Reproducible and Accurate Matrix Multiplication in ExBLAS for High-Performance Computing

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SCAN 2014, 16th GAMM-IMACS International Symposium on Scientific Computing, Computer Arithmetic and Validated Numerics
Würzburg, Germany, September 21-26, 2014


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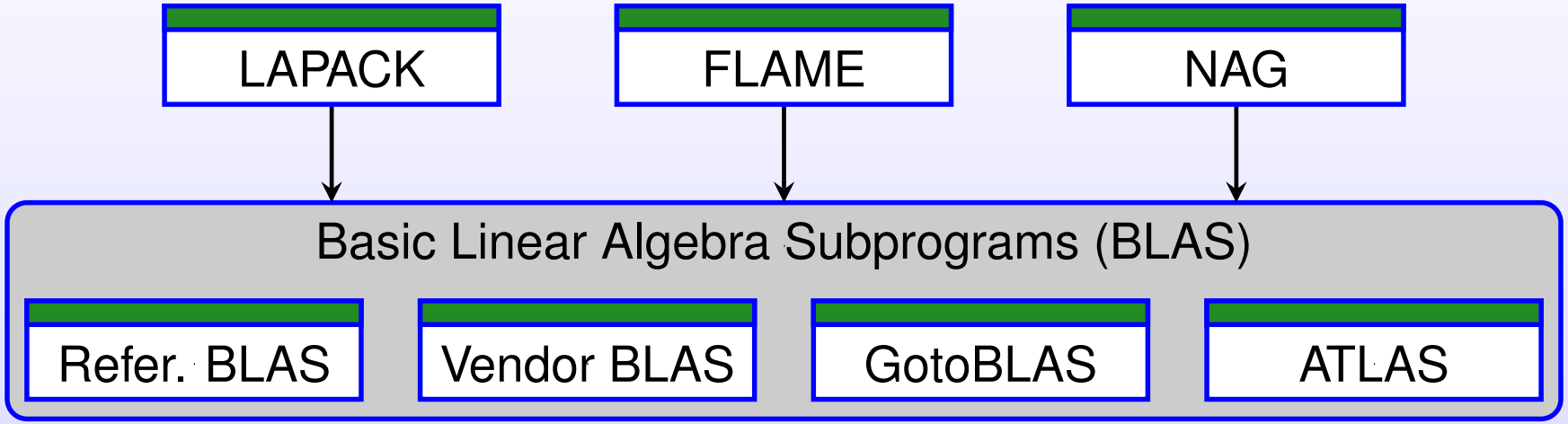
LIP6

Motivation



$\Downarrow$

BLAS-1:	$y := y + \alpha x$ $\alpha := \alpha + x^T y$	$\alpha \in R; x, y \in R^n$	$2/3$
BLAS-2:	$A := A + xy^T$ $y := A^{-1}x$	$A \in R^{n \times n}; x, y \in R^n$	2
BLAS-3:	$C := C + AB$ $C := A^{-1}B$	$A, B, C \in R^{n \times n}$	$n/2$

Ultimate Goal

- To compute BLAS operations with floating-point numbers efficiently and with the best possible accuracy on a wide range of architectures

ExBLAS – **Ex**act **BLAS**

- ExBLAS-1: `ExSCAL`, `ExDOT`, `ExAXPY`, ...
- ExBLAS-2: `ExGER`, `ExGEMV`, `ExTRSV`, `ExSYR`, ...
- ExBLAS-3: `ExGEMM`, `ExTRSM`, `ExSYR2K`, ...

Outline

Problems

- Floating-point arithmetic suffers from rounding errors
- Floating-point operations $(+, \times)$ are commutative but non-associative

$$(-1 + 1) + 2^{-53} \neq -1 + (1 + 2^{-53})$$ in double precision

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- Consequence: results of floating-point computations depend on the order of computation
- Results computed by performance-optimized parallel floating-point libraries may be often inconsistent: each run returns a different result

Reproducibility at ExaScale (I)

- **Reproducibility** – ability to obtain bit-wise identical results from run-to-run on the same input data on the same or different architectures
- **ExaScale** – ability to perform exaflops (10^{18} floating-point operations) per second

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Challenges

- Increasing power of current computers
  - $\rightarrow$ GPU accelerators, Intel Phi processors, etc.
- Enable to solve more complex problems
  - $\rightarrow$ Quantum field theory, supernova simulation, etc.
- A high number of floating-point operations performed
  - $\rightarrow$ Each of them leads to round-off error

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Difficult to obtain accurate and reproducible results

Needs for Reproducibility

- Debugging
  - Look inside the code step-by-step and might need to rerun multiple times on the same input data
- Understanding the reliability of output
- Contractual reasons (for security, ...)
- etc.

Sources of Non-Reproducibility

Performance-optimized floating-point libraries are prone to non-reproducibility for various reasons:

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Performance-optimized floating-point libraries are prone to non-reproducibility for various reasons:

- Changing Data Layouts:
  - Data partitioning
  - Data alignment
- Changing Hardware Resources
  - Number of threads
  - Fused Multiply-Add support
  - Intermediate precision (64 bits, 80 bits, 128 bits, etc)
  - Data path (SSE, AVX, GPU warp, etc)
  - Cache line size
  - Number of processors
  - Network topology

Existing Solutions

- **Fix the Order of Computations**
  - Sequential mode: intolerably costly at large-scale systems
  - Fixed reduction trees: substantial communication overhead

  → Example: Intel **C**onditional **N**umerical **R**eproducibility (slow, no accuracy guarantees)

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- **Eliminate/Reduce the Rounding Errors**
  - Fixed-point arithmetic: limited range of values
  - Fixed FP expansions with Error-Free Transformations (EFT)
  - → Example: double-double or quad-double (Briggs, Bailey, Hida, Li) (work well on a set of relatively close numbers)
  - "Infinite" precision: reproducible independently from the inputs
  - → Example: Kulisch accumulator (considered inefficient)

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- **Libraries**
  - ReproBLAS: Reproducible BLAS (Demmel and Nguyen)

