Reproducible level 1 BLAS on massively parallel systems

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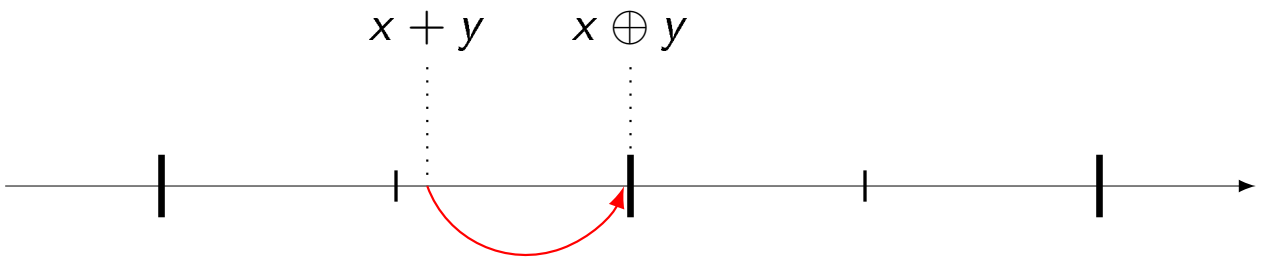
Introduction and problematic

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

- $A \oplus (B \oplus C) \neq (A \oplus B) \oplus C$.
- Catastrophic cancelation : $M = 2^{53}$; $0 = -M \oplus (M \oplus 1) \neq (-M \oplus M) \oplus 1 = 1$.

Non-reproducibility of summation

- For a sum $(\sum_{i=1}^{n} X_i)$, the final result depends on the order of the computations.
- Why should operations order be different.
  - Different micro-architectures (different instruction sets).
  - Different compilers (or even versions of compilers).
  - Data alignment.
  - Dynamic scheduling.
  - Non-deterministic reduction.

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"

How to fix the numerical reproducibility problem ?

Parallel libraries solutions

- Static scheduling.
- Deterministic reduction.
  - Available on OpenMP and TBB.
  - Recommended in MPI 3.0 standard.
- MKL (Conditional Numerical Reproducibility).

Algorithmic solutions

- Deterministic error (Demmel and Nguyen, 2013).
  - ReprodSum.
  - FastReprodSum.
  - OneReduction.
- Enhanced precision.
  - Higher precision (quadruple precision for instance).
    - Improve accuracy and consistency (Villa and al., 2009).
    - Reproducibility is not always guaranteed.
  - Correctly rounded arithmetic.
    - FP expansions + Super accumulators (S. Collange and al., 2014).

Our aim

Guarantee the numerical reproducibility for BLAS (Basic Linear Algebra Subroutines)

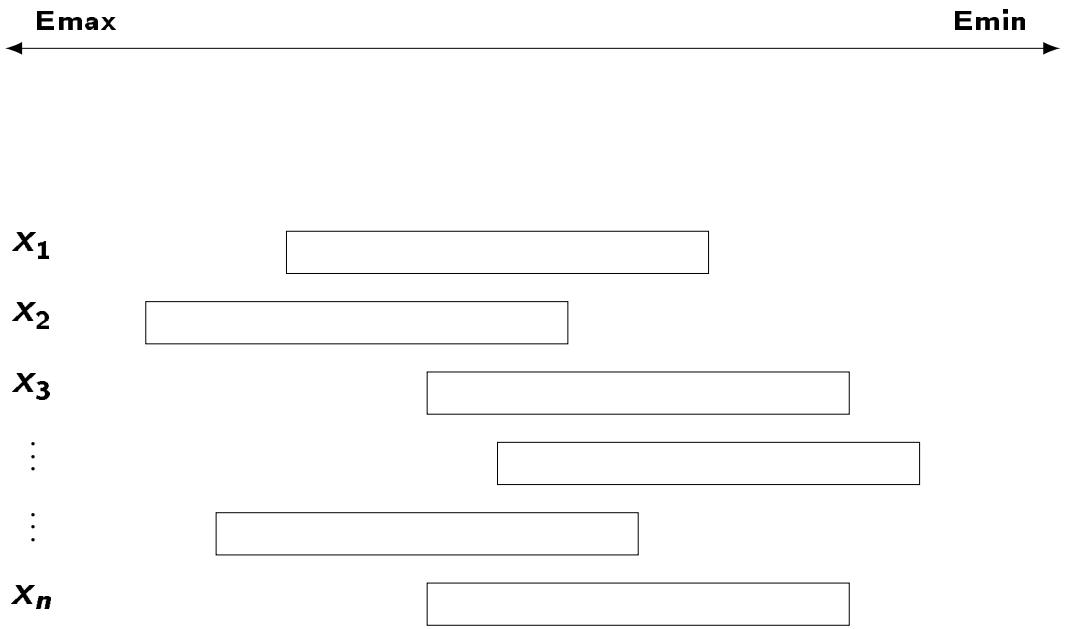
- Level 1 : max, min, scal, axpy, norm, asum, dot.
- dot can be transformed to a sum $\sum_{i=1}^{n} X_i \cdot Y_i = \sum_{i=1}^{2n} Z_i$.

Compute an accurate sum

- Several algorithms available.
- Is the cost acceptable ?

Table of contents

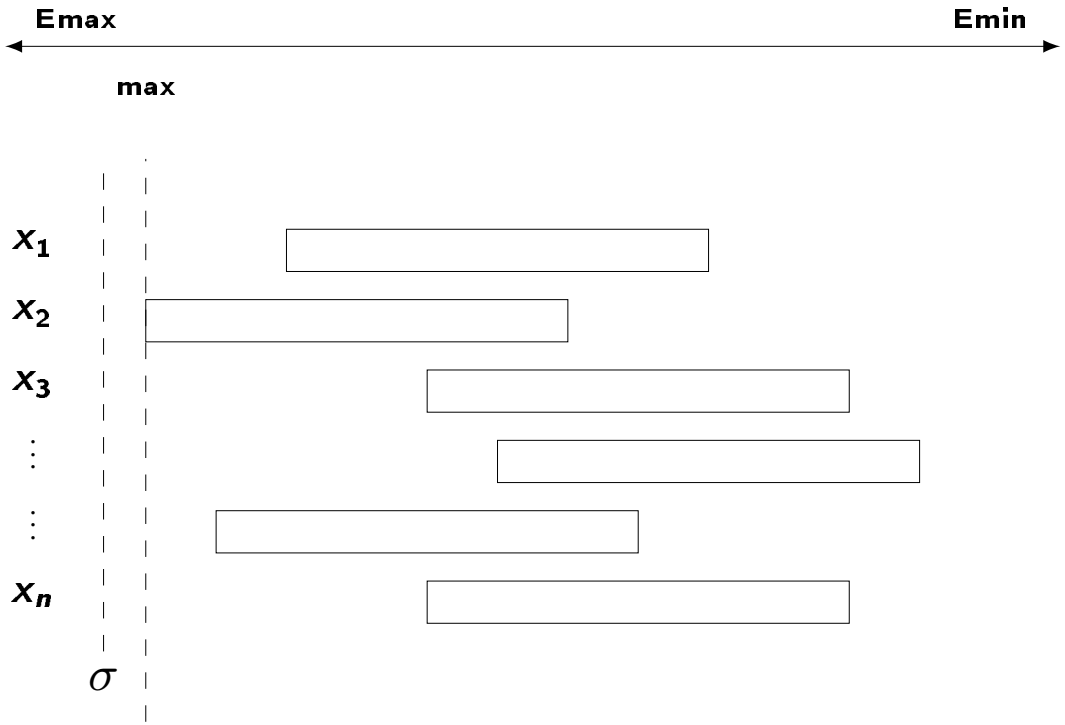
ReprodSum and FastReprodSum (Demmel and Nguyen, 2013)



Steps for sequential

- Compute max.

ReprodSum and FastReprodSum (Demmel and Nguyen, 2013)



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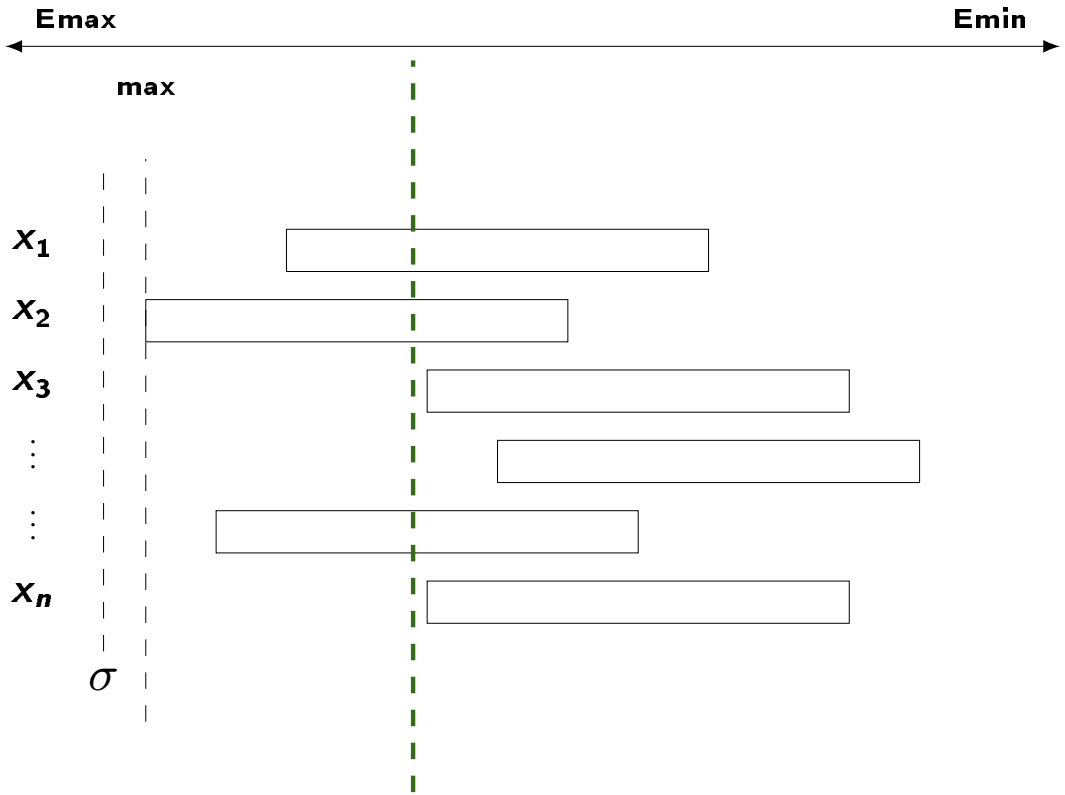

