Towards Fast, Accurate and Reproducible LU Factorization

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Linear Algebra Libraries

BLAS-1 [1979]:	$y := y + \alpha x$ $\alpha := \alpha + x^T y$	$\alpha \in \mathbb{R}; x, y \in \mathbb{R}^n$	$2/3$
BLAS-2 [1988]:	$A := A + xy^T$ $y := A^{-1}x$	$A \in \mathbb{R}^{n \times n}; x, y \in \mathbb{R}^n$	2
BLAS-3 [1990]:	$C := C + AB$ $C := A^{-1}B$	$A, B, C \in \mathbb{R}^{n \times n}$	$n/2$

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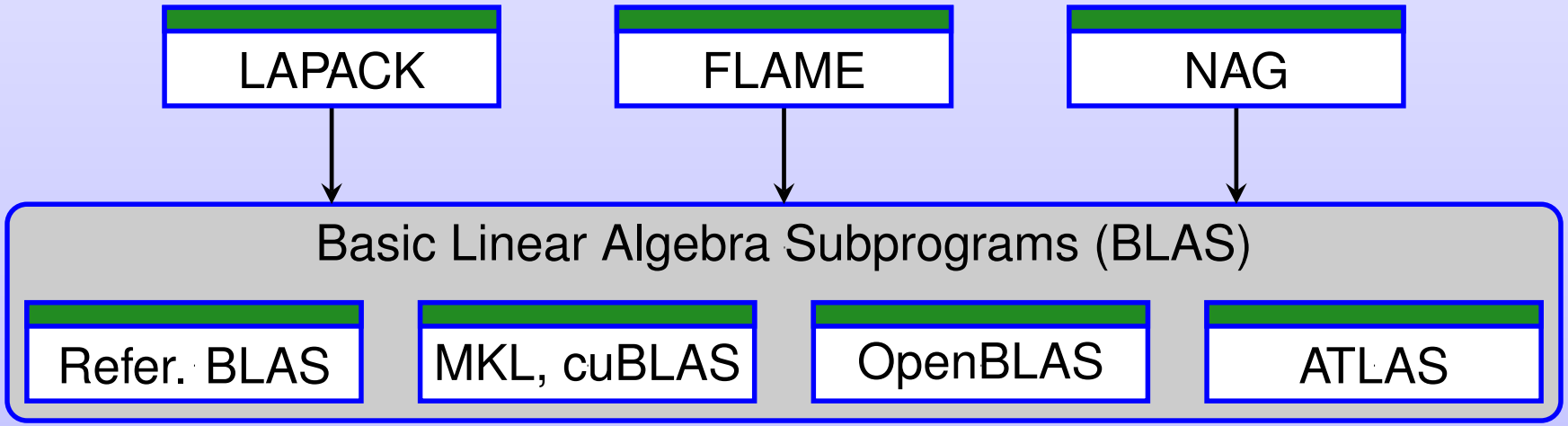

Goals

- To compute BLAS operations with floating-point numbers fast and precise, ensuring their numerical reproducibility, on a wide range of architectures

ExBLAS – **Ex**act **BLAS**

- **Ex**BLAS-1: `ExSUM`, `ExSCAL`, `ExDOT`, `ExAXPY`, ...
- **Ex**BLAS-2: `ExGER`, `ExGEMV`, `ExTRSV`, `ExSYR`, ...
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- Use the ExBLAS kernels to construct exact higher-level operations such as the LU factorization

Outline

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Accuracy and Reproducibility

Problems

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

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

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

- 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** – ability to obtain bit-wise identical results from run-to-run on the same input data on the same or different architectures

Existing Solutions

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

  $\rightarrow$ Example: Intel **C**onditional **N**umerical **R**eproducibility ($\sim 2x$ for datum, 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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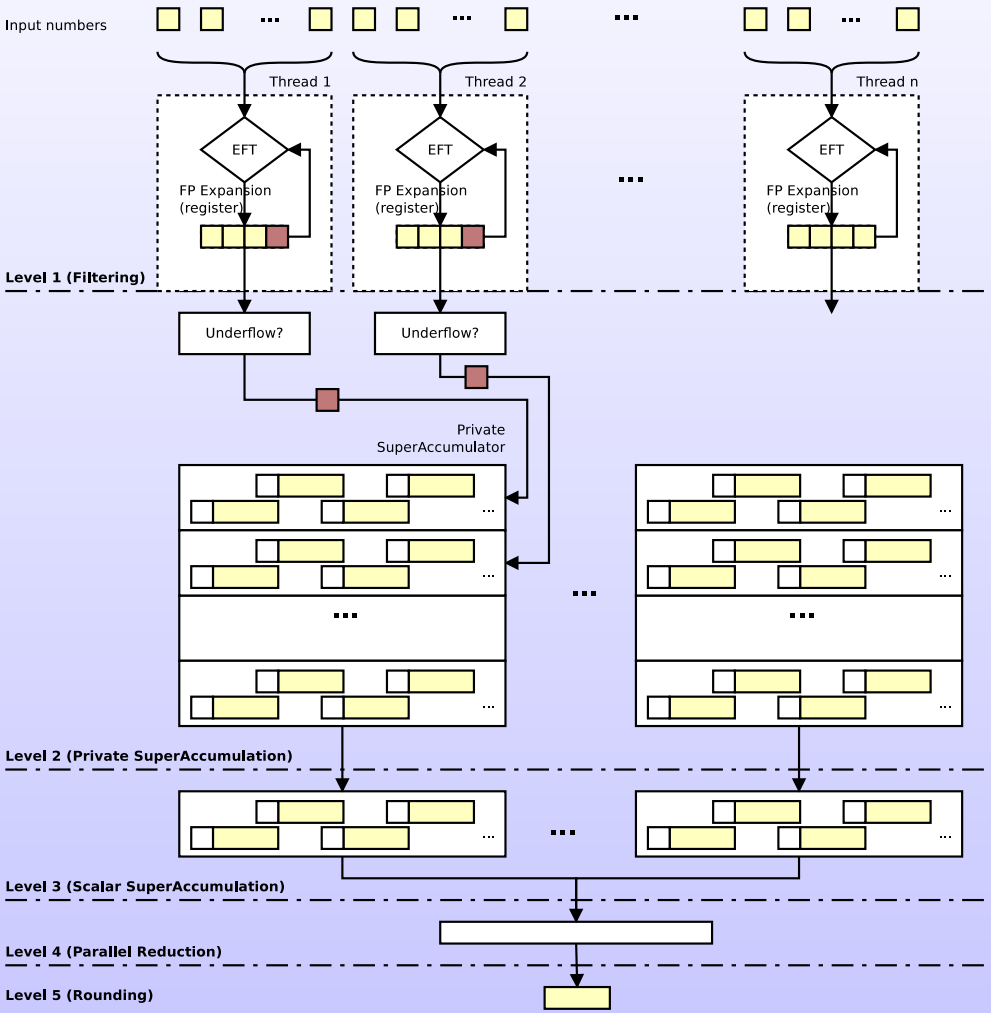
- **Libraries**
  - ReproBLAS: Reproducible BLAS (Demmel, Nguyen, Ahrens)

  → For BLAS-1, GEMV, and GEMM on CPUs

  - RARE-BLAS: Repr. Accur. Rounded and Eff. BLAS (Chohra, Langlois, Parello) → For BLAS-1 and GEMV on CPUs