  → For BLAS-1 on CPUs only

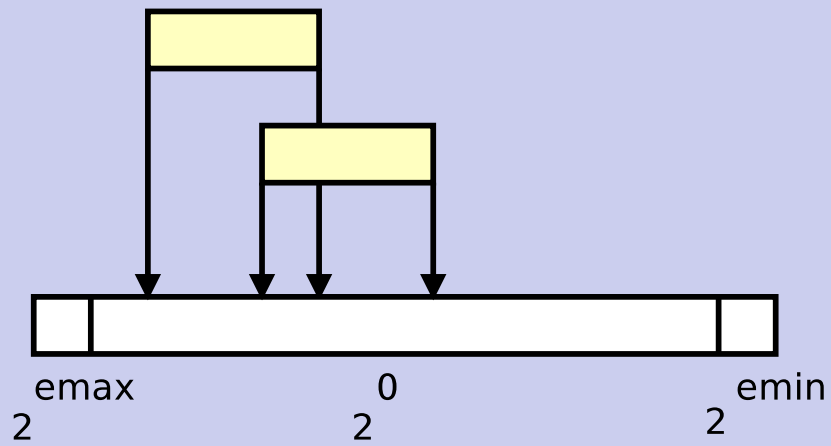
Our Approach

Algorithm 1 EFT of size 2 (Dekker and Knuth)

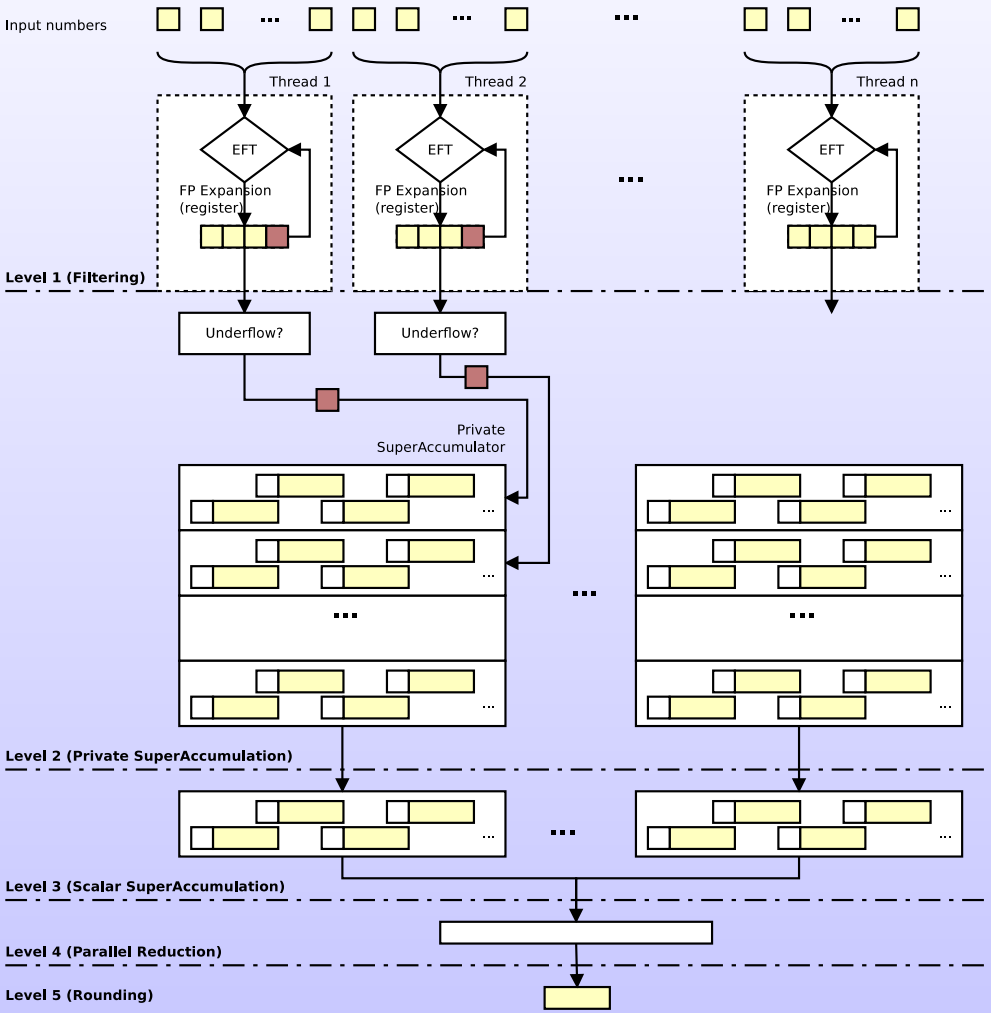
function$[r, s]$ = TwoSum(a, b)

1: $r \leftarrow a + b$
2: $z \leftarrow r - a$
3: $s \leftarrow (a - (r - z)) + (b - z)$