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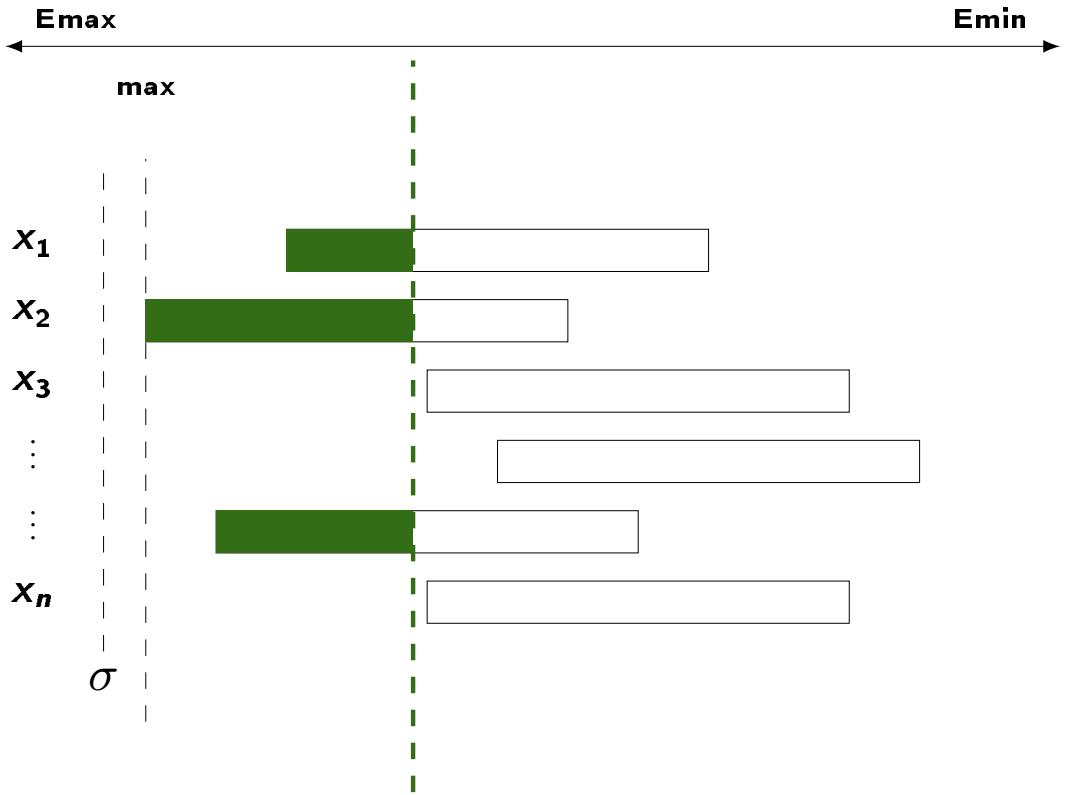
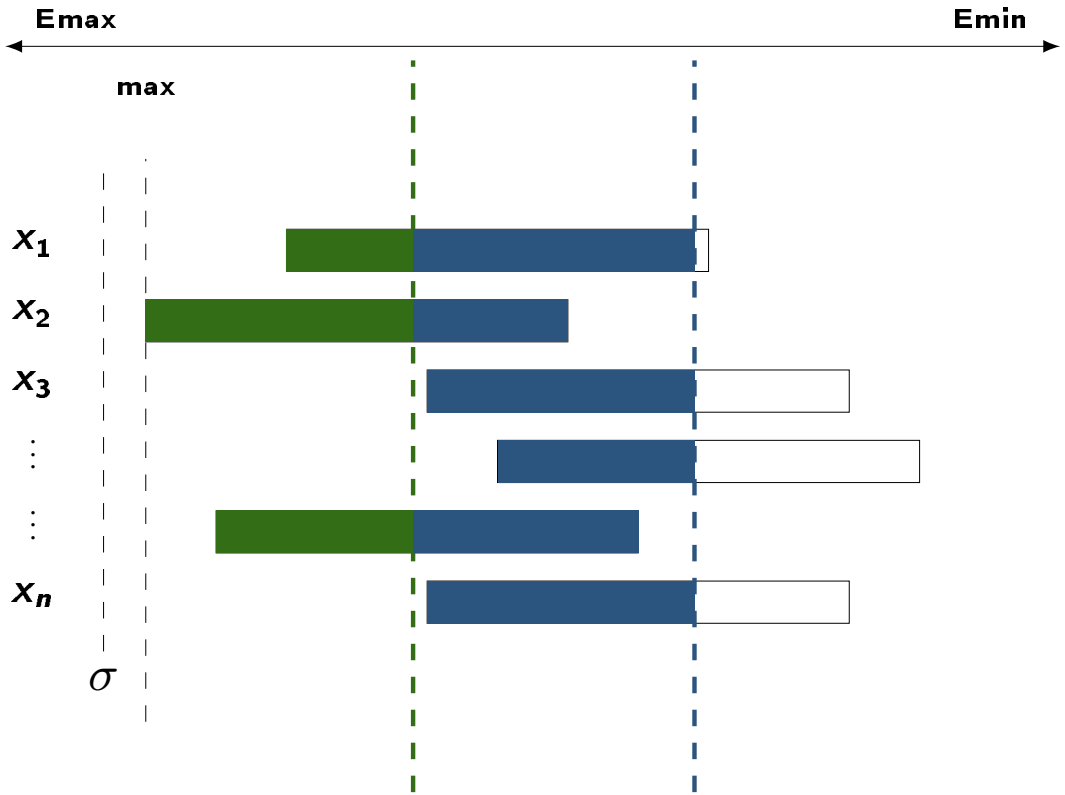


Steps for sequential

- Compute max.
- Sum each fold.

ReprodSum and FastReprodSum (Demmel and Nguyen, 2013)



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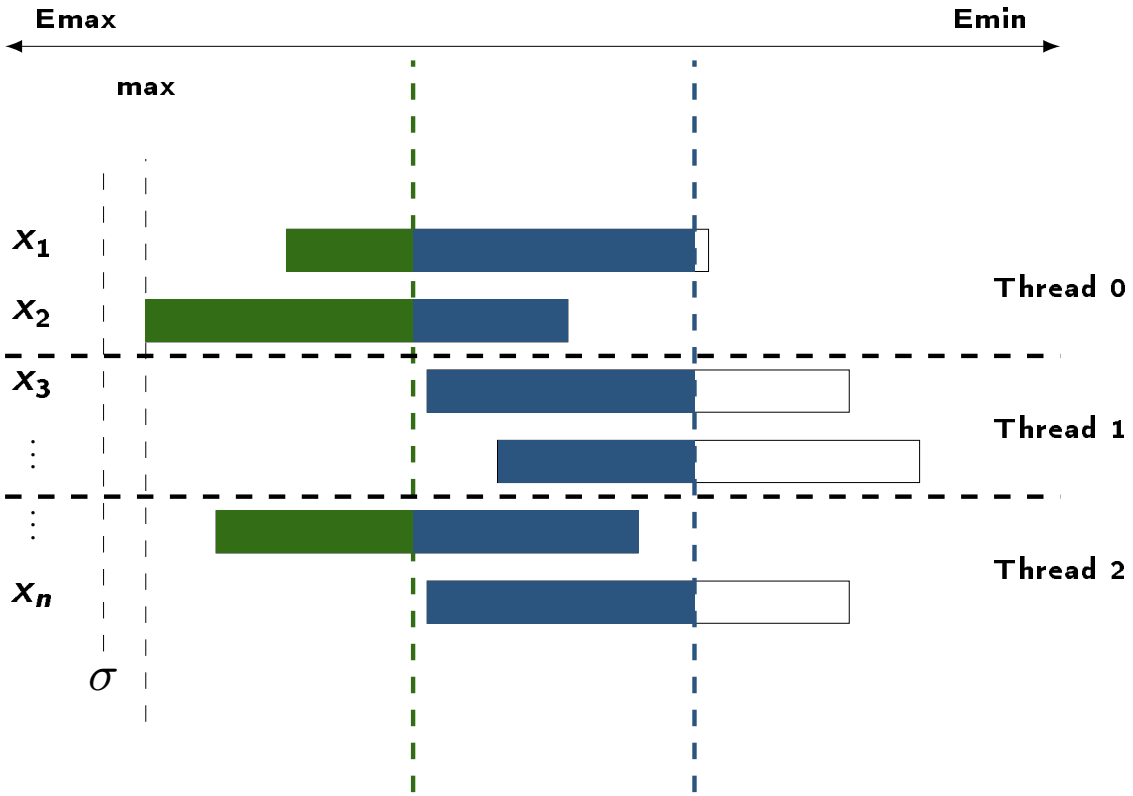