Outline

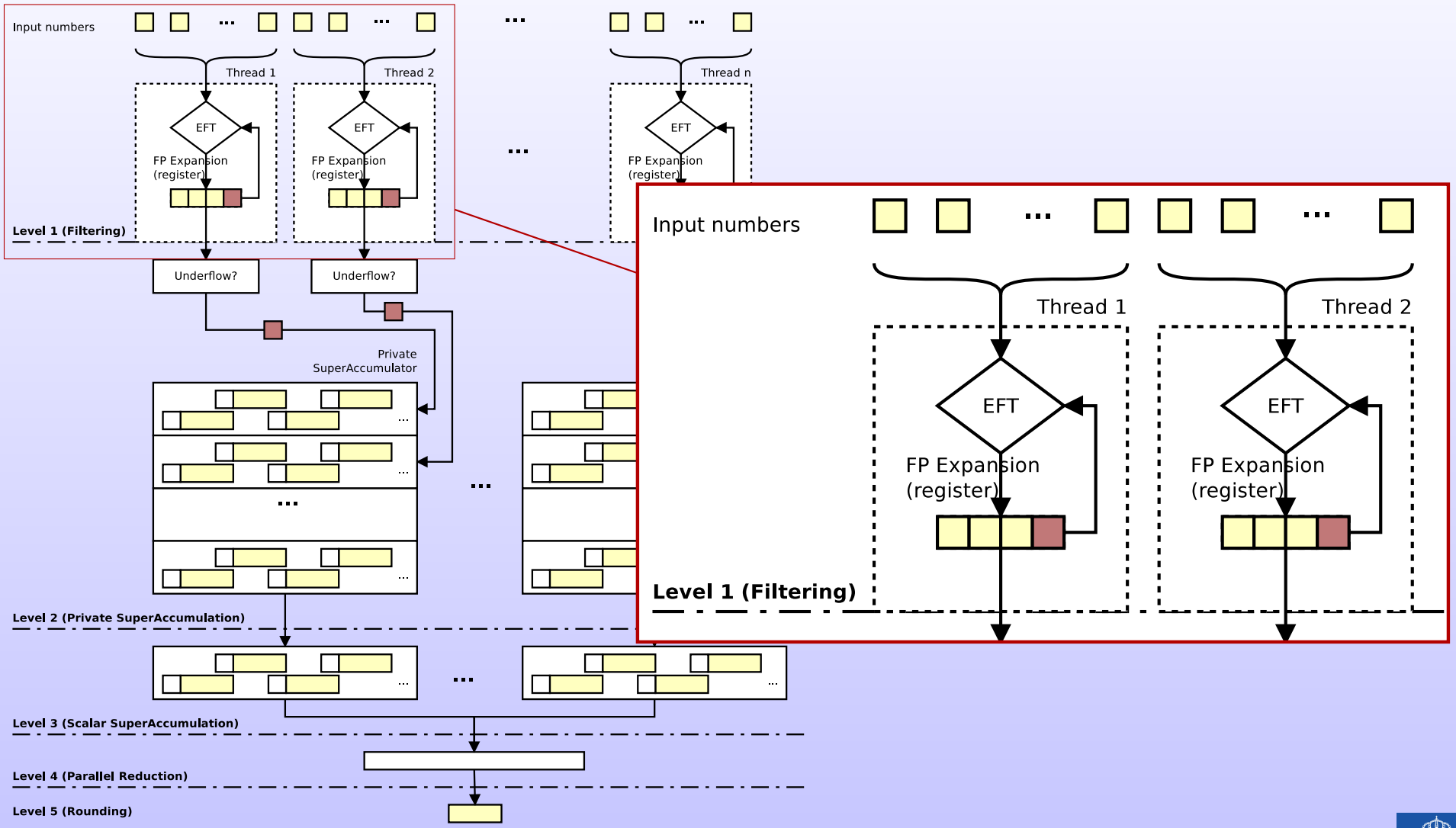
Our Multi-Level Reproducible Summation



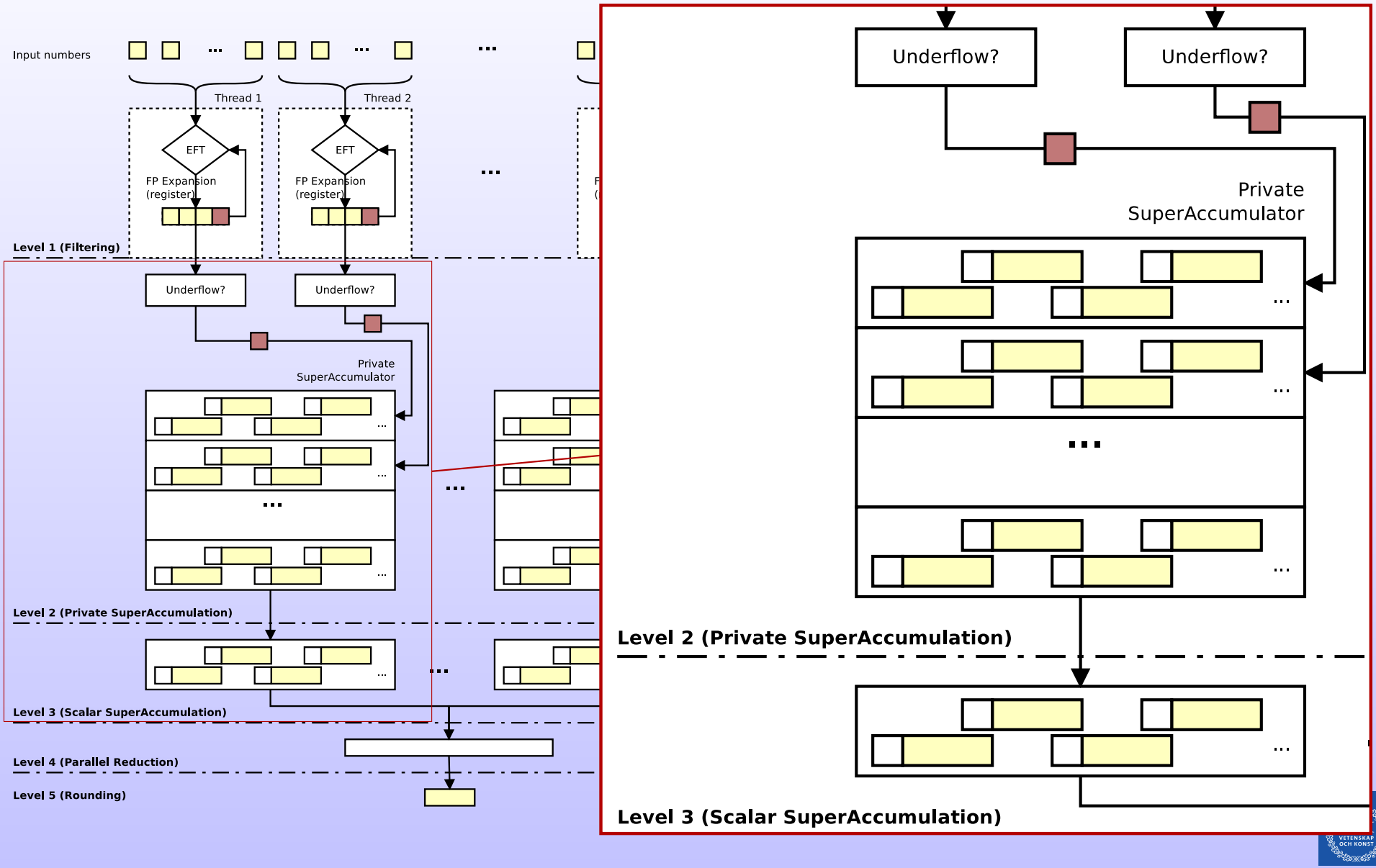
- Parallel algorithm with 5-levels
- Suitable for today's parallel architectures
- Based on FPE with EFT and Kulisch accumulator
- Guarantees "inf" precision