Kulisch long accumulator



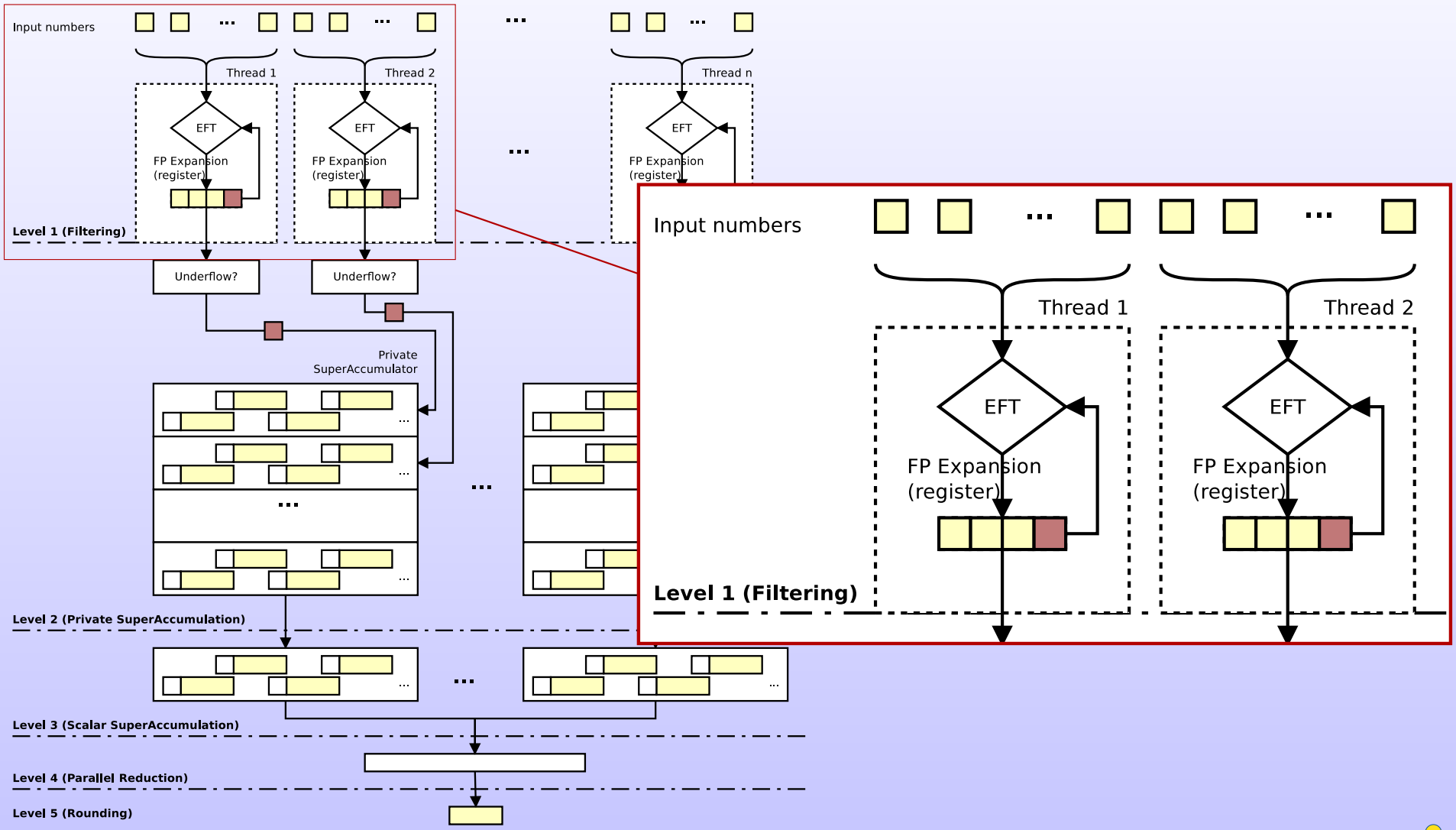
Multi-Level Reproducible Summation



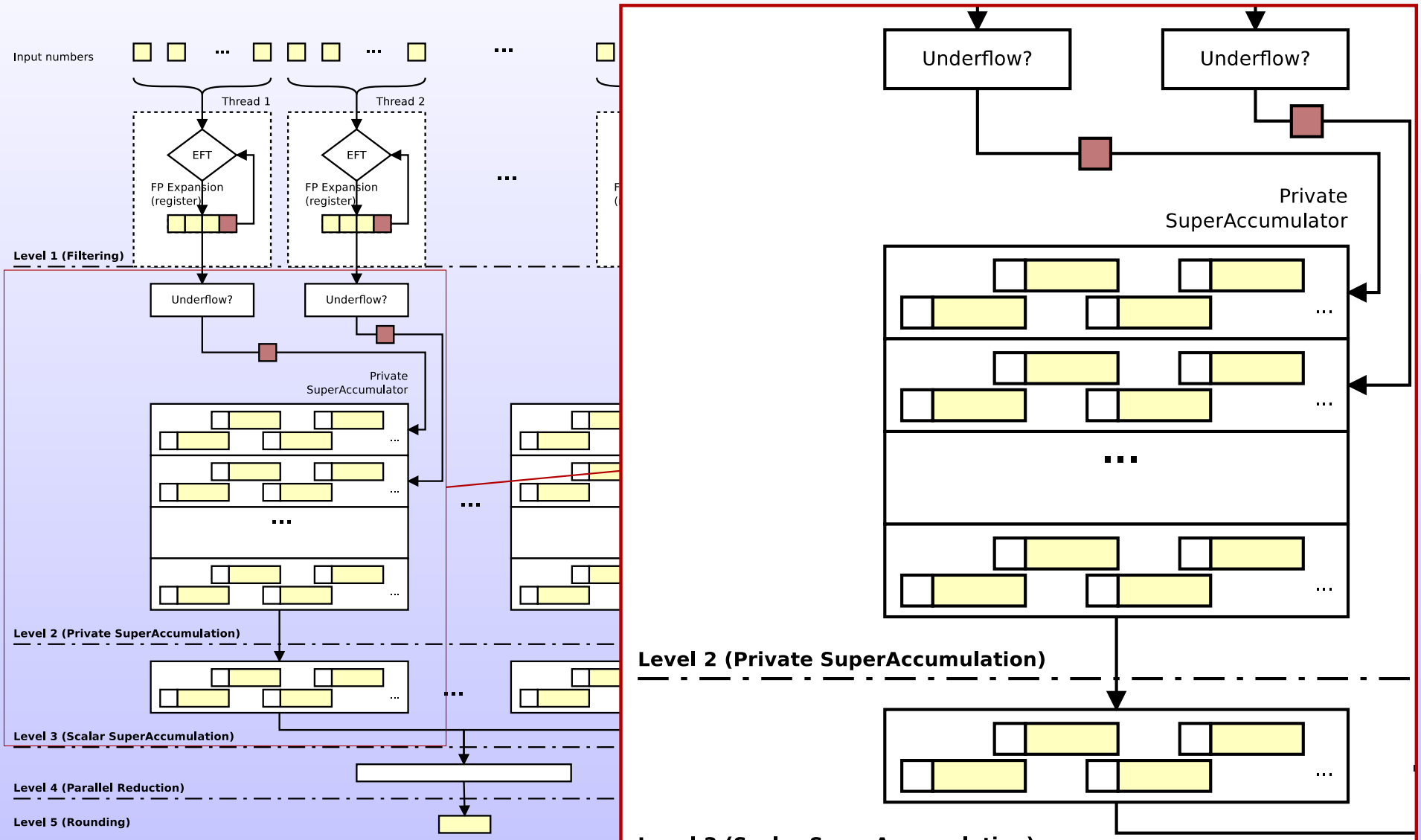
- Parallel algorithm with 5-levels
- Suitable for today's parallel architectures
- Based on FPE with EFT and Kulisch accumulator
- Guarantees "inf" precision