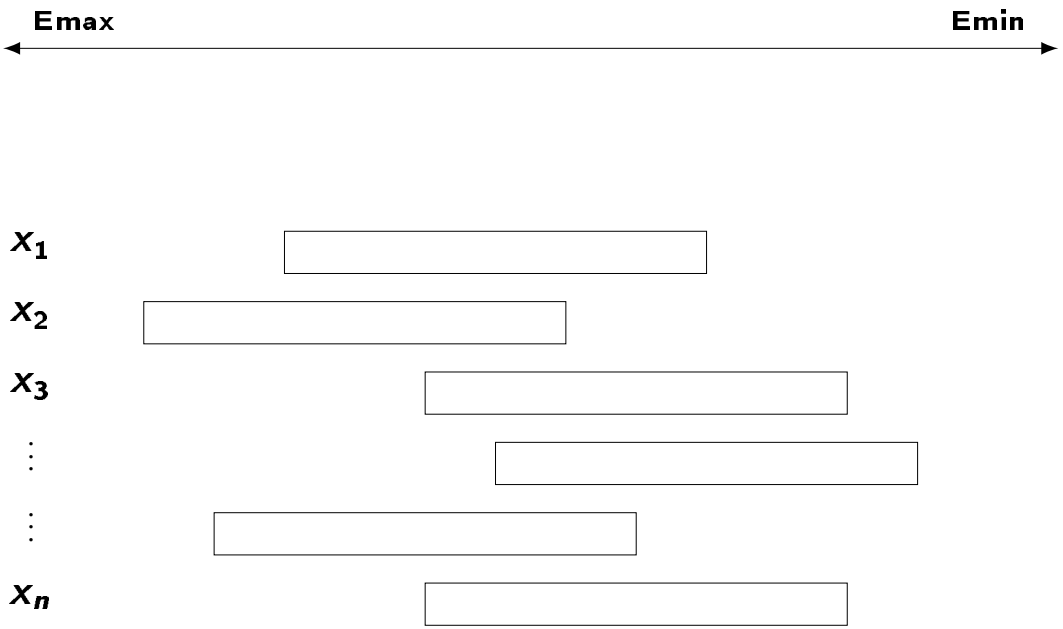
Steps for sequential

- 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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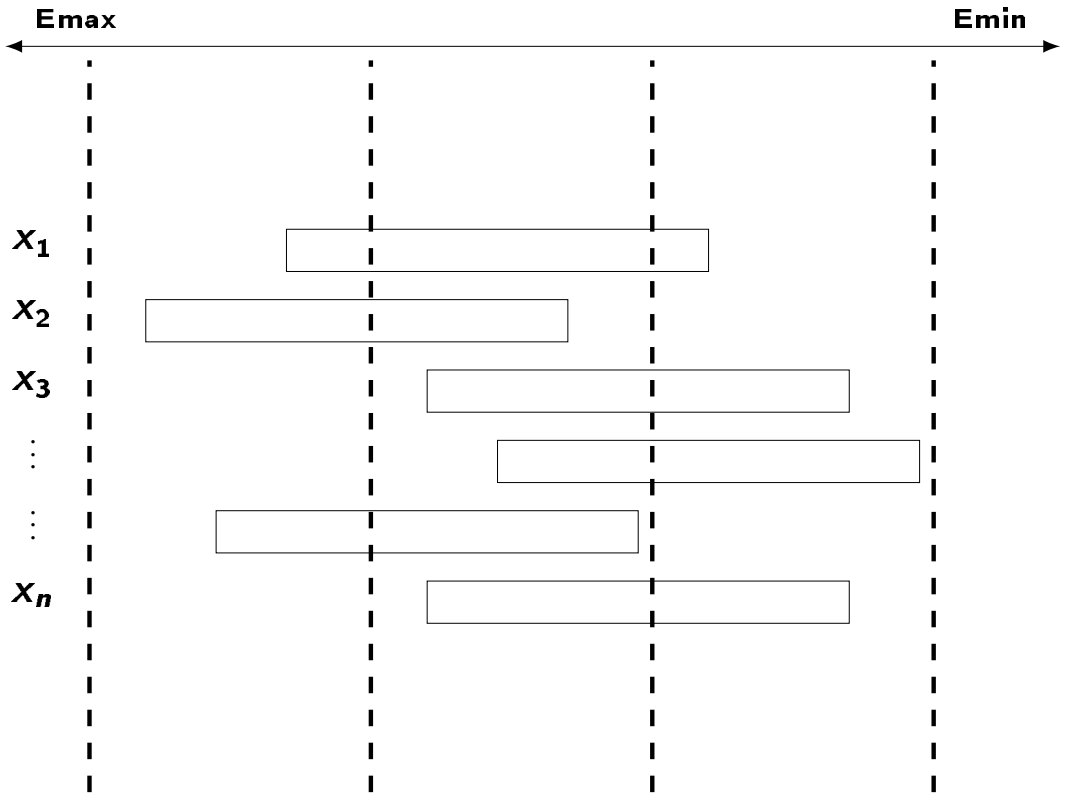

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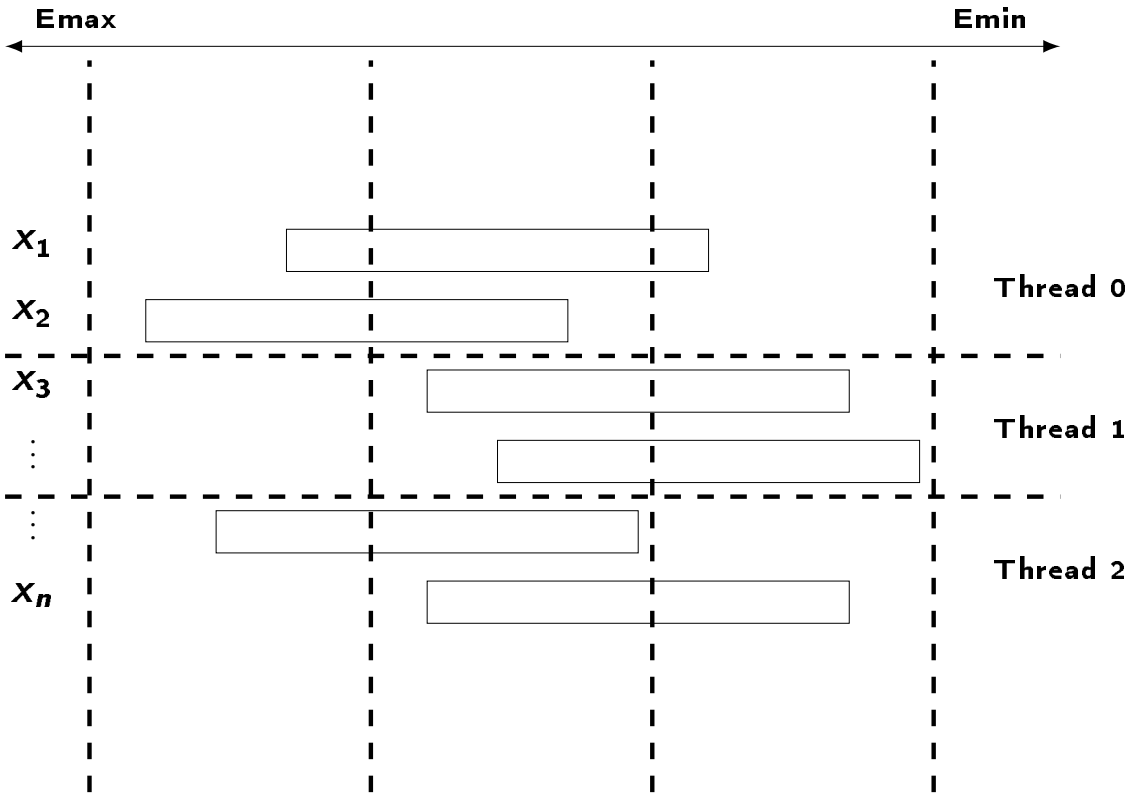

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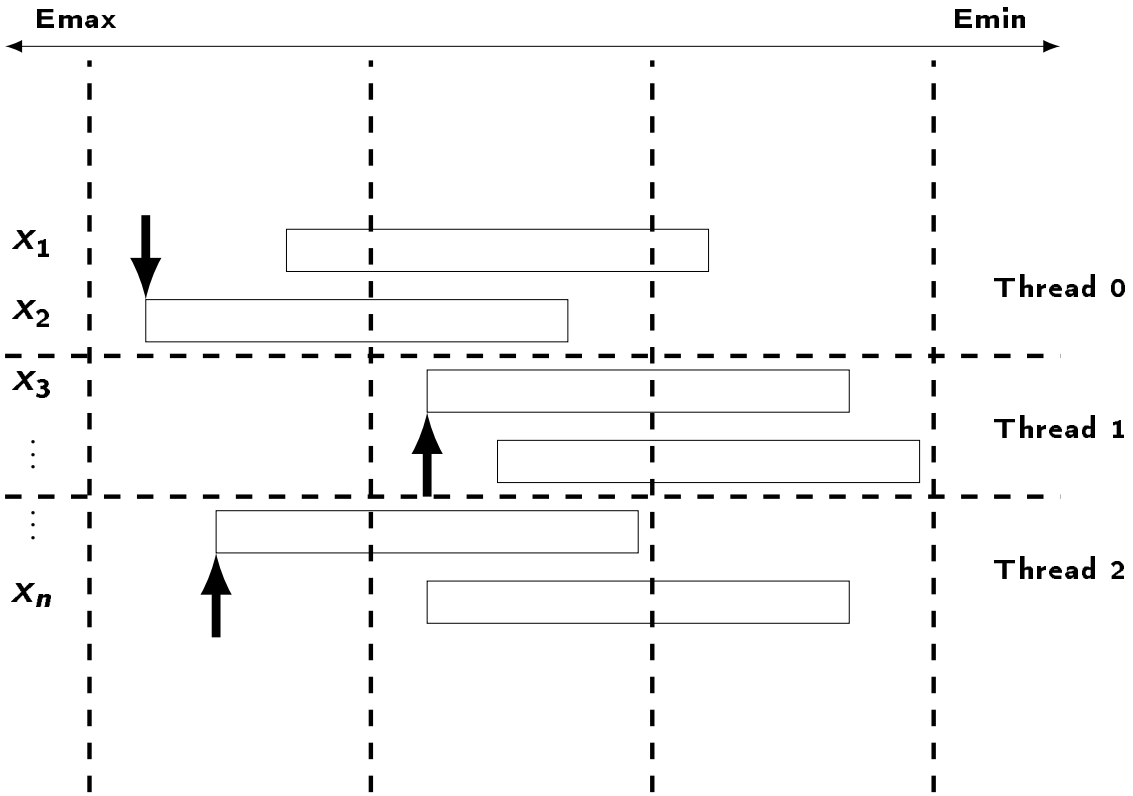