→ **bit-wise reproducibility**

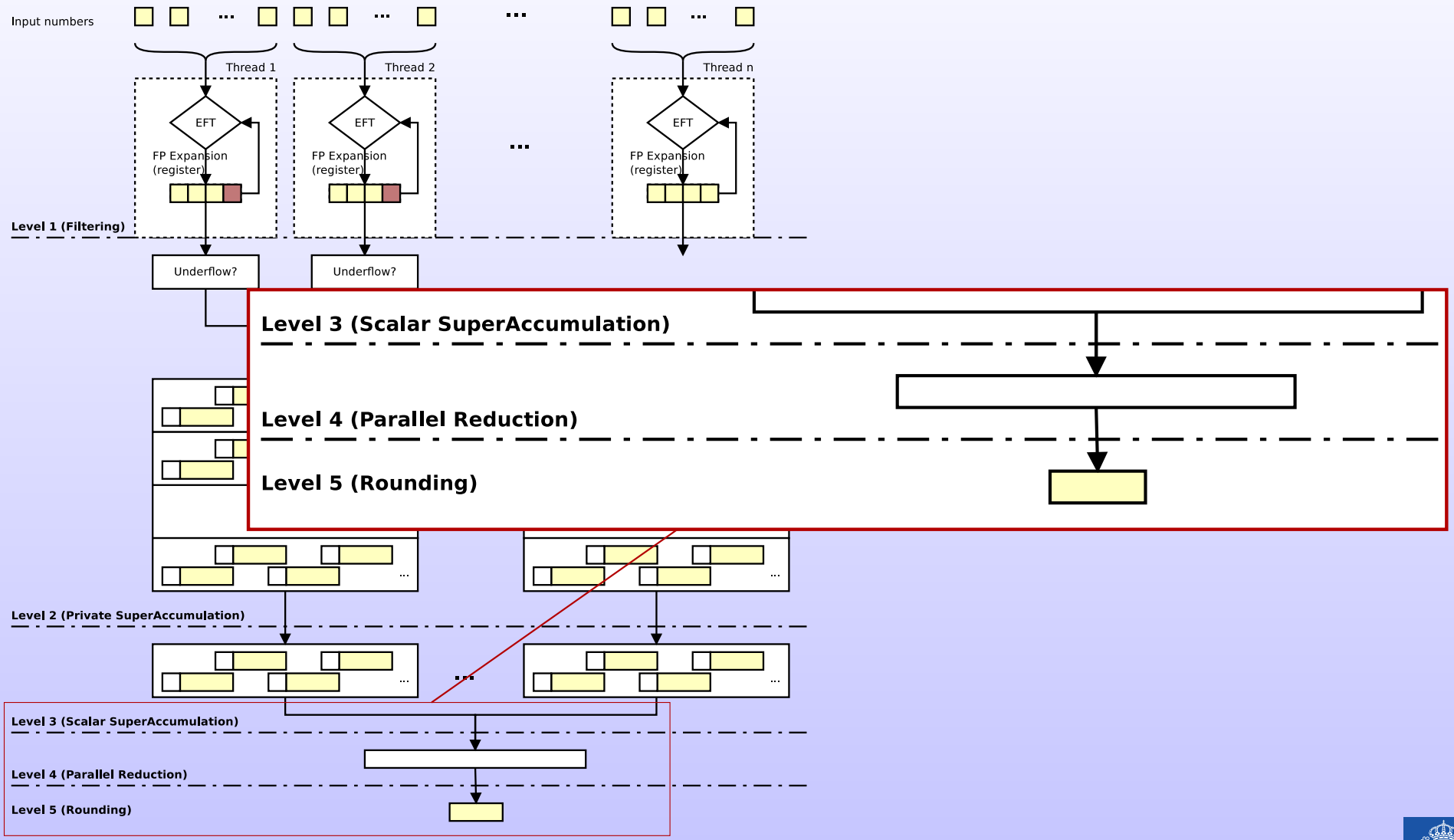
Level 1: Filtering



Level 2 and 3: Scalar Superaccumulator



Level 4 and 5: Reduction and Rounding



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- $x := \alpha * x \rightarrow$ correctly rounded and reproducible

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- $x := \alpha * x \rightarrow$ correctly rounded and reproducible
- Within LU: $x := 1/\alpha * x \rightarrow$ not correctly rounded

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ExGER

- General case: $A := \alpha * x * y^T + A$

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ExSCAL

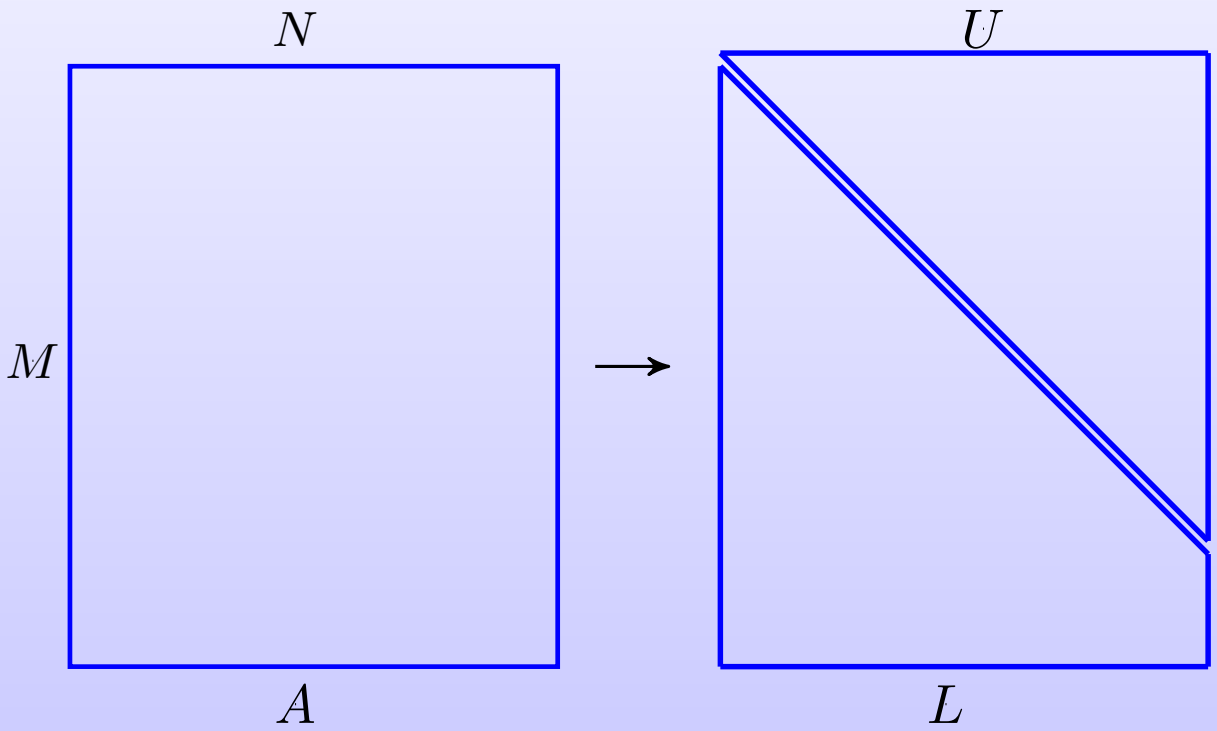
- $x := \alpha * x \rightarrow$ correctly rounded and reproducible
- Within LU: $x := 1/\alpha * x \rightarrow$ not correctly rounded
- ExInvSCAL: $x := x/\alpha \rightarrow$ correctly rounded and reproducible

ExGER

- General case: $A := \alpha * x * y^T + A$
- Within LU: $A := x * y^T + A$. Using FMA $\rightarrow$ correctly rounded and reproducible