→ bit-wise reproductibility

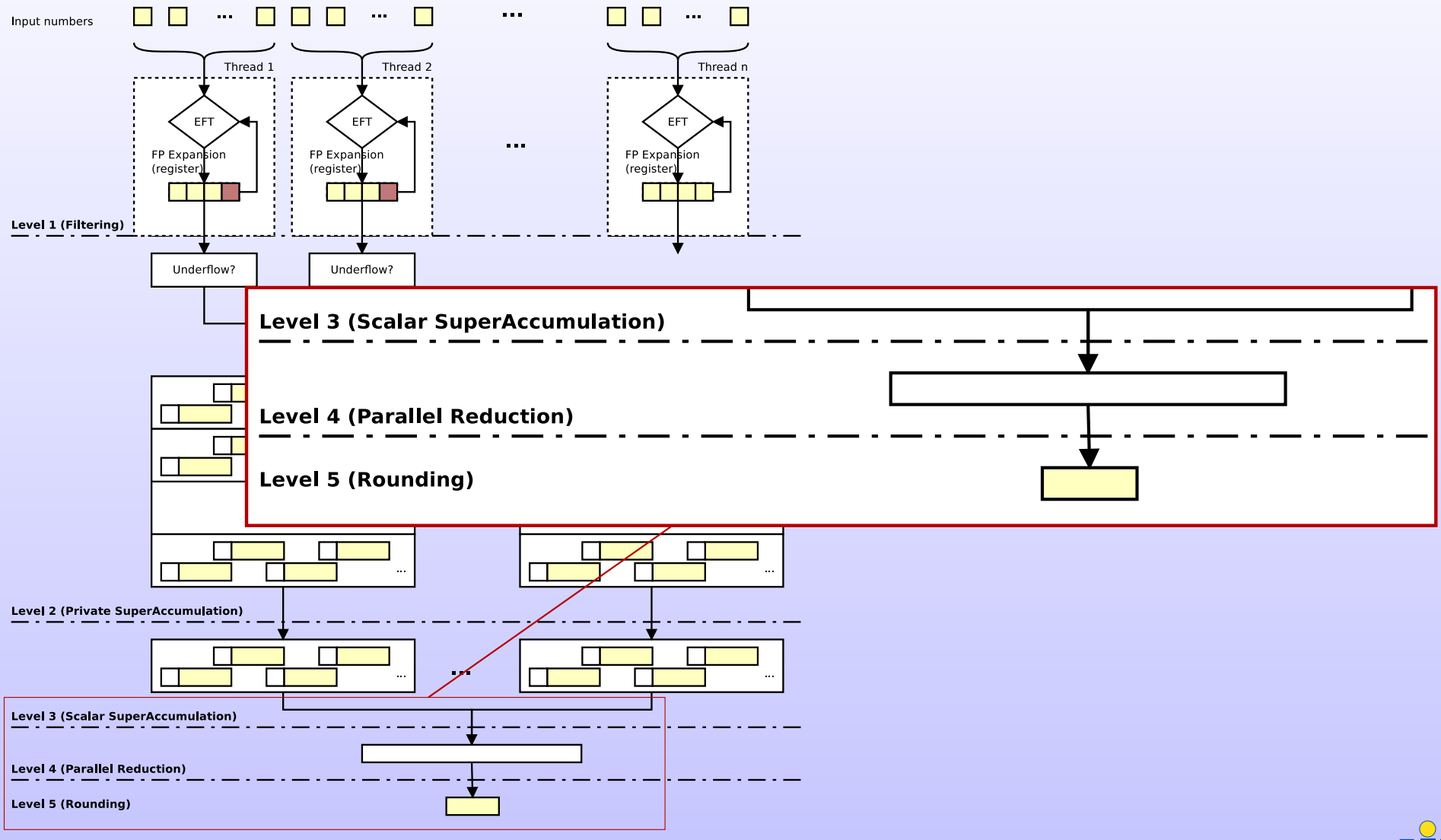
Level 1: Filtering



Level 2 and 3: Scalar Superaccumulator

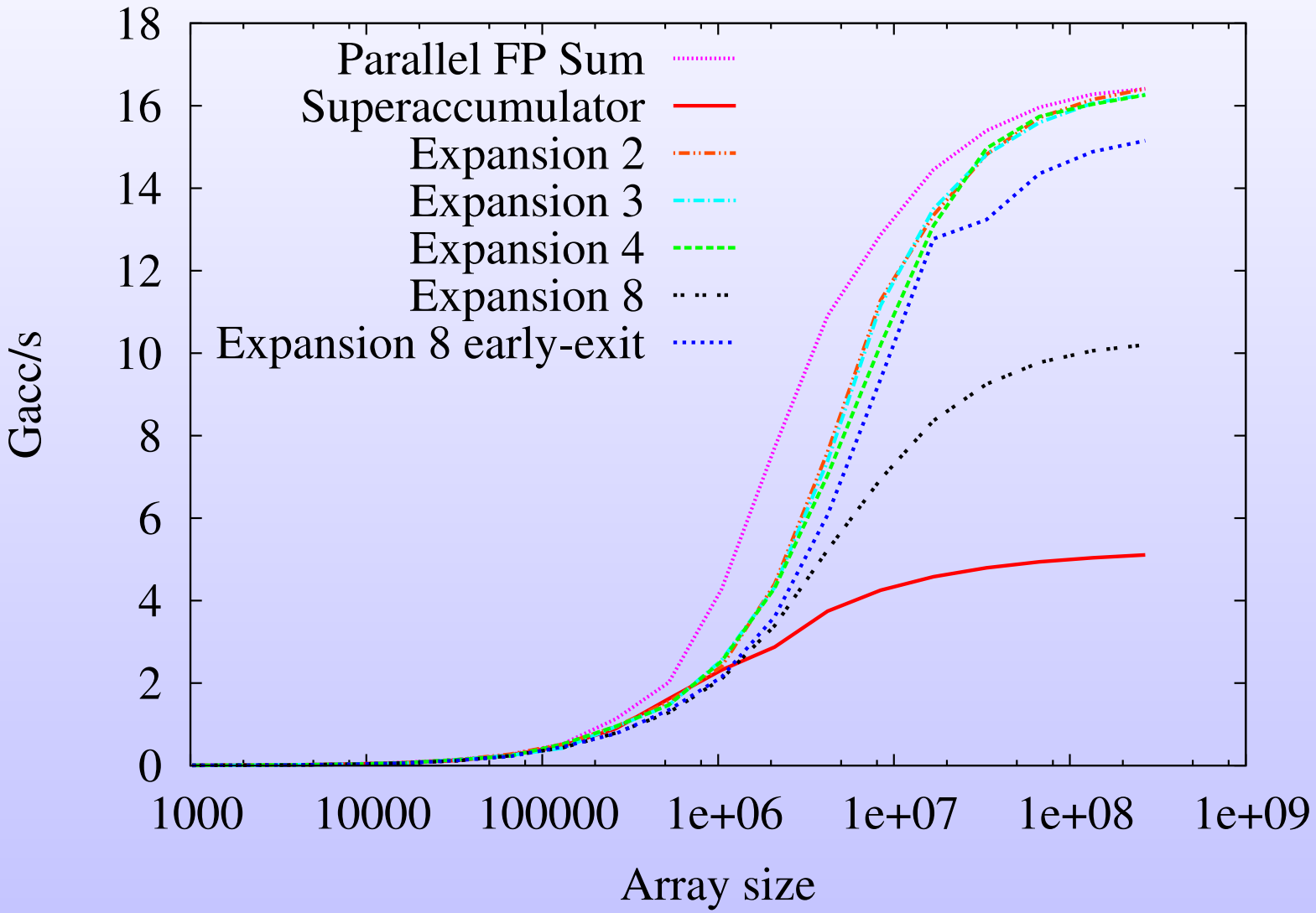