Steps for parallel

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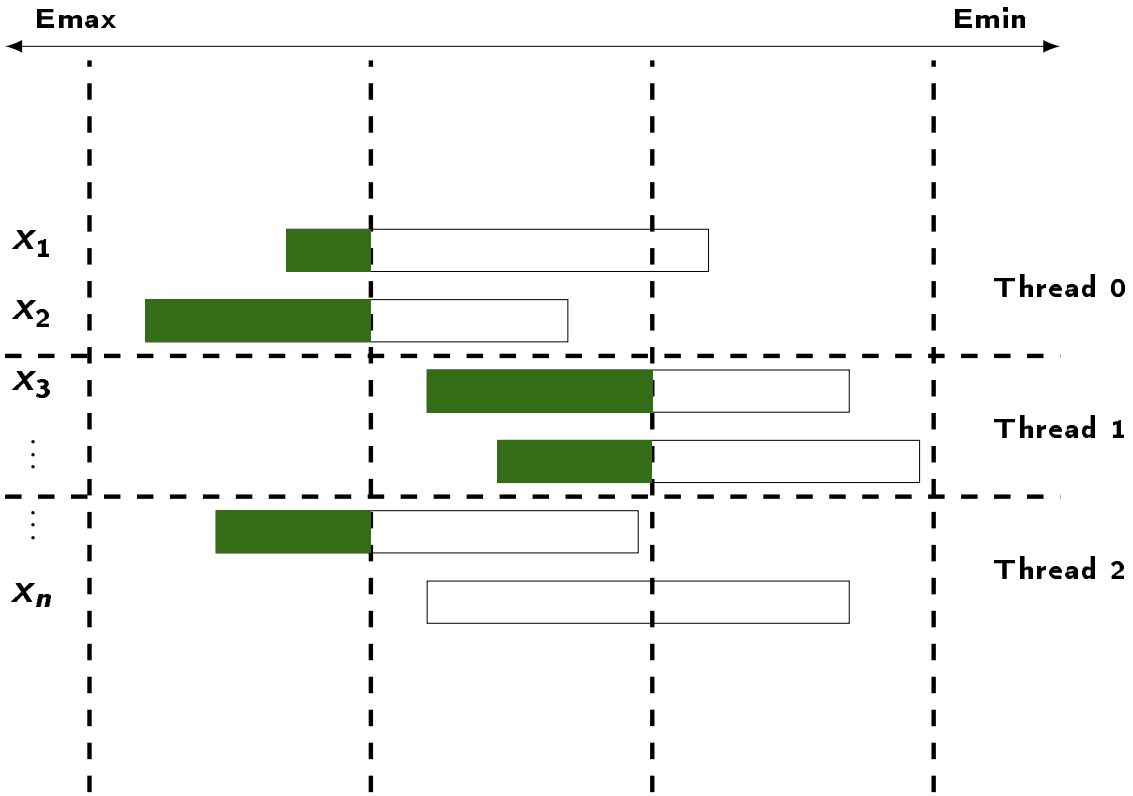

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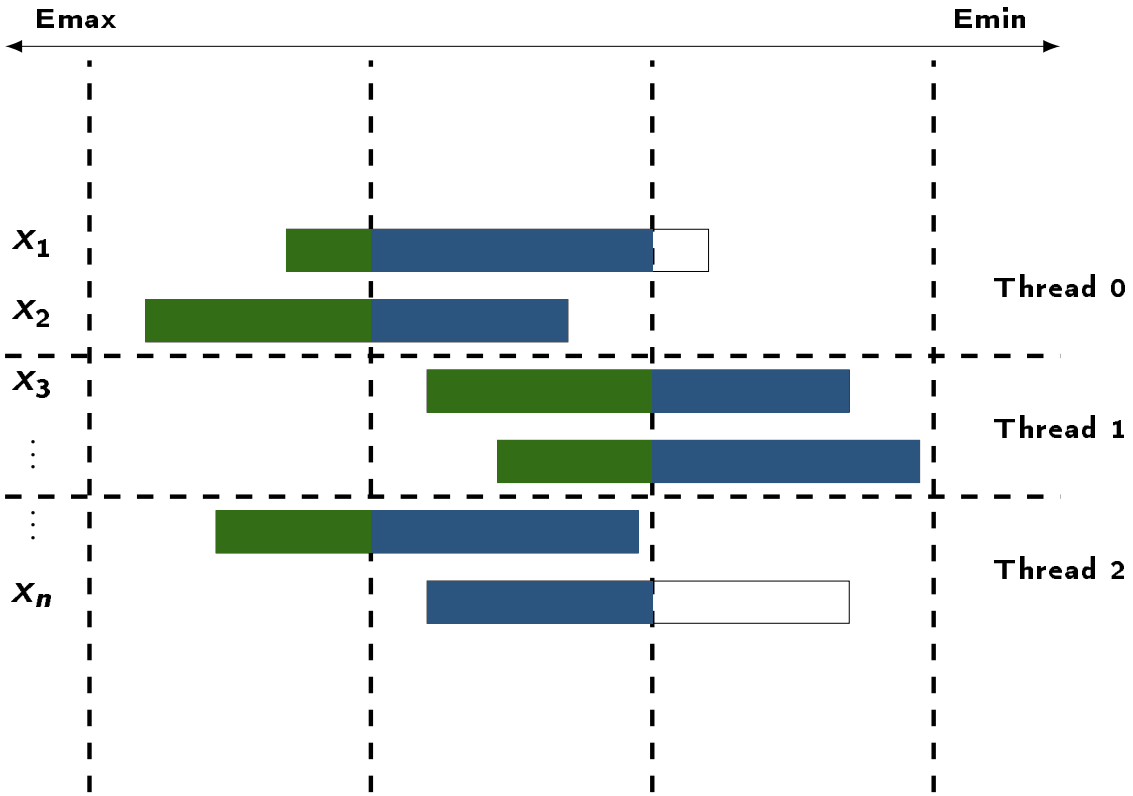