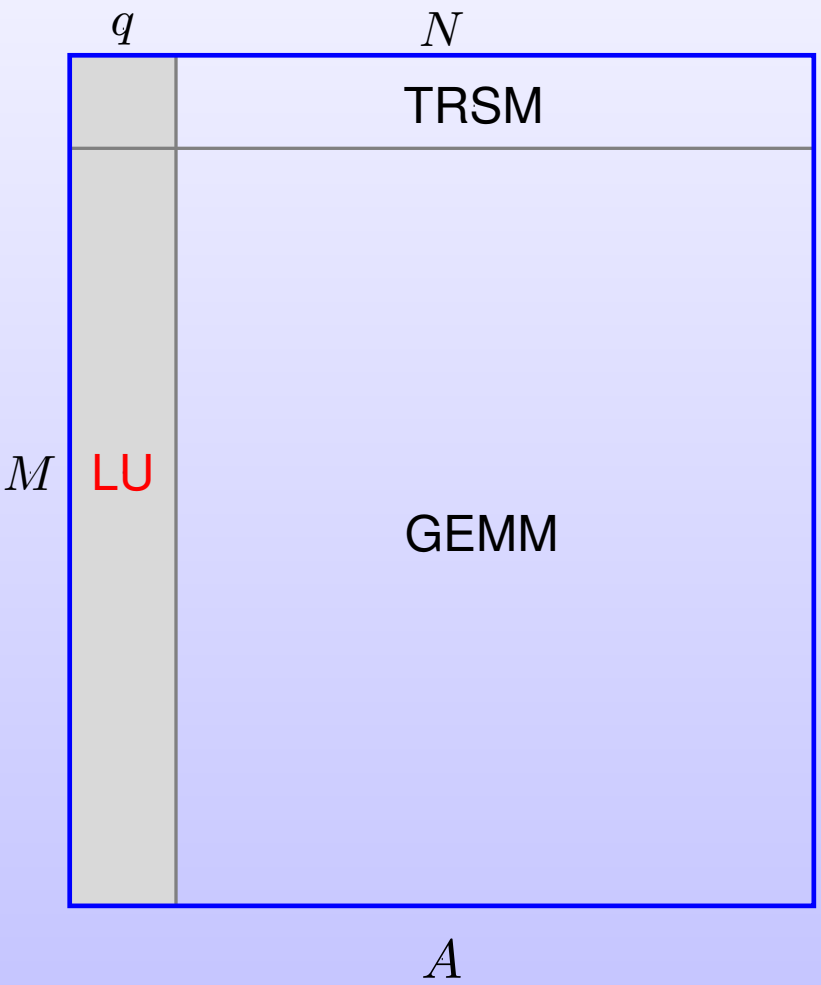
LU Factorization

$$\boxed{Ax = b} \Rightarrow \boxed{A = LU}$$



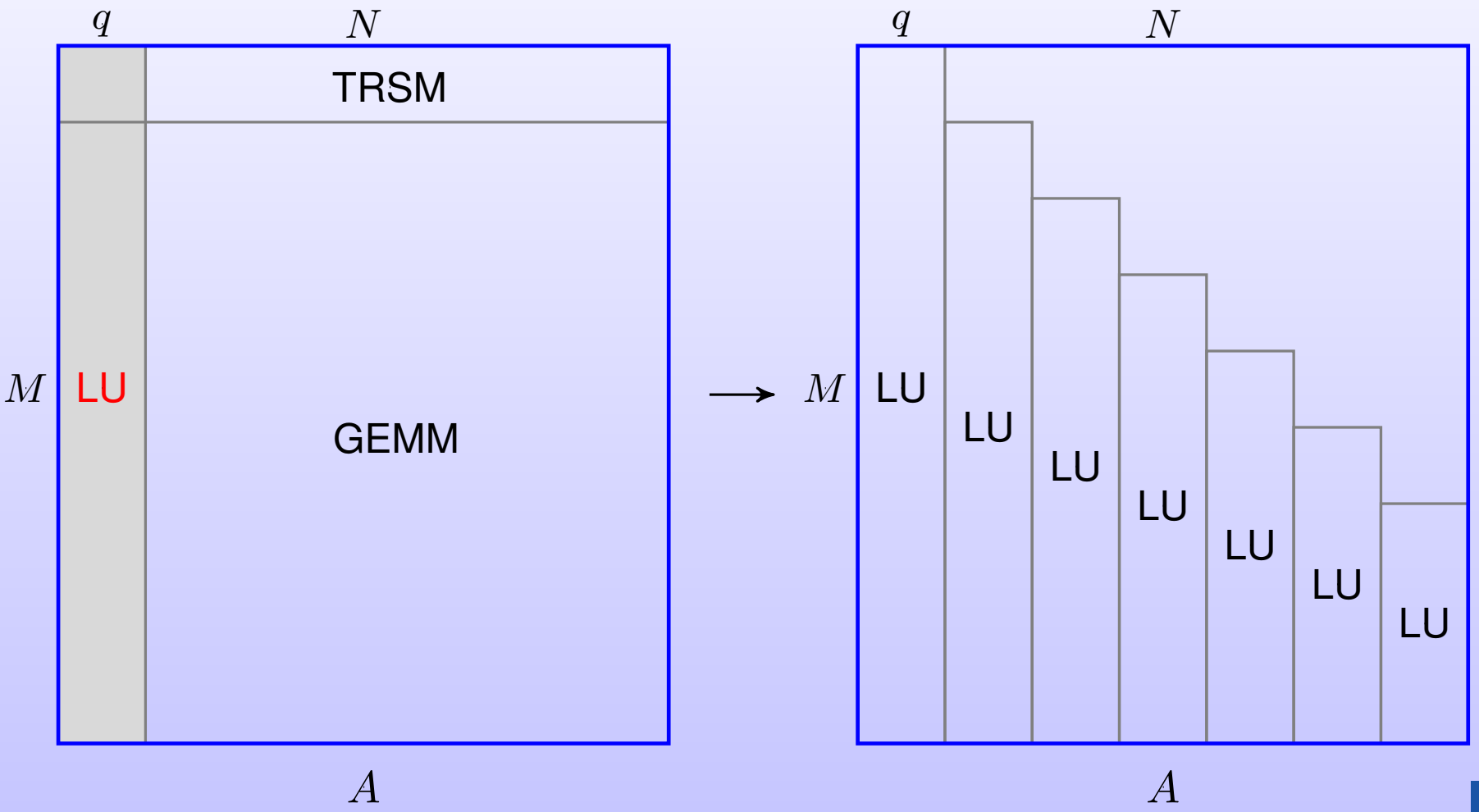
LU Factorization

$$\boxed{A = LU}$$



LU Factorization

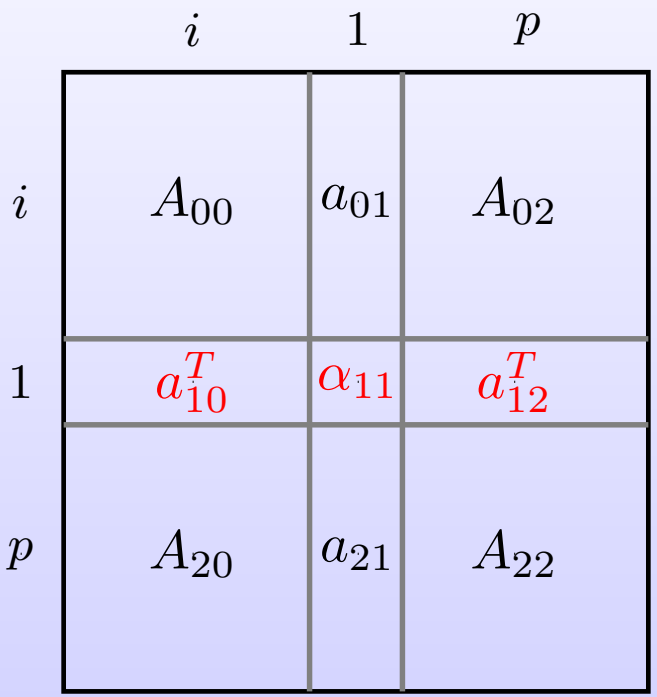
$$A = LU$$



An unblocked LU Factorization

LU Factorization

$$
\begin{array}{ll}
a_{10}^T := a_{10}^T U_{00}^{-1} & \texttt{TRSV} \\
\alpha_{11} := \alpha_{11} - a_{10}^T a_{01} & \texttt{DOT} \\
a_{12}^T := a_{12}^T - a_{10}^T A_{02} & \texttt{GEMV}
\end{array}
$$