Level 4 and 5: Reduction and Rounding



Parallel Summation

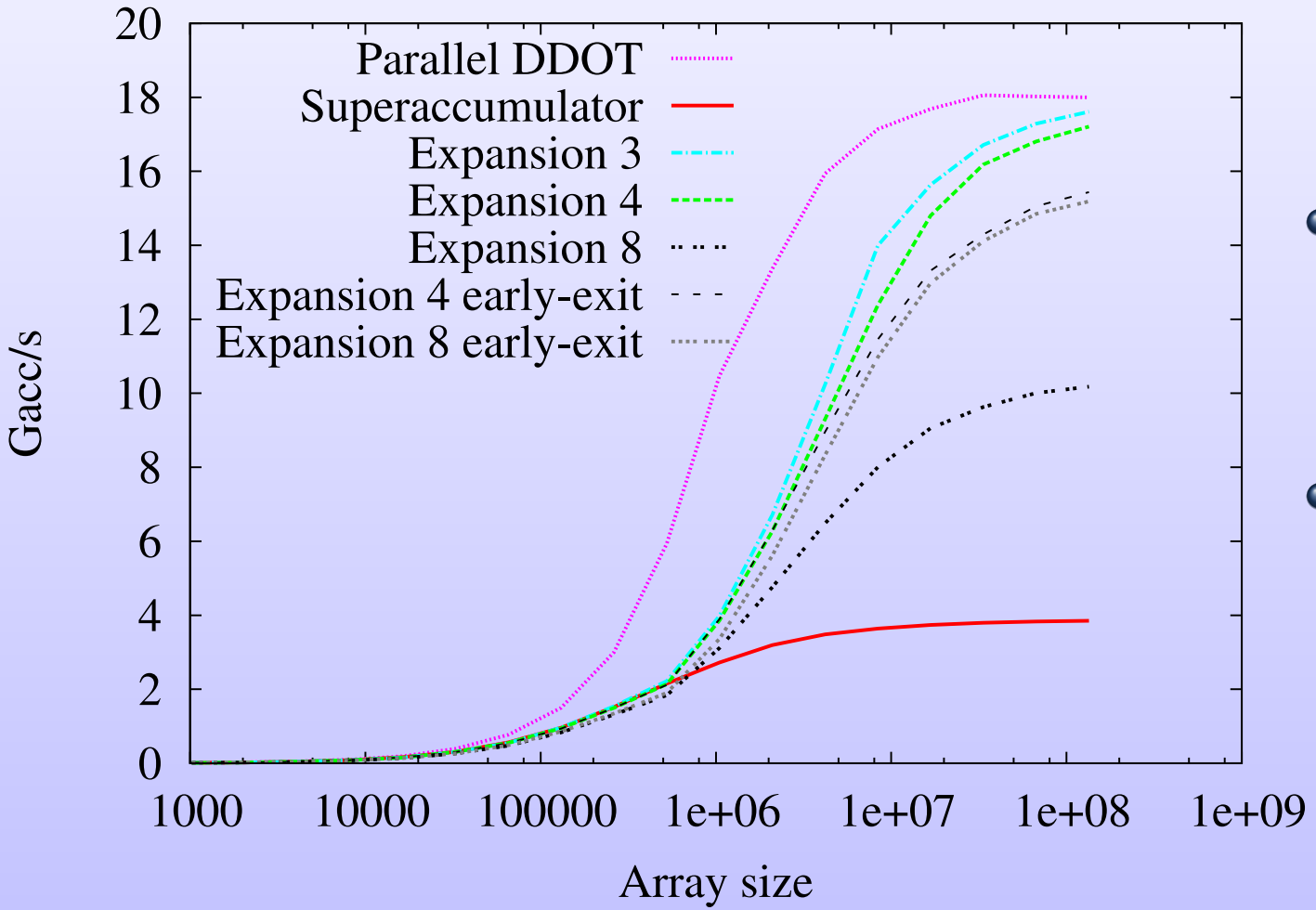
Performance Scaling on NVIDIA Tesla K20c



