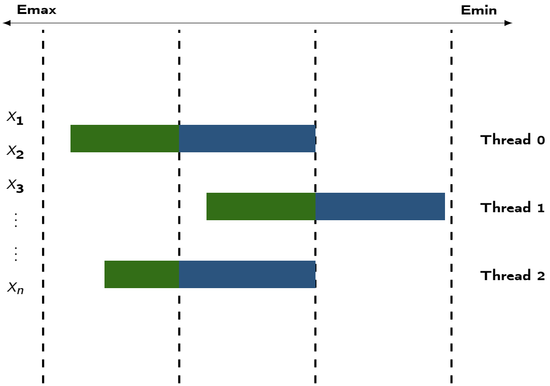
OneReduction (Demmel and Nguyen, 2013)



Steps for Parallel

- Max (Compute).
- Sum (Compute).

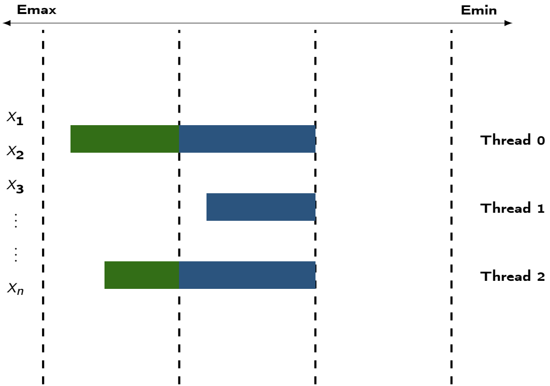
OneReduction (Demmel and Nguyen, 2013)



Steps for Parallel

- Max (Compute).
- Sum (Compute).

OneReduction (Demmel and Nguyen, 2013)



Steps for Parallel

- Max (Compute).
- Sum (Compute).
- Sum (Reduce).

OneReduction (Demmel and Nguyen, 2013)

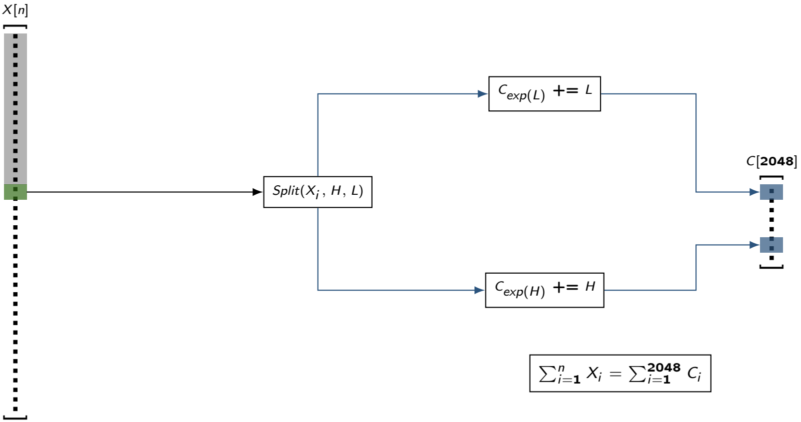
Pros

- Always reproducible result.
- Easy to enhance precision.
- Single communication.

Cons

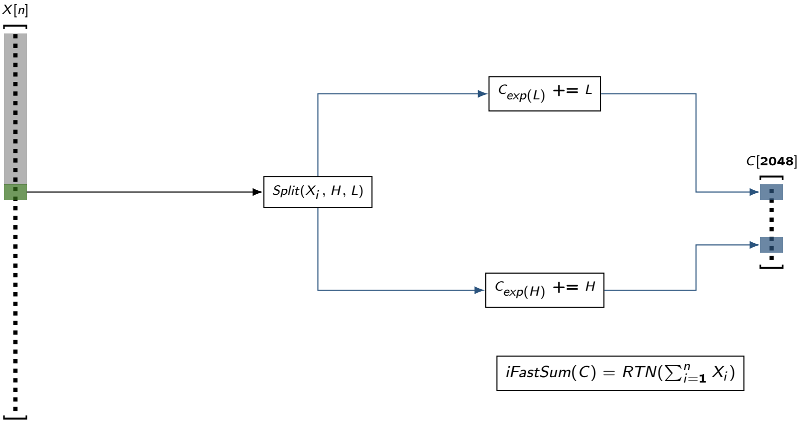
- Accuracy problem on ill-conditioned sums.

Algorithm HybridSum (Zhu and Hayes, 2009)

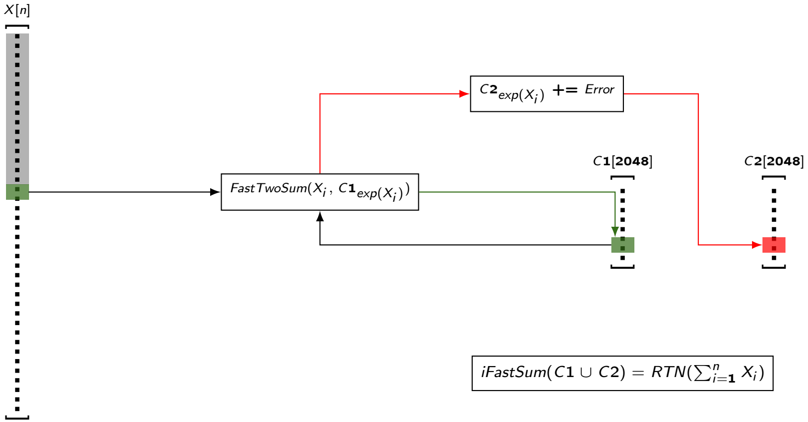


$$\sum_{i=1}^{n} X_i = \sum_{i=1}^{2048} C_i$$

Algorithm HybridSum (Zhu and Hayes, 2009)



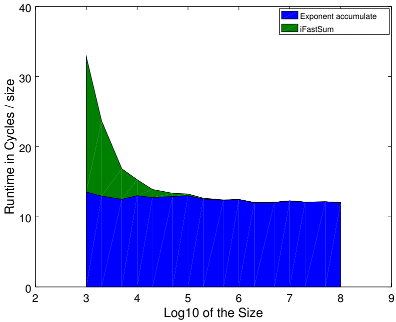
Algorithm OnlineExact (Zhu and Hayes, 2010)



Efficiency of the Algorithm OnlineExact

Implementation

- Entry vector condition number $= 10^{16}$.



Note

- The transformation cost is linear to vector size.
- Post-transformation process cost is negligible for large vectors.
- It is better to use an iterative algorithm on small datasets.