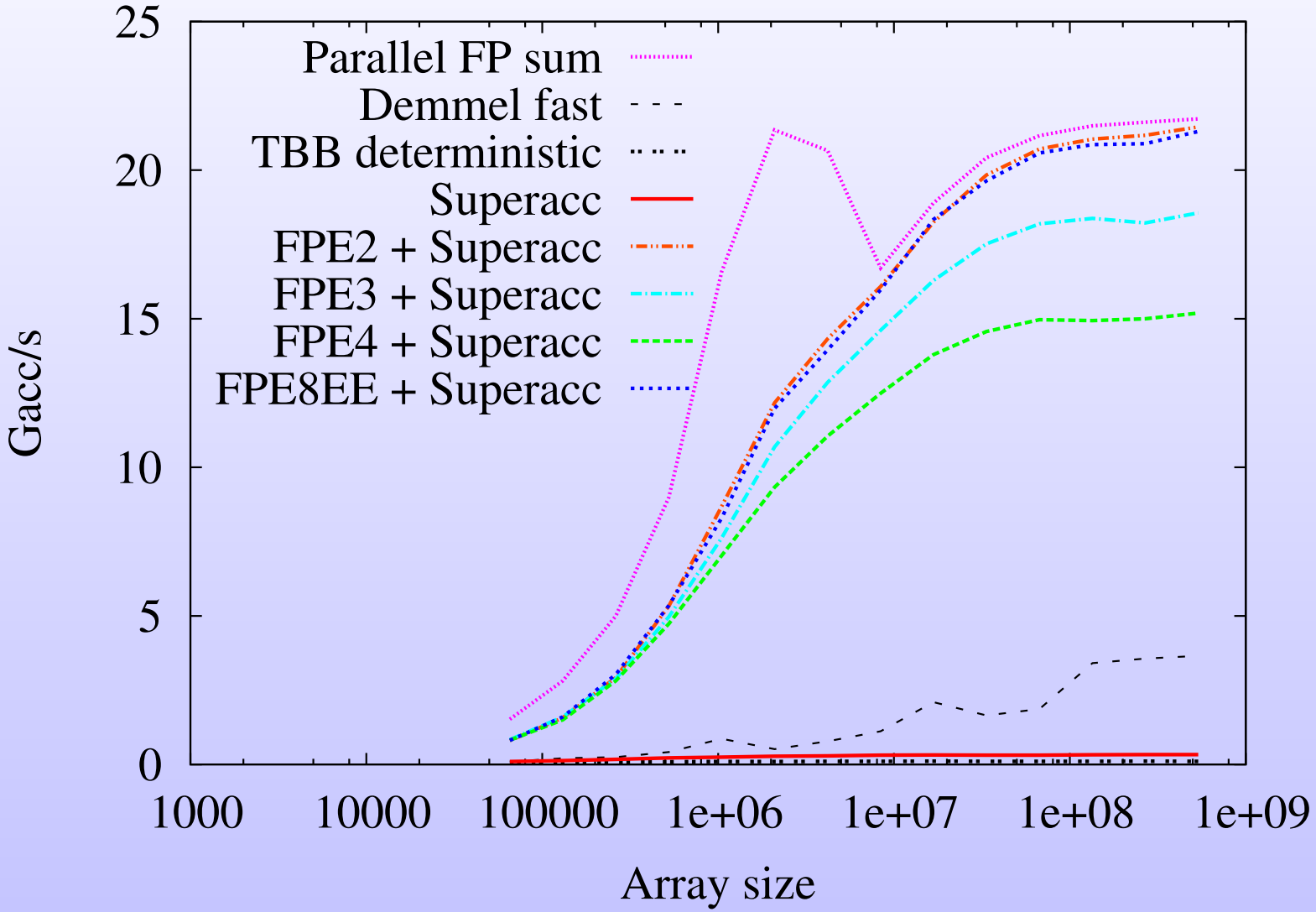


3×3 partitioning of A

Outline

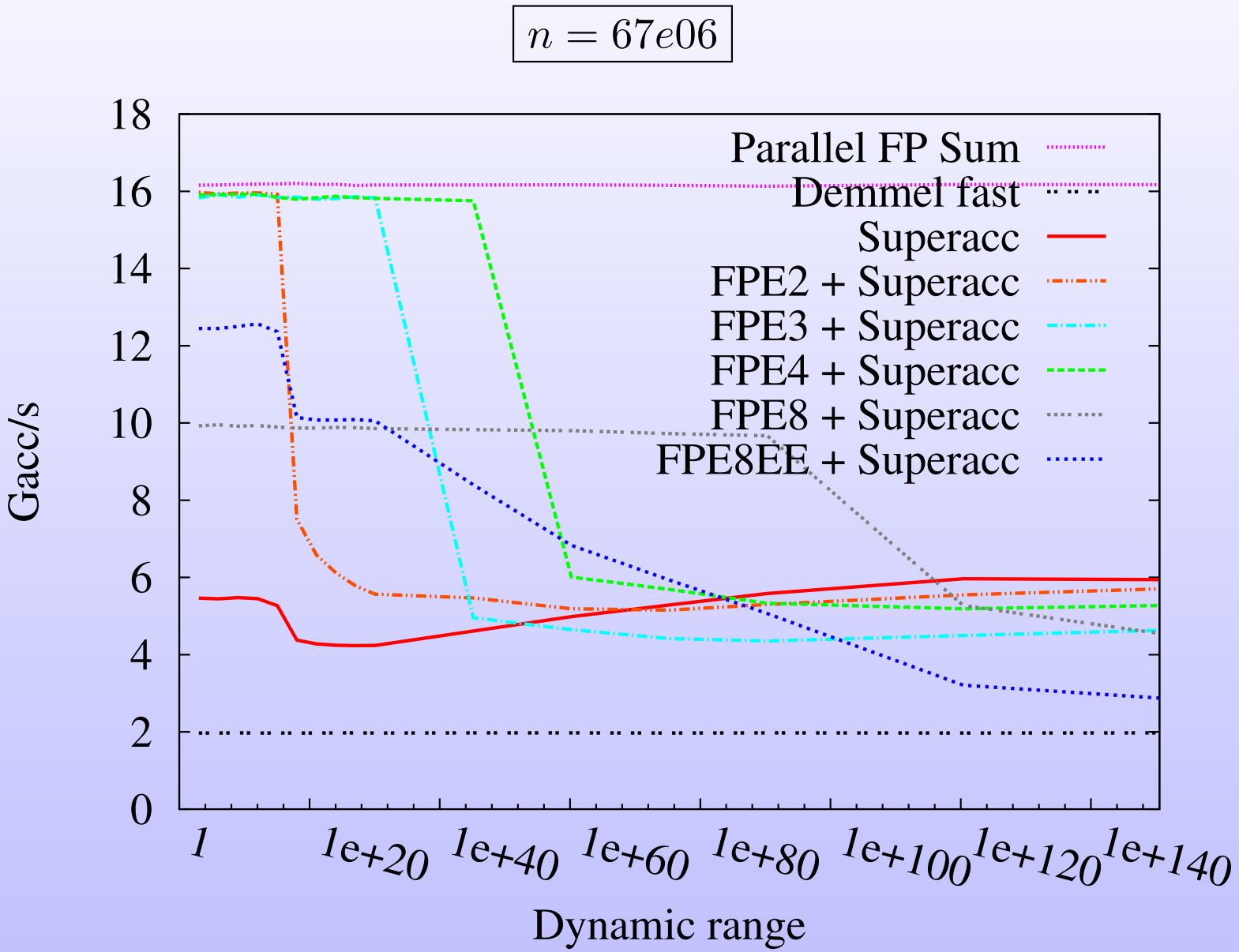
Parallel Reduction

Performance Scaling on Intel Xeon Phi



Parallel Reduction

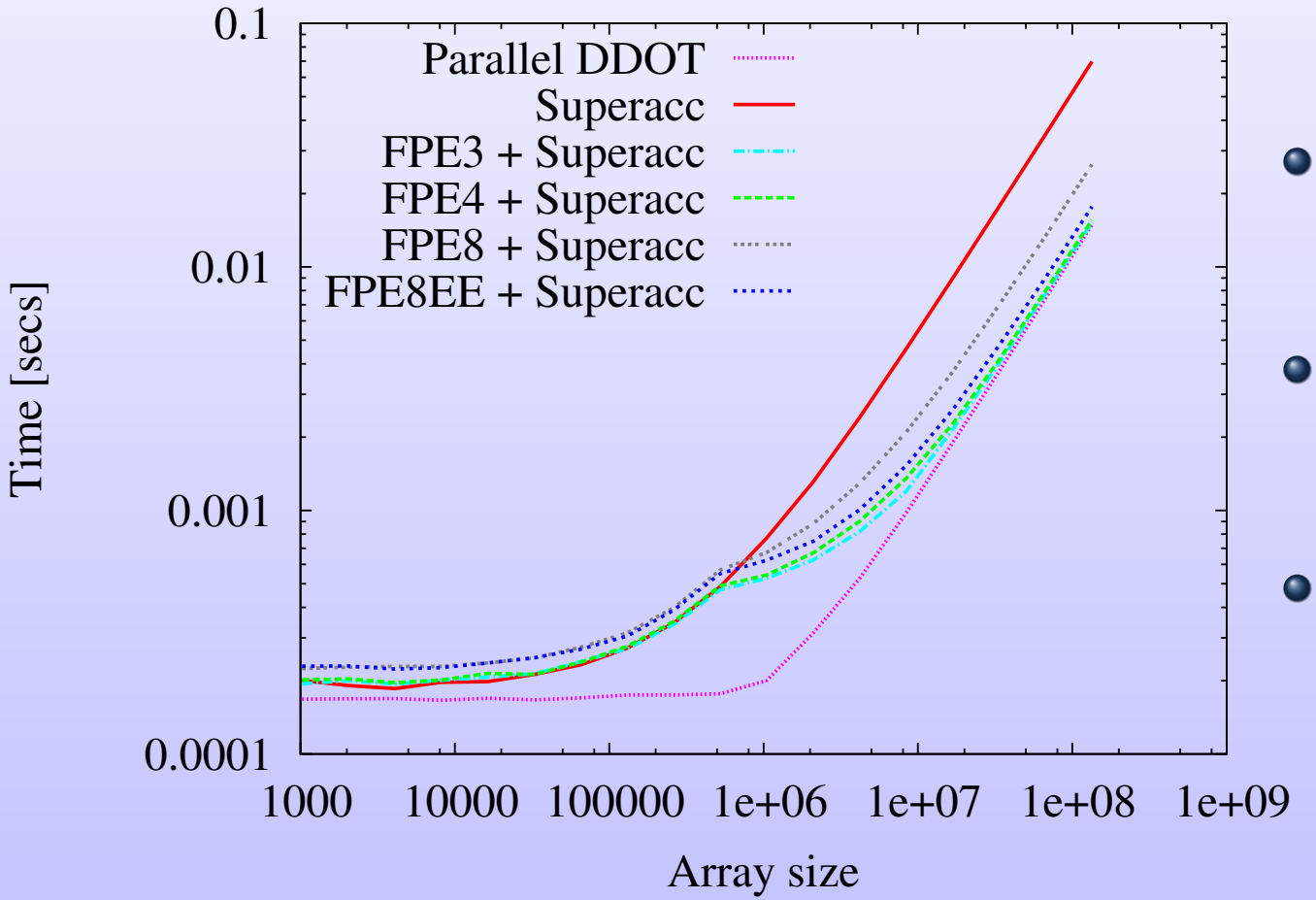
Data-Dependent Performance on NVIDIA Tesla K20c