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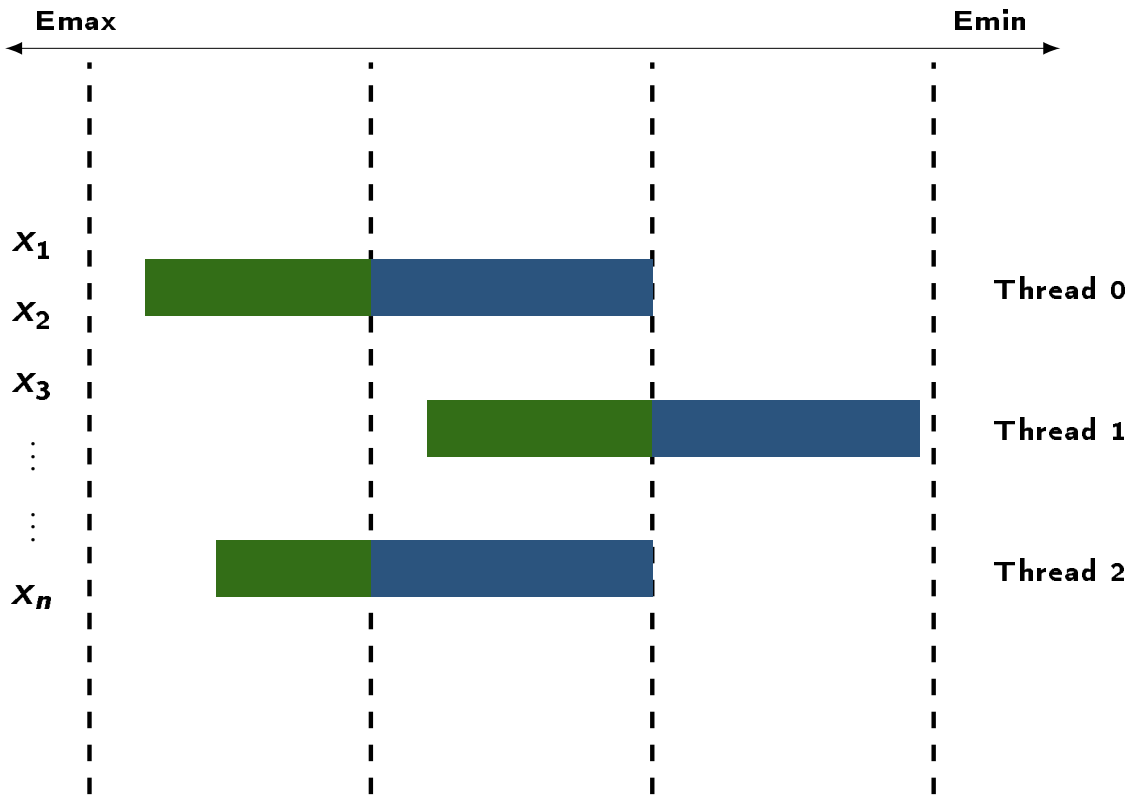
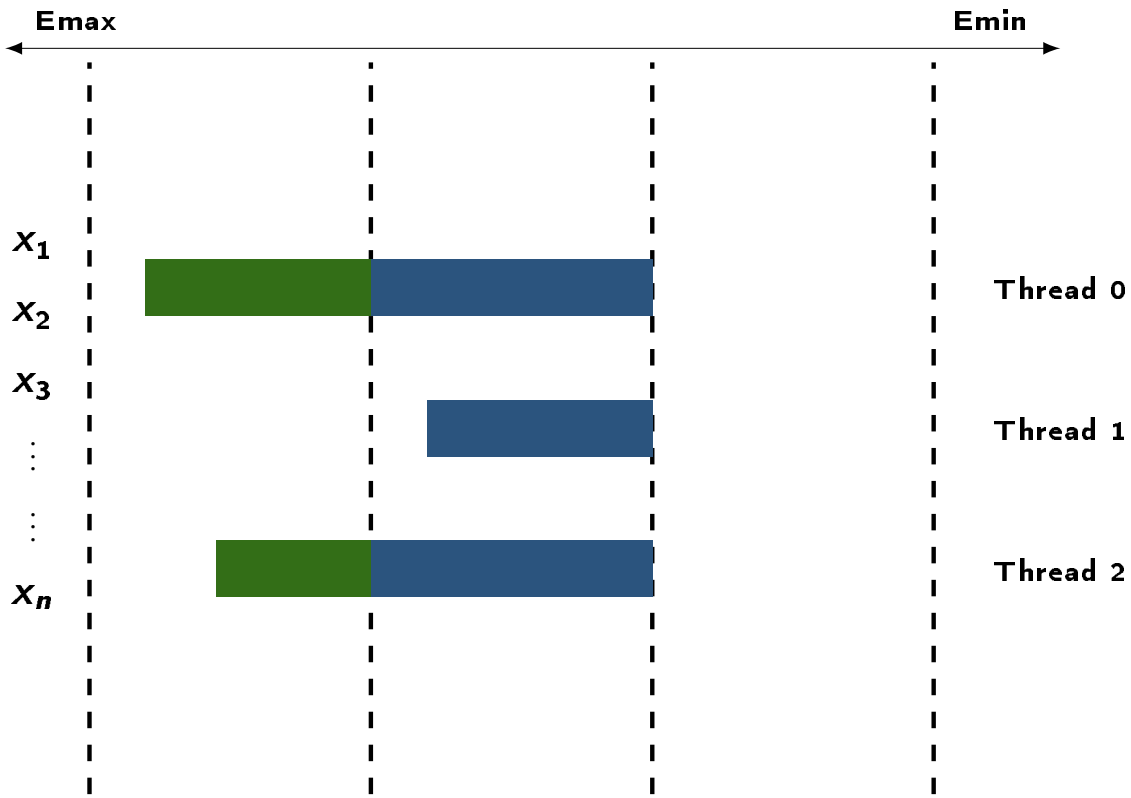


Steps for parallel

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

OneReduction (Demmel and Nguyen, 2013)



Steps for parallel

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

Table of contents

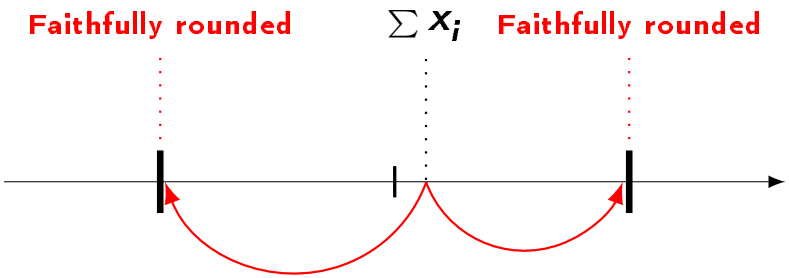
Precise summation algorithms

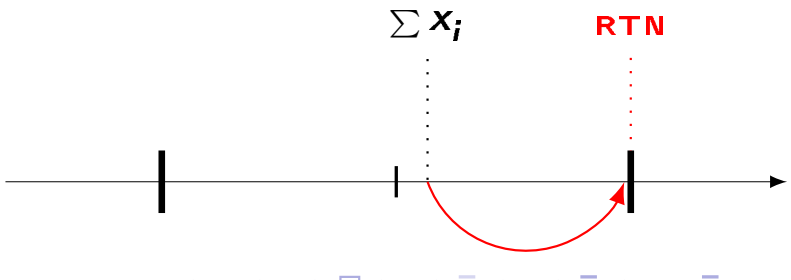
Faithfully rounded (one of the floating-point neighbors)

- FastSum (Zhu and Hayes, 2005).
- AccSum (Rump and al., 2008).
- FastAccSum (Rump, 2008).

Correctly rounded (according to the rounding mode)

- NearSum (Rump and al., 2008).
- iFastSum (Zhu and Hayes, 2009).
- HybridSum (Zhu and Hayes, 2009).
- OnlineExact (Zhu and Hayes, 2010).





Experimental framework

Implementation

- Implemented using C language.

Compiler

- Intel ICC 14.0.2.
- Options : -O3 -xHost -fp-model double -fp-model strict -funroll-all-loops.

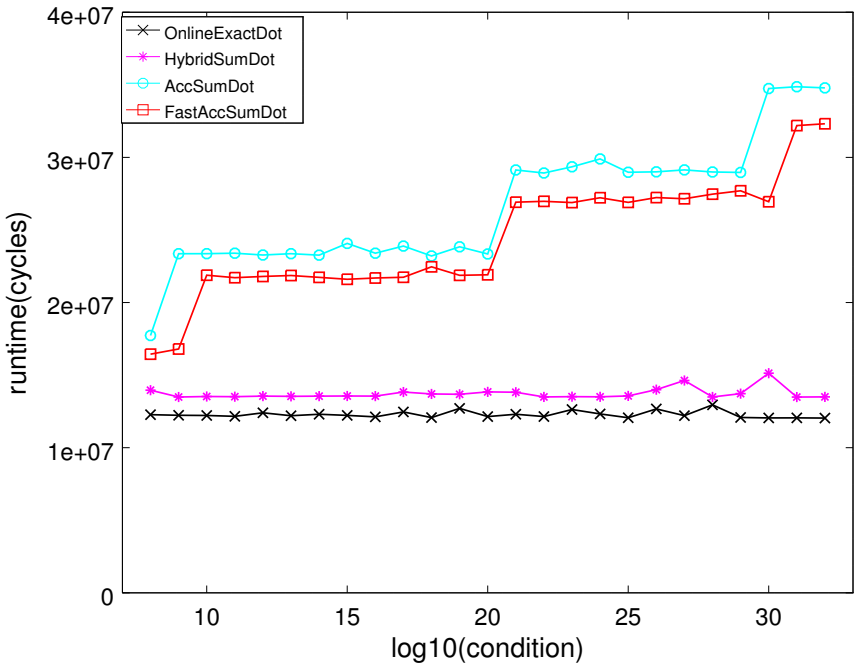
Hardware

- i7-3540M at 3 GHz.
- Turbo boost turned off.

HybridSum and OnlineExact do not depend on the condition number

Implementation

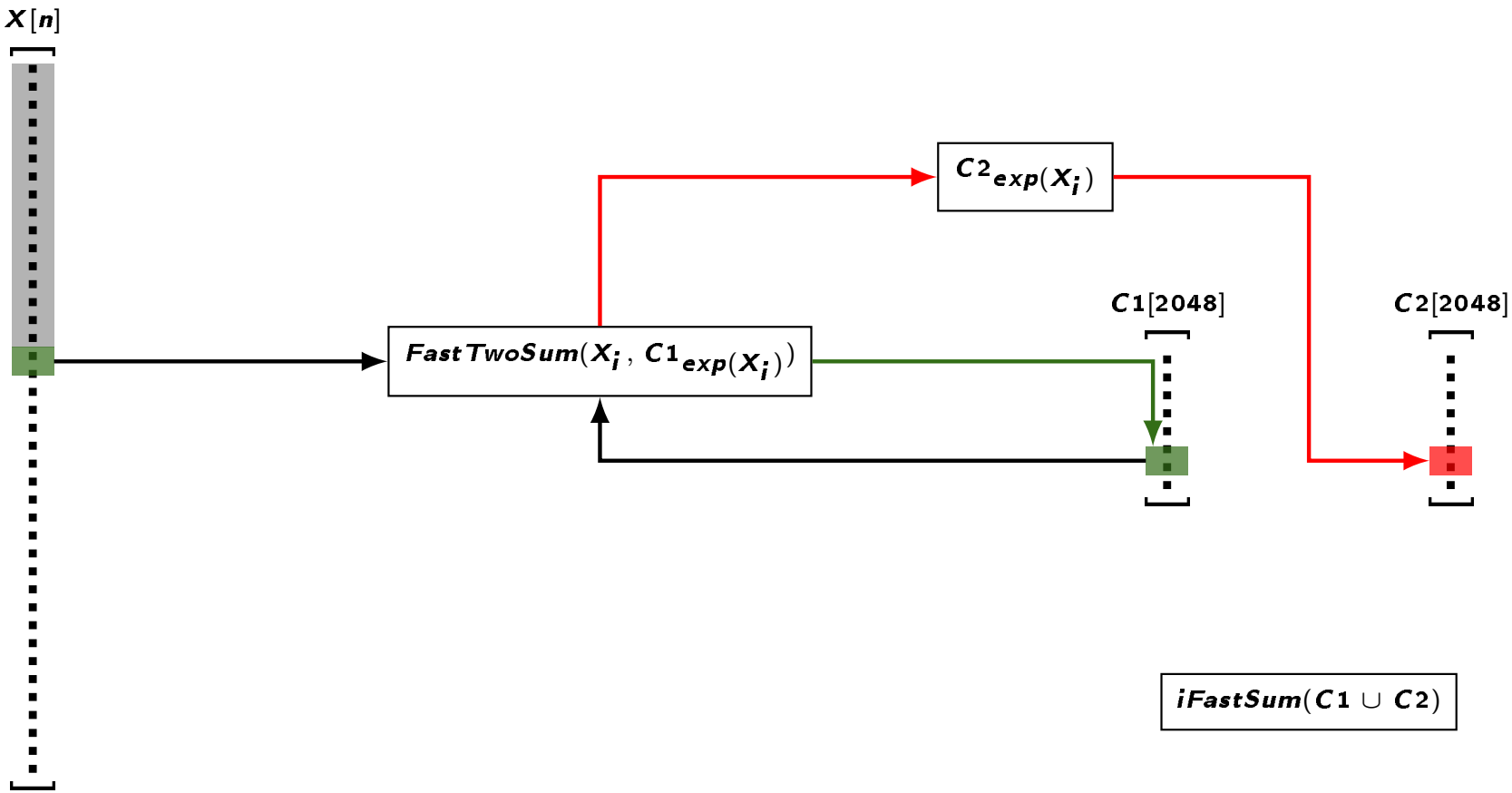
- Manually optimized version for all algorithms.
- Entry vectors size = 10^6.