Parallel Dot Product

Performance Scaling on NVIDIA Tesla K20c

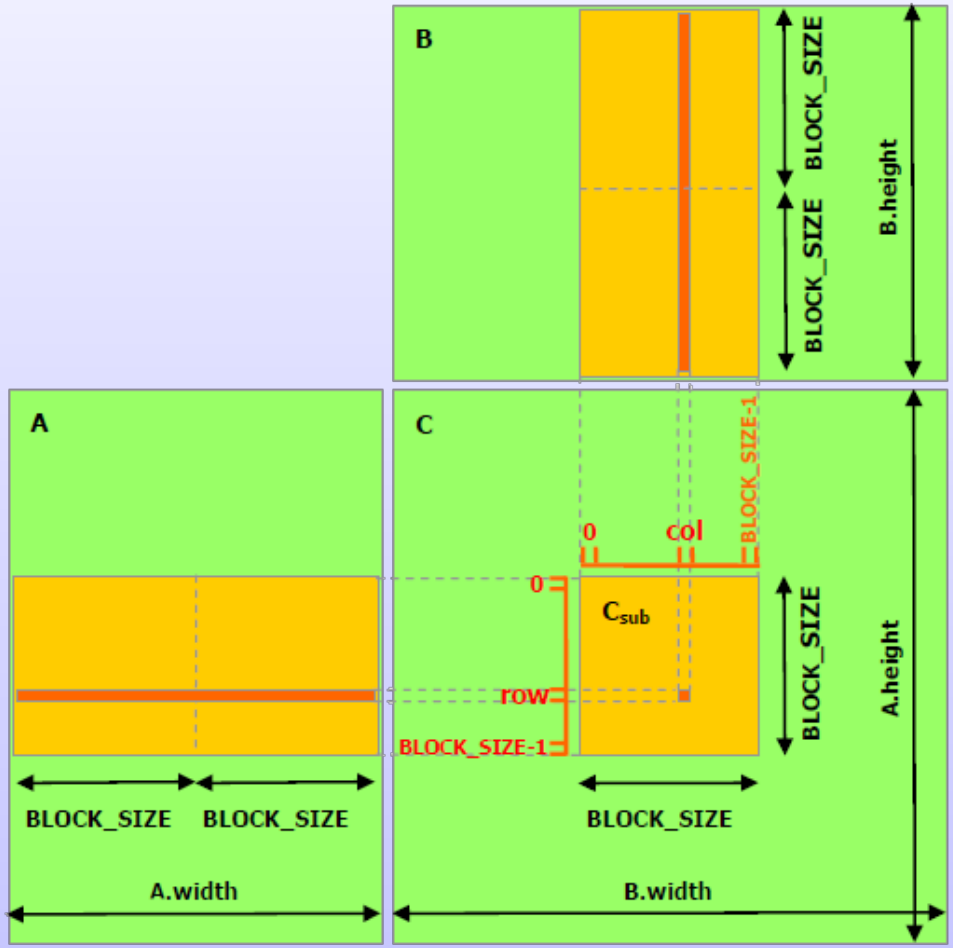
DDOT: $\alpha := x^T y = \sum_i^N x_i y_i$



- Based on TwoProduct and Reproducible Summation
- TwoProduct relies on FMA

Multi-Level Reproducible DGEMM

DGEMM: $C := \alpha AB + \beta C$



Source: CUDA C Programming Guide

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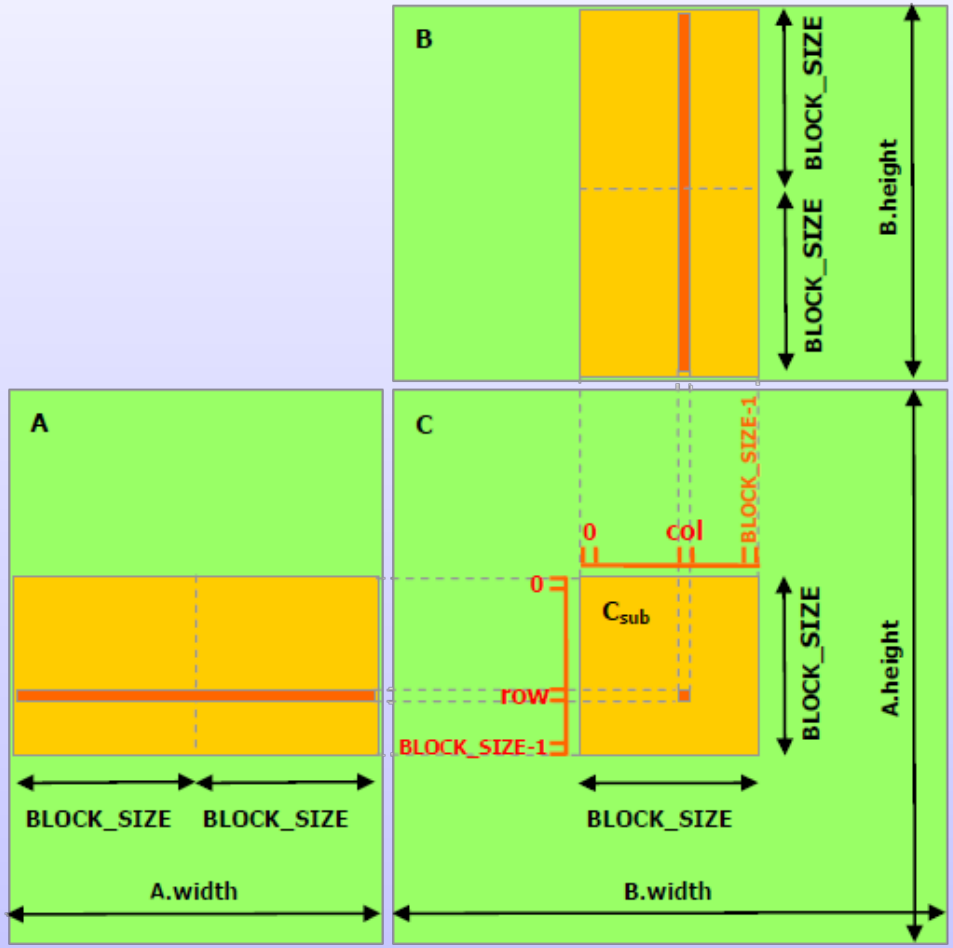

Source: CUDA C Programming Guide

- One FPE and Kulisch accumulator per thread
- Algorithm consists of 3 steps:
  - Filtering
  - Private SuperAccumulation
  - Rouding
- Each thread computes multiple elements of matrix C to reduce memory pressure