Dot Product

Performance Scaling on NVIDIA Tesla K20c

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

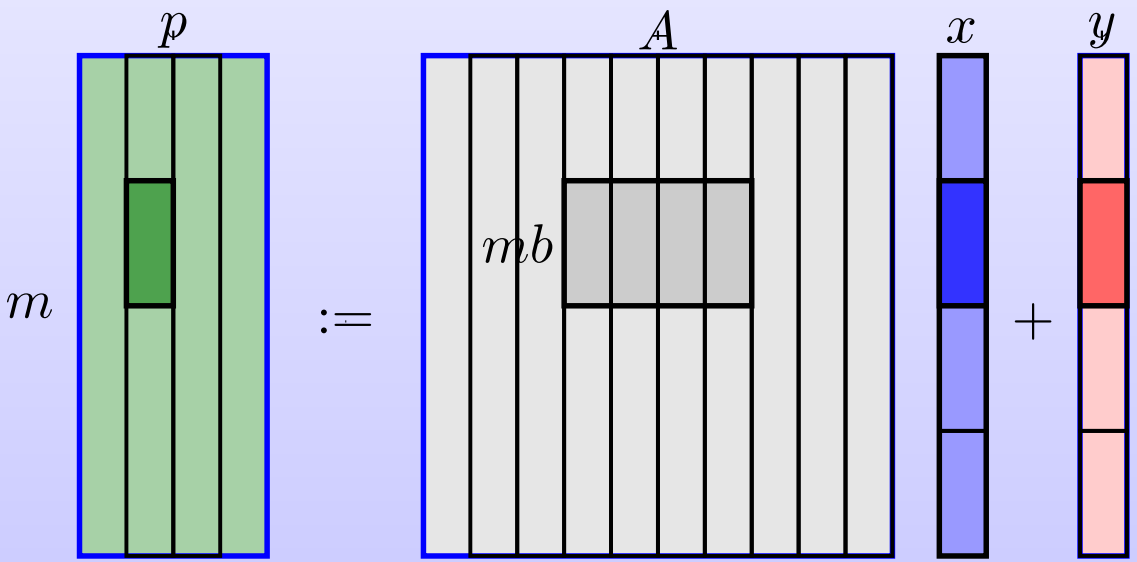


- Based on TwoProduct and Reproducible Summation
- TwoProduct(a, b)
  1: $r \leftarrow a * b$
  2: $s \leftarrow fma(a, b, -r)$
- $fma(a, b, c) = a * b + c$

Matrix-Vector Product

Performance Scaling on NVIDIA Tesla K80

DGEMV: $y := \alpha Ax + \beta y$



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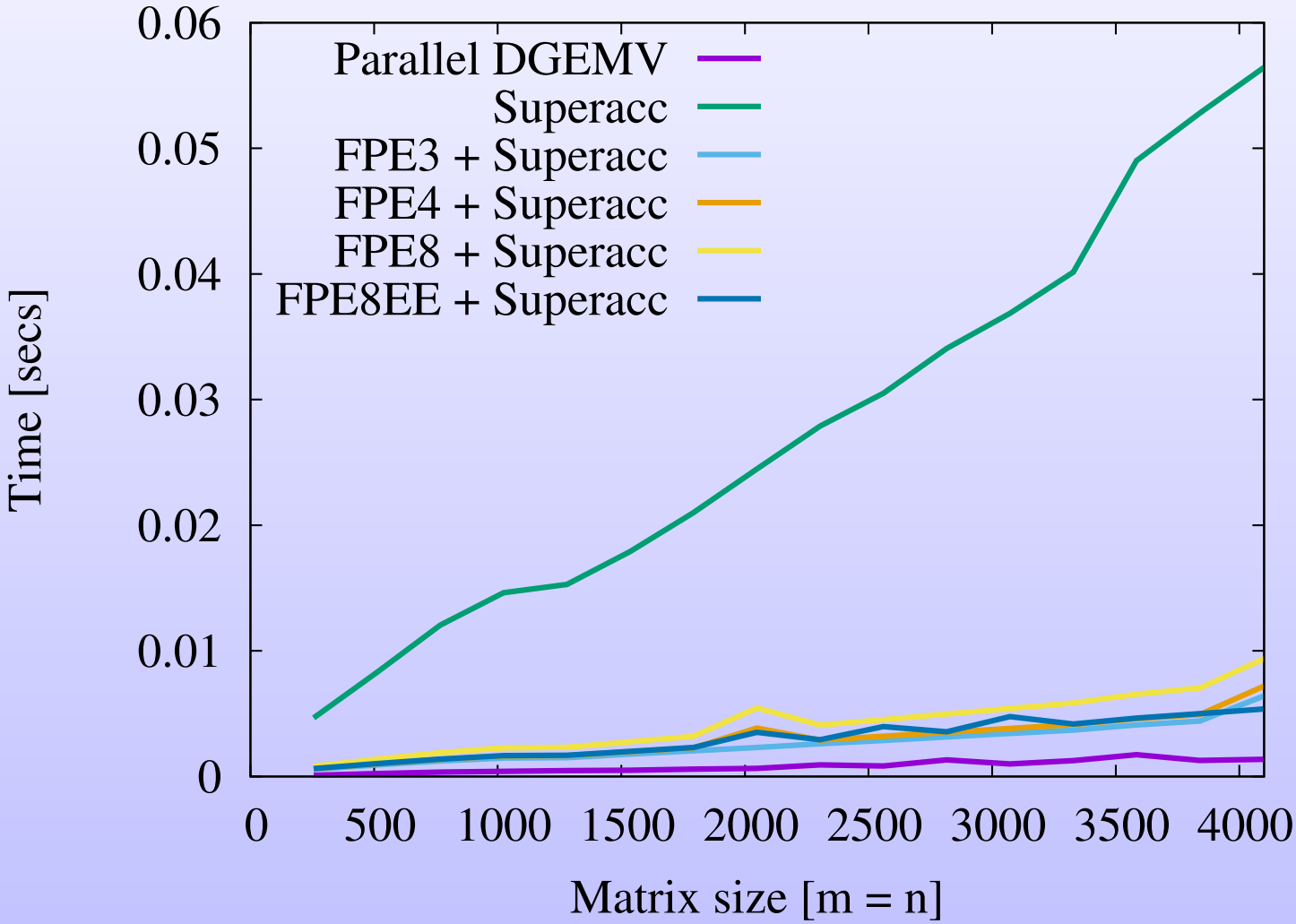