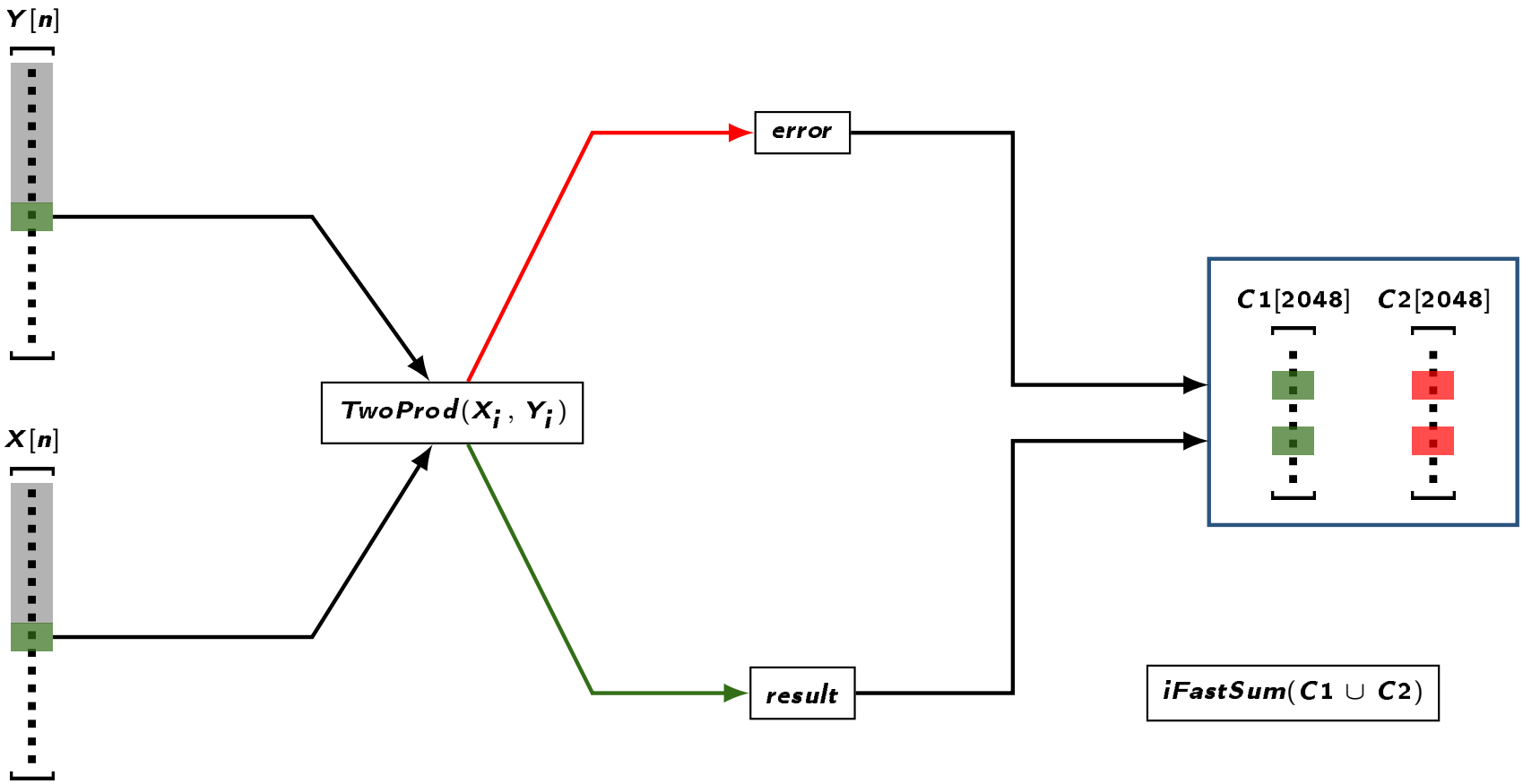
Note

- HS and OLE : condition number independents.

Algorithm OnlineExact (Zhu and Hayes, 2010)



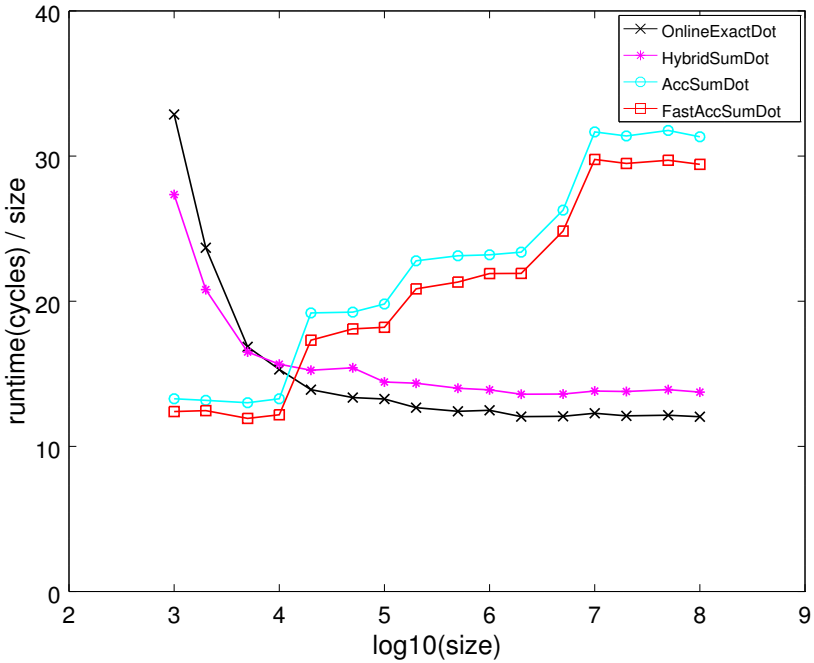
Dot with OnlineExact (Zhu and Hayes, 2010)



HybridSum and OnlineExact are not efficient for small vectors

Implementation

- Manually optimized version for all algorithms.
- Entry vectors condition = 10^{16}.

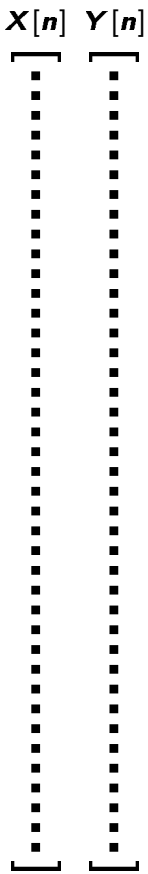


Note

- HS and OLE : more efficient for large vectors.
- Mixed solution is possible.