Parallel Matrix Multiplication

Performance Scaling on NVIDIA Tesla K20c

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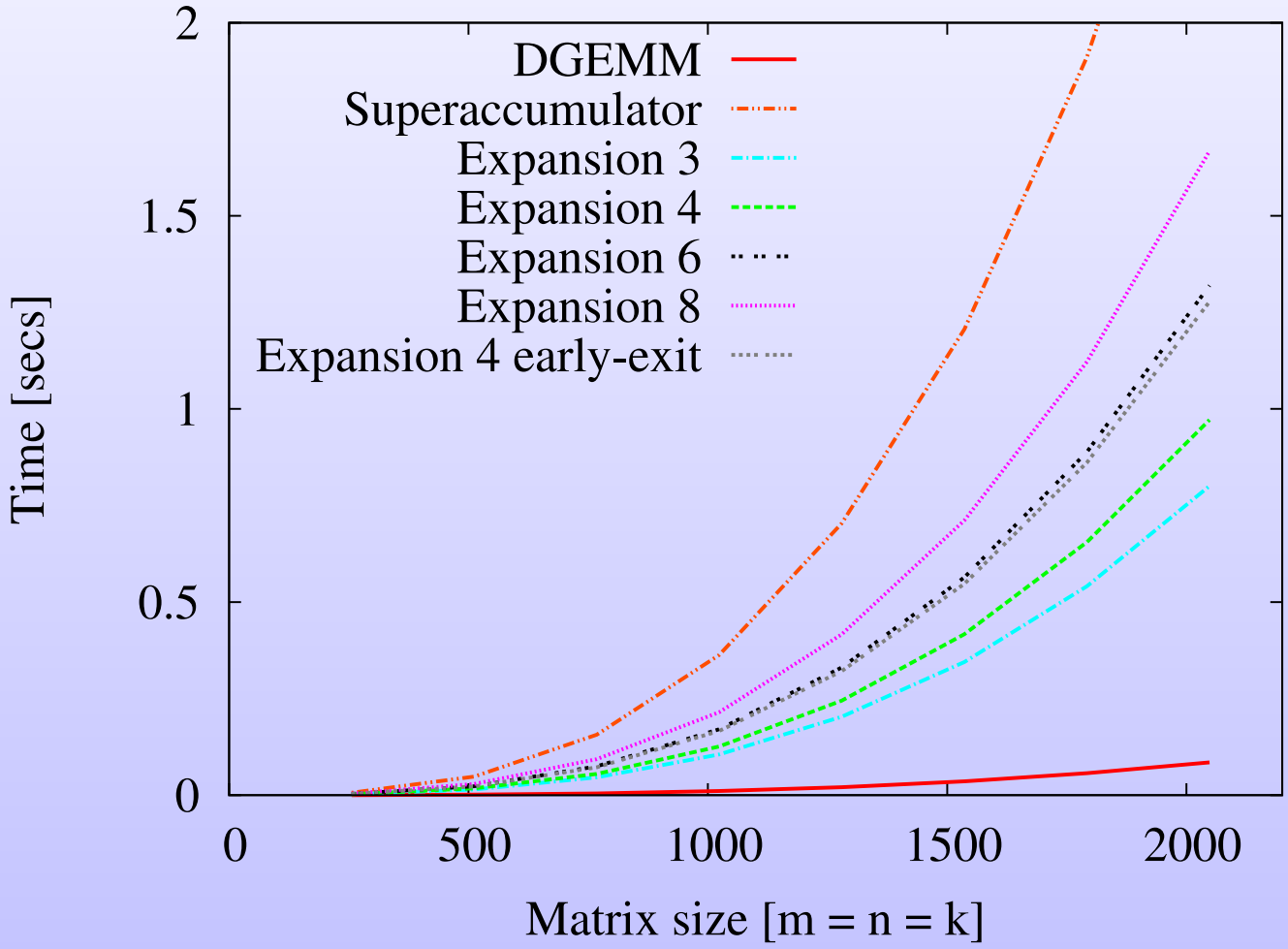

- $12dn^3$ Flops more, d is size of FPE
- Up to $76n^3$ more memory usage

The Proposed Multi-Level Algorithm

- Computes the results with no errors due to rounding
- Provides bit-wise identical reproducibility, regardless of
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- Scales perfectly with the increase of the problem size or the number of cores

Conclusions

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- Provides bit-wise identical reproducibility, regardless of
  - Data permutation, data assignment
  - Thread scheduling, etc.
- Is efficient – delivers comparable performance to the standard parallel summation and dot product
- Scales perfectly with the increase of the problem size or the number of cores
- For DGEMM the performance needs to be enhanced

Future Work

- ExGEMM on Intel Phi and also Intel CPUs
- The algorithm is suitable for large scale systems (ExaScale) with one more reduction step between nodes