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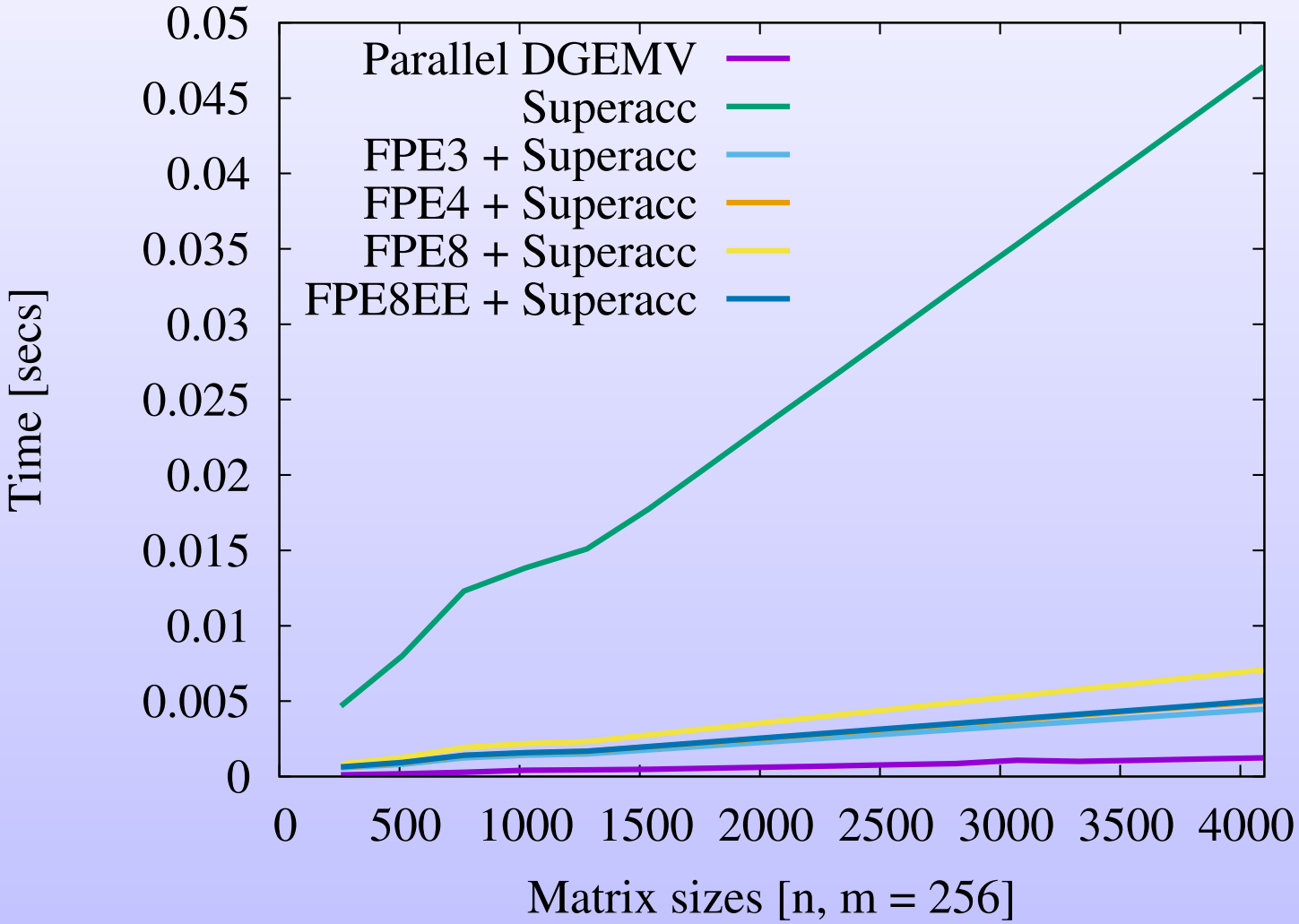
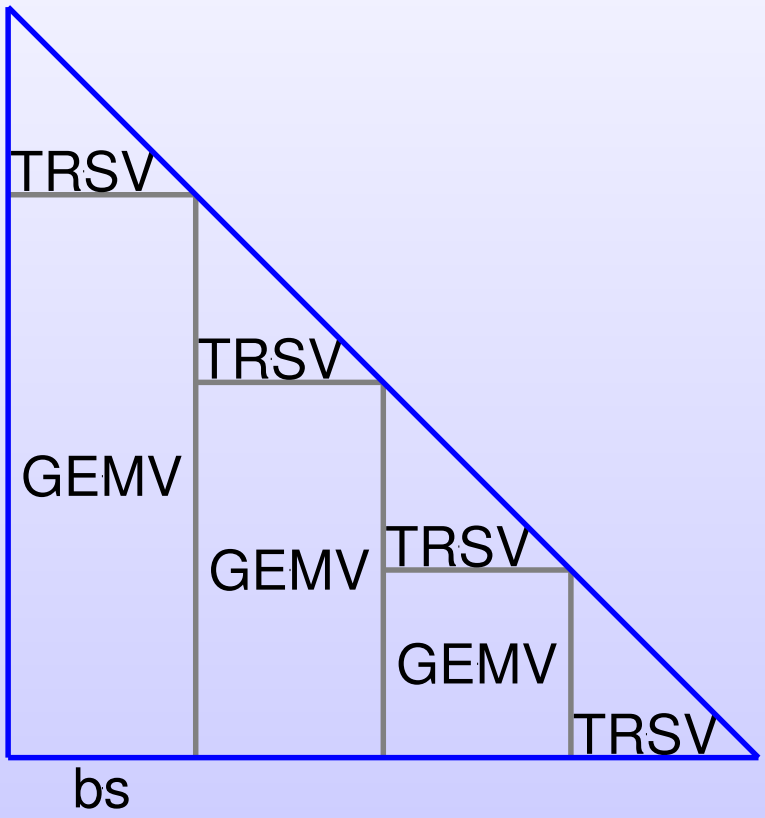
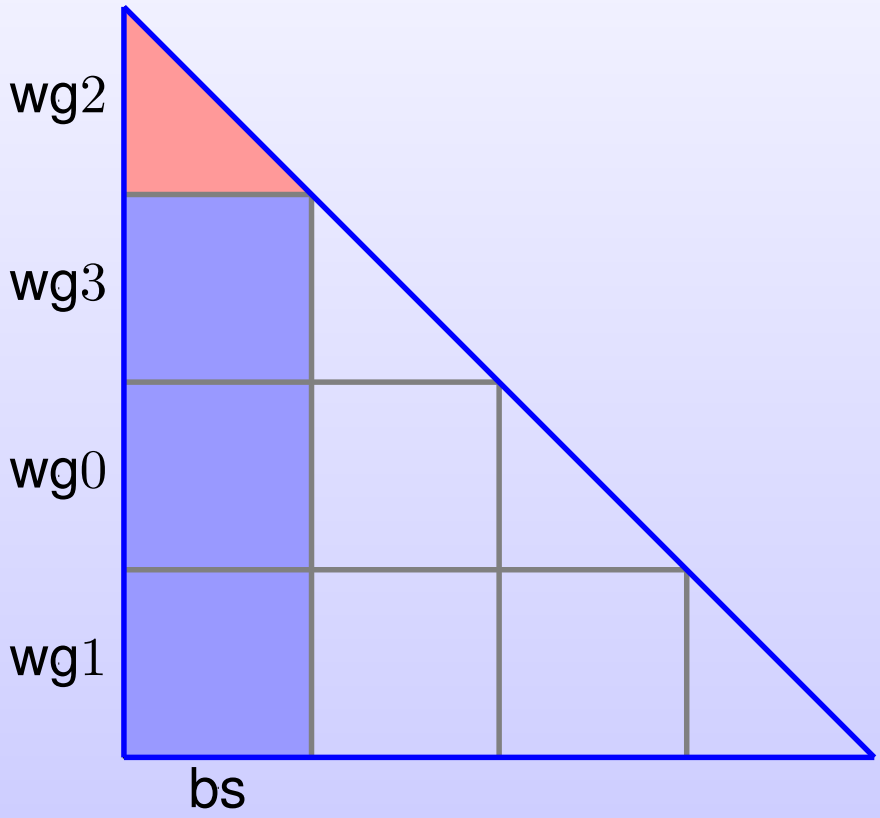