Table of contents

Parallel OnlineExact (2 processors case)



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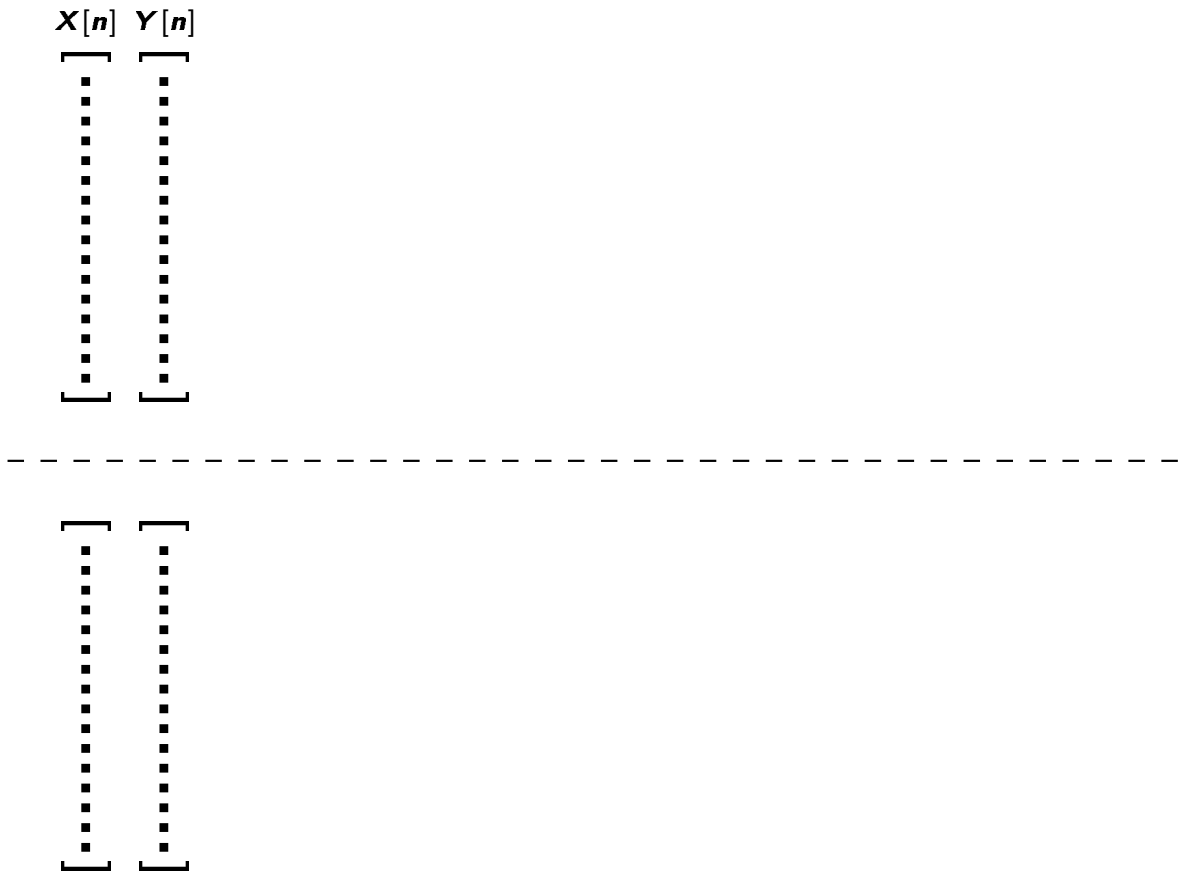

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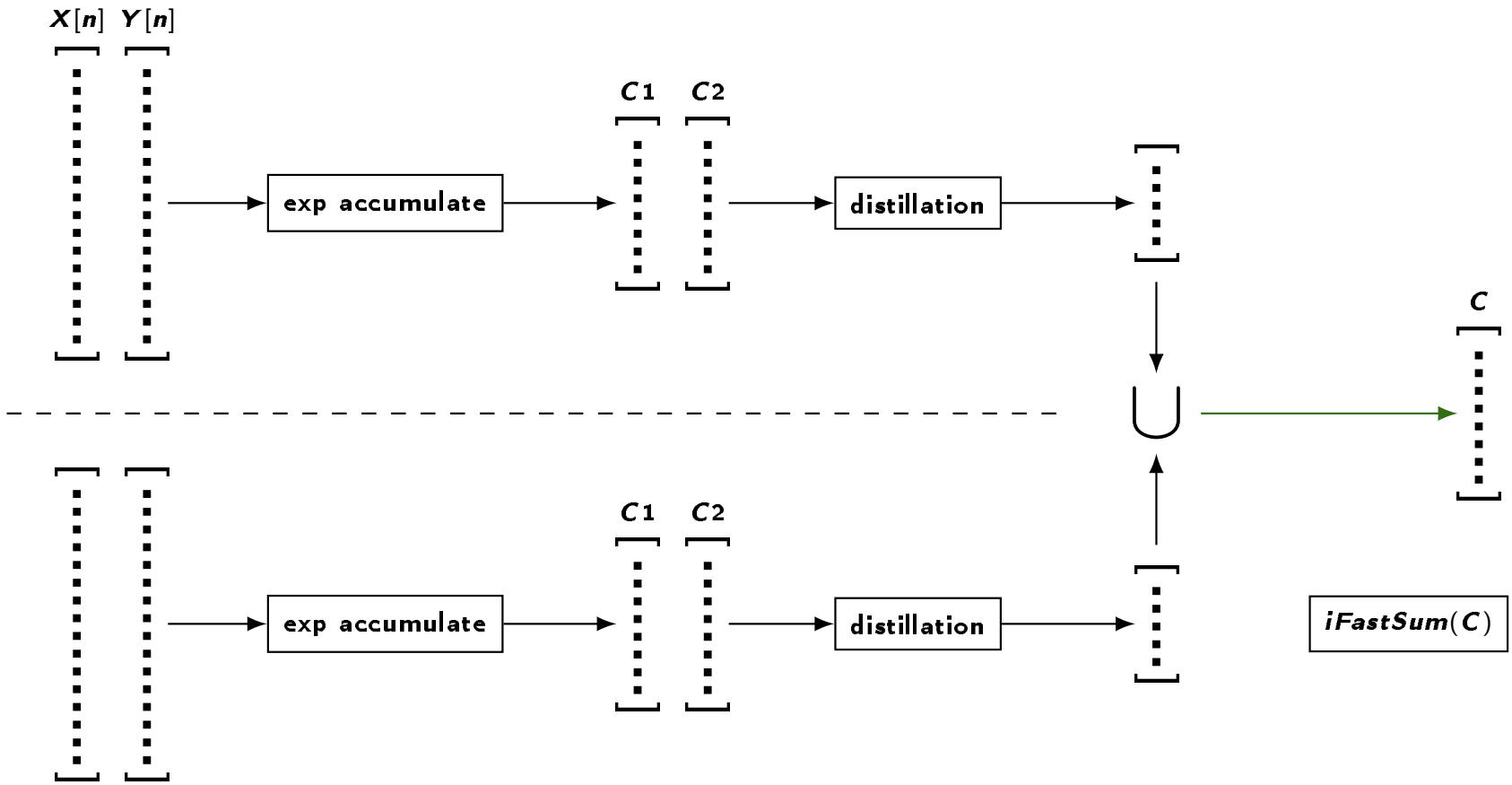


Experimental framework

Hardware

- OCCIGEN (26^{th} supercomputer in top500 list).
- 4212 Xeon E5-2690 v3 socket (L3 cache = 30 M).
- 12 cores on each socket.

Software

- Intel ICC 15.0.0.
- OpenMP 4.0 (Intra socket parallelism).
- OpenMPI (Inter socket communications).

Algorithms

- Classic dot (MKL implementation + MPI reduction).
- Reproducible dot (ReprodDot, FastReprodDot, OneReduction).
- Correctly rounded dot (Parallel version of OnlineExact and HybridSum).

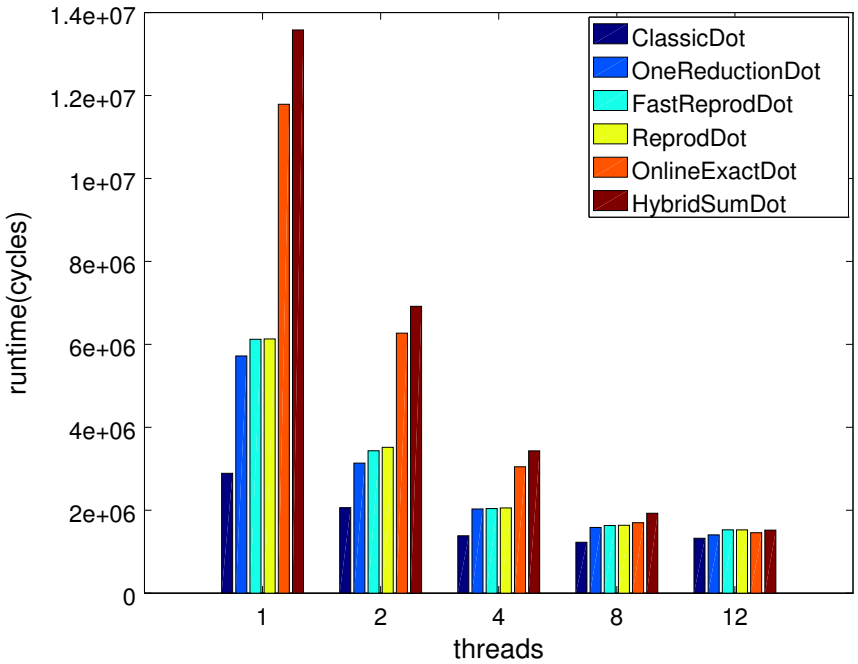
Single socket results

configurations

- #sockets = 1.
- #threads = 1 .. 12 on single socket.

dataset

- Entry vectors size = 10^6.
- Condition number = 10^{32}.



Note

- Classic dot is memory bounded.
- Data hold in level 3 cache.
- ReprodDot and FastReprodDot avoid second memory access.