→ Parallelization with MPI

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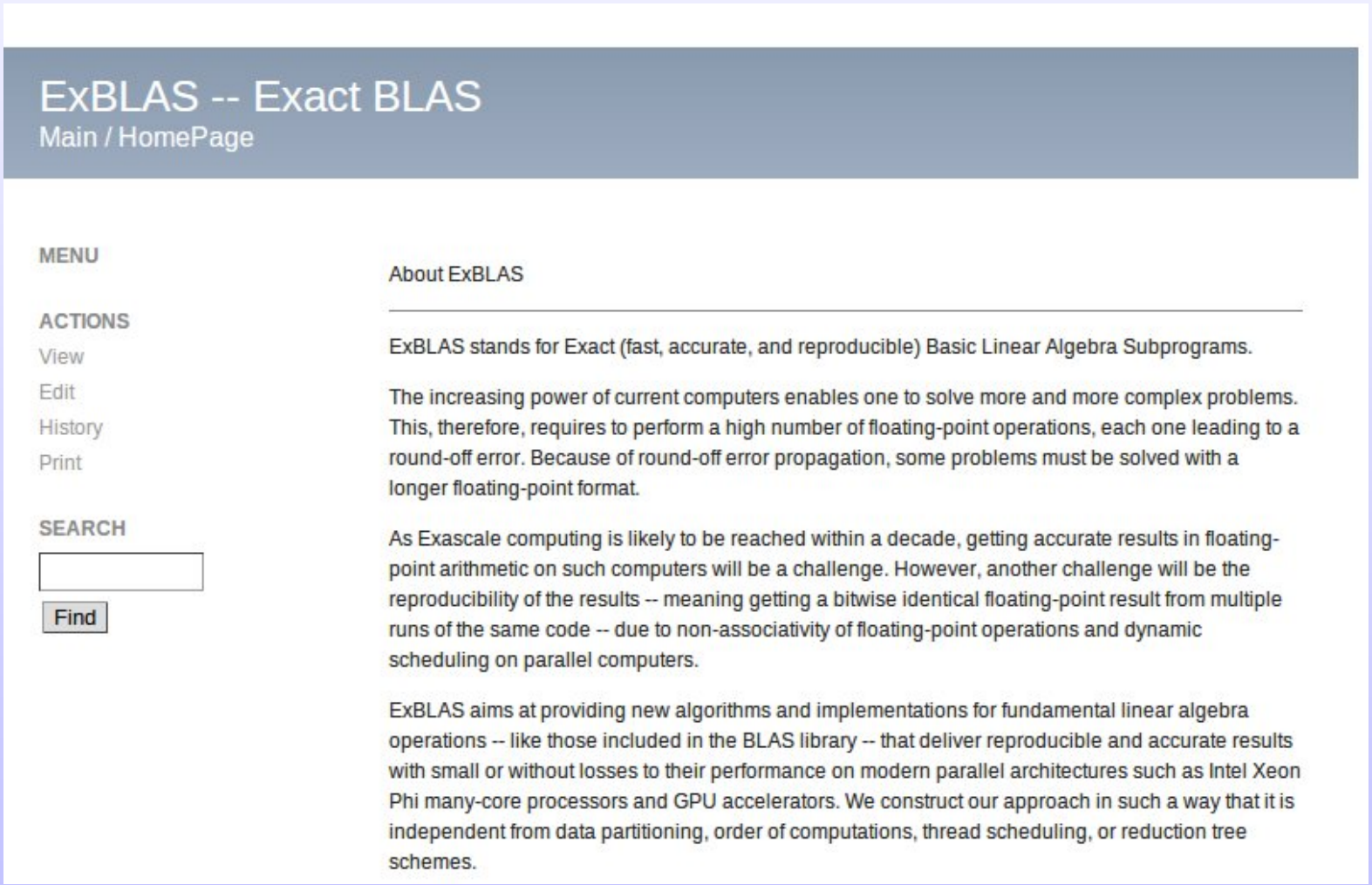
Acknowledgement

Thank you for your attention!

→ This work undertaken (partially) in the framework of CALSIMLAB is supported by the public grant ANR-11-LABX-0037-01 overseen by the French National Research Agency (ANR) as part of the “Investissements d’Avenir” program (reference: ANR-11-IDEX-0004-02).

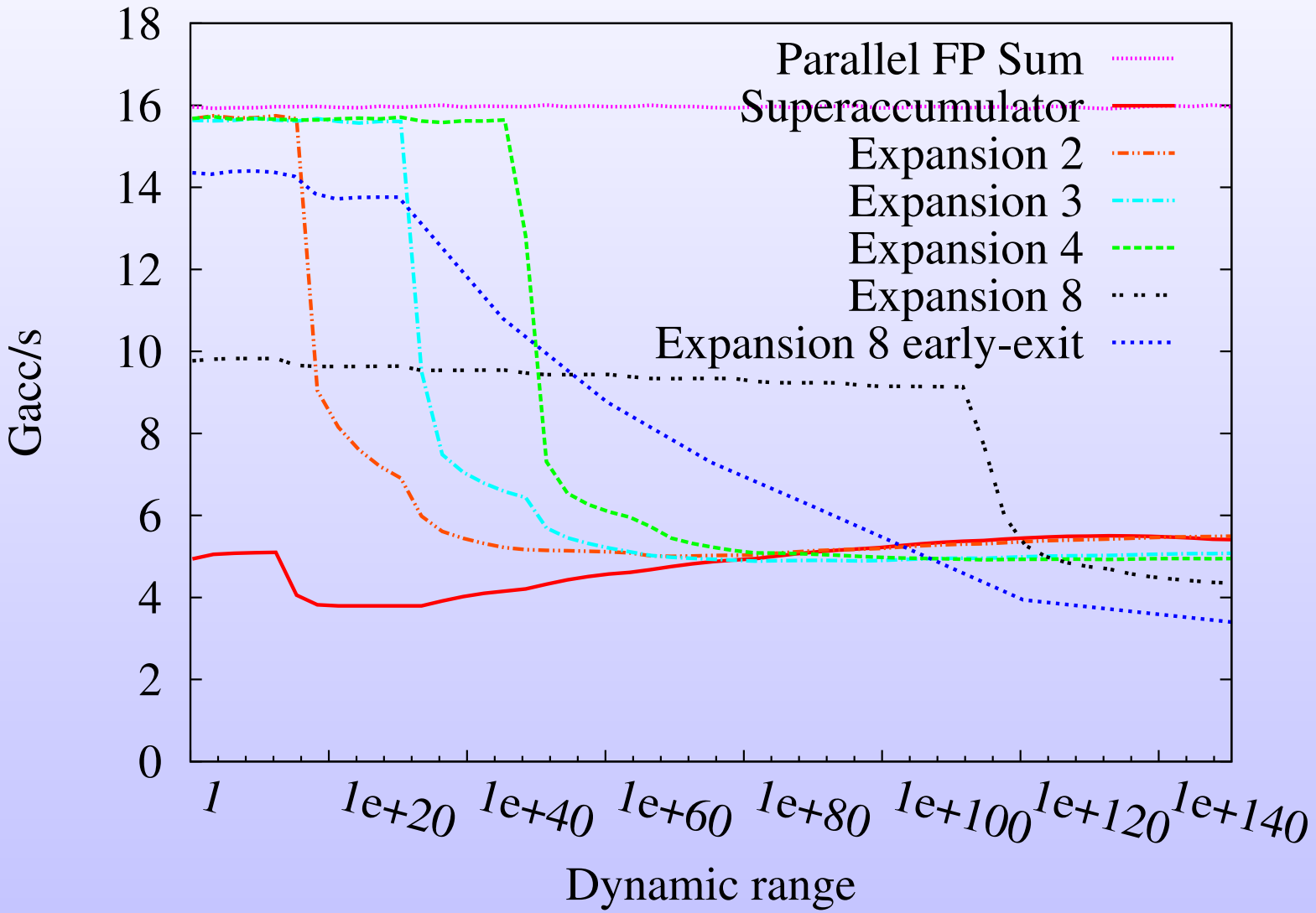
On the Web

URL: `https://exblas.lip6.fr`



Parallel Summation

Data-Dependent Performance on NVIDIA Tesla K20c



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