Triangular Solver

Matrix Partitioning



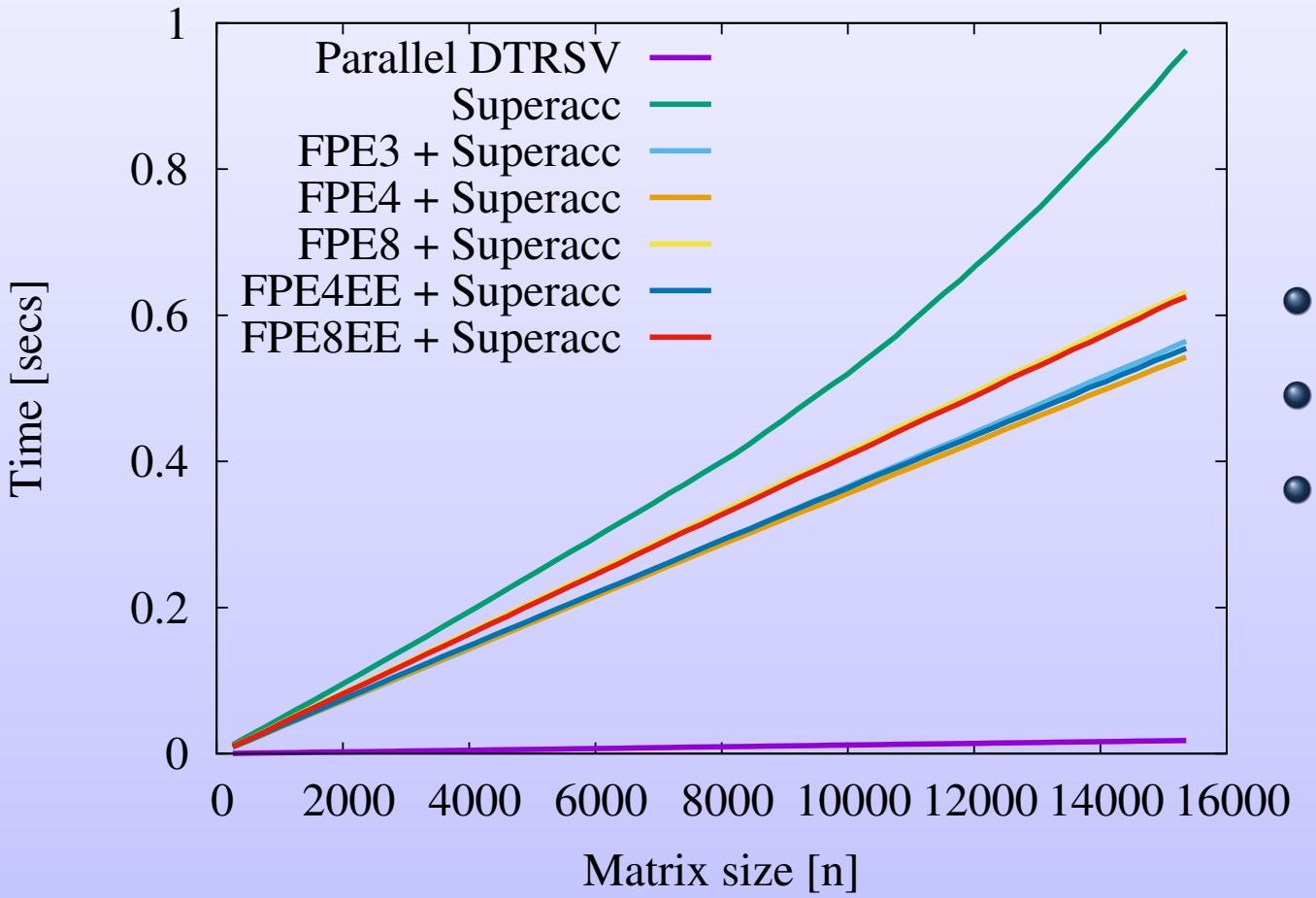


Partitioning of a lower triangular matrix L

Triangular Solver

Performance Scaling on NVIDIA Tesla K20c

DTRSV: $Ax = b$

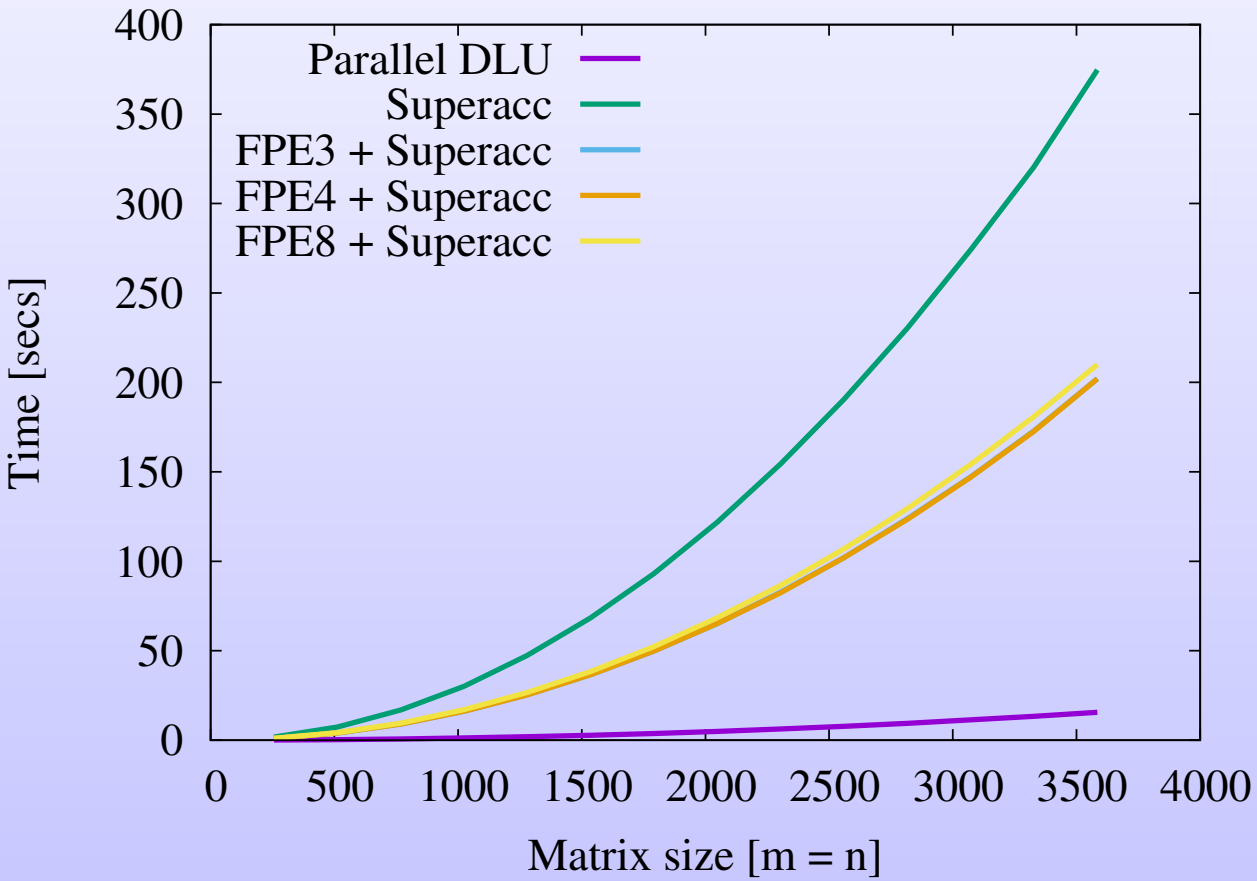


- Blocked ExTRSV
- Based on ExDOT
- Internal ExGEMV

LU Factorization

Performance Scaling on NVIDIA Tesla K80

$$\boxed{A = LU}$$



$$a_{10}^T \leftarrow a_{10}^T U_{00}^{-1} \qquad \texttt{trsv}$$
$$\alpha_{11} \leftarrow \alpha_{11} - a_{10}^T a_{01} \qquad \texttt{dot}$$
$$a_{12}^T \leftarrow a_{12}^T - a_{10}^T A_{02} \qquad \texttt{gemv}$$

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Conclusions and Future Work

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  - Thread scheduling
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  - Reduction trees

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Future directions

- Enhance compute-intensive operations and the LU factorization
- Cover the other variants of the unblocked LU factorization
- Application of our implementations in real-world codes

Thank you for your attention!

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

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[a] Routines in blue are already in ExBLAS