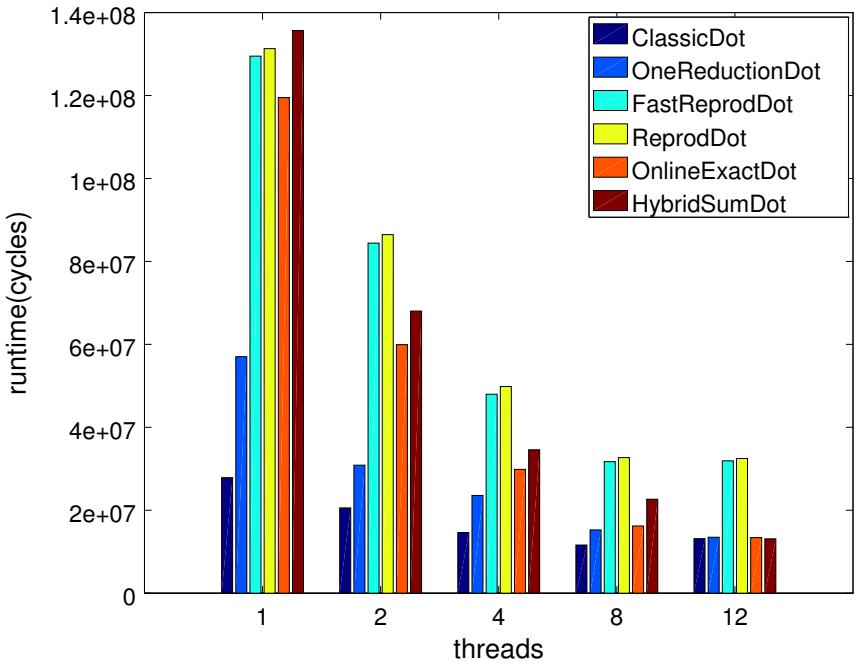
Single socket results

configurations

- #sockets = 1.
- #threads = 1 .. 12 on single socket.

dataset

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



Note

- Data do not hold in cache.
- Memory cost is more important for ReprodDot and FastReprodDot.

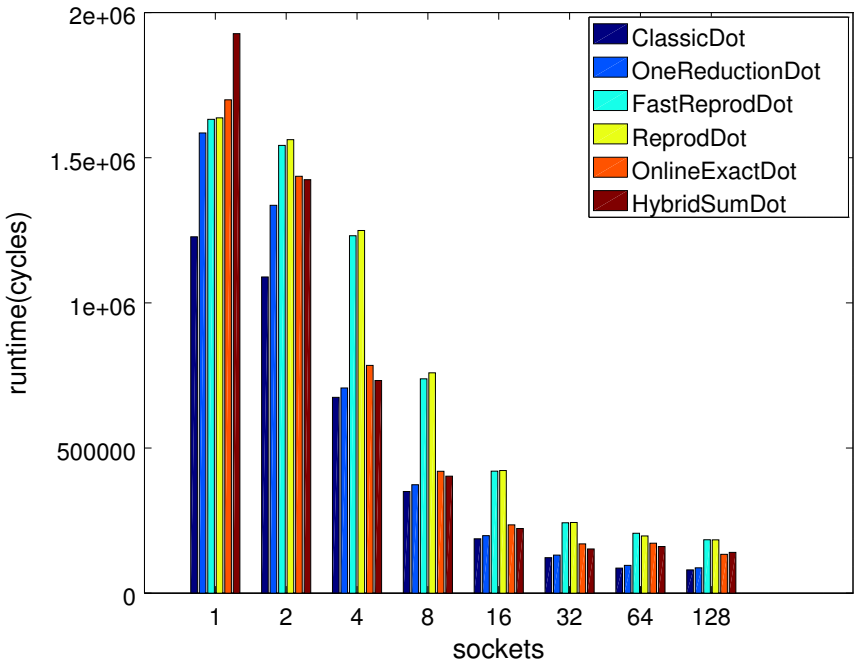
Multi-socket results

configurations

- #sockets = 1 .. 128.
- #threads = 8 per socket.

dataset

- Entry vectors size = 10^6.
- Condition number = 10^{32}.



Note

- Small dataset.
- We do not need too much sockets.

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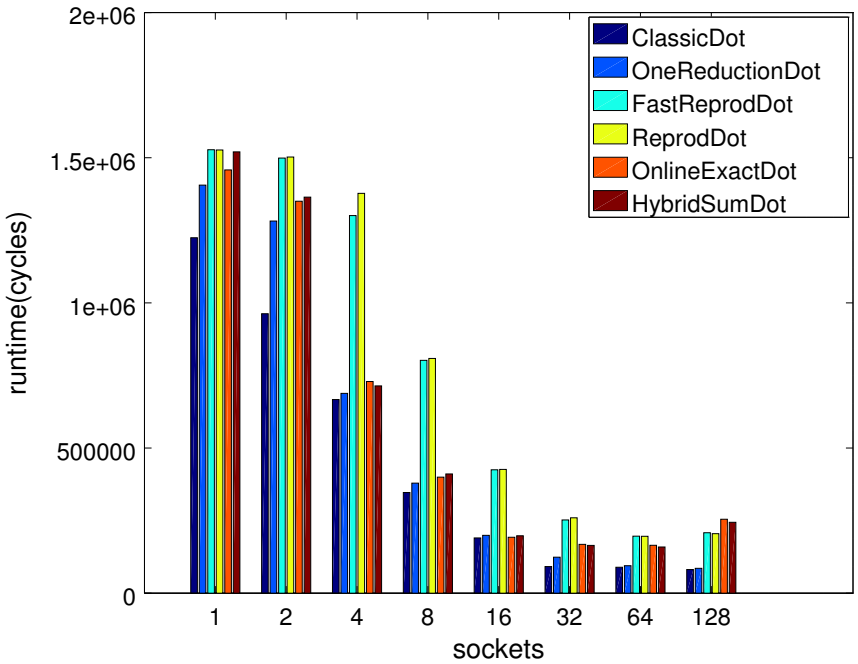

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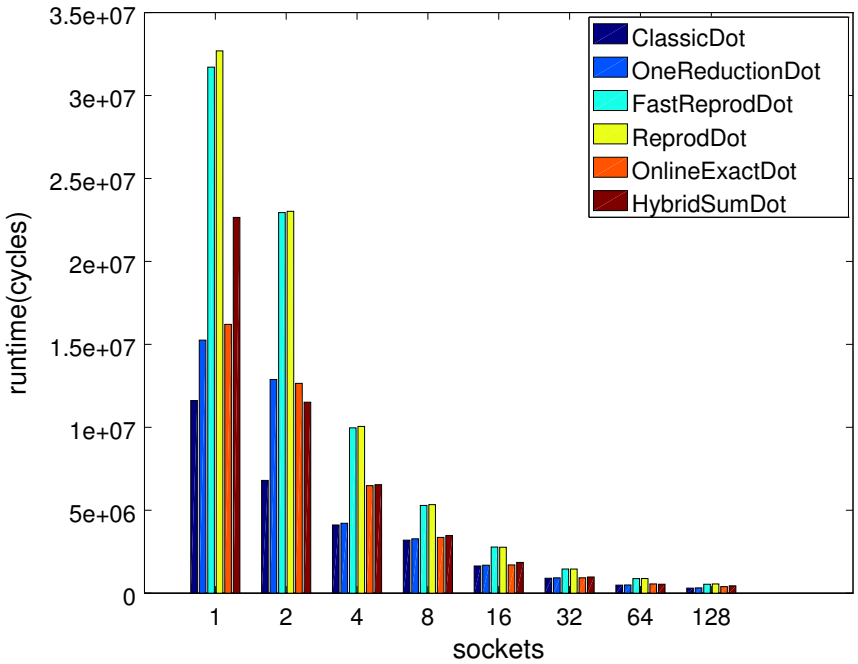

Note

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

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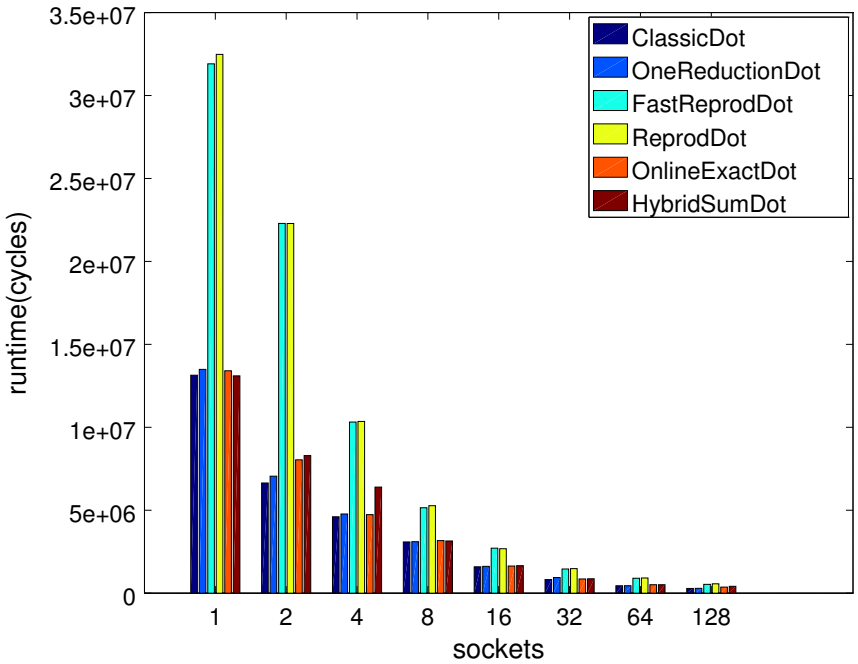

Note

- Good scaling for large datasets.
- Two communications cost limits ReprodDot and FastReprodDot.
- We need only one communication for OneReduction, HybridSum and OnlineExact.
- Using all cores : advantageous for RTN implementations.

Table of contents

Conclusion

Reproducible level 1 BLAS

- RTN cost for level 1 BLAS is acceptable on massively multi-thread systems.
- Our solution do not depend on condition.
- Intra-socket performance for classic dot is memory bounded.
- Only one communication is required.
- Scale correctly up to 128 sockets.

Future work

Future work

- Level 2 BLAS.
  - GEMV.
  - TRSV.
- Level 3 BLAS will not be easy.
  - DGEMM utilise 95% of peak performance.
  - Used algorithms are not adapted to work on blocks.
  - Some operations can not be vectorised.
  - No balance between FP additions and multiplications.

THANK YOU
FOR
YOUR ATTENTION