High performance computer algebra: how to use floating point arithmetic exactly?

Journée Informatique et Calcul

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Exact linear algebra

Coefficient domains:

Word size:
- integers with a priori bounds
- $\mathbb{Z}/p\mathbb{Z}$ for p of ≈ 32 bits

Multi-precision: $\mathbb{Z}/p\mathbb{Z}$ for p of $\approx 100, 200, 1000, 2000, \ldots$ bits

Arbitrary precision: $\mathbb{Z}, \mathbb{Q}$

Polynomials: $\mathsf{K}[X]$ for K any of the above

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Need for genericity.

Exact linear algebra

Motivations

Comp. Number Theory:	CharPoly, LinSys, Echelon, over $\mathbb{Z}, \mathbb{Q}, \mathbb{Z}/p\mathbb{Z}$, Dense
Graph Theory:	MatMul, CharPoly, Det, over $\mathbb{Z}$, Sparse
Discrete log.:	LinSys, over $\mathbb{Z}/p\mathbb{Z}$, $p \approx 120$ bits, Sparse
Integer Factorization:	NullSpace, over $\mathbb{Z}/2\mathbb{Z}$, Sparse
Algebraic Attacks:	Echelon, LinSys, over $\mathbb{Z}/p\mathbb{Z}$, $p \approx 20$ bits, Sparse & Dense
List decoding of RS codes:	Lattice reduction, over GF$(q)[X]$, Structured

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Need for high performance.

Outline

1. Choosing the underlying arithmetic
   - Using machine word arithmetic
   - Larger field sizes
2. Algorithmic: reductions and building blocks
3. Parallel exact linear algebra

Outline

Achieving high practical efficiency

Most of linear algebra operations boil down to (a lot of)

$$\texttt{y} \leftarrow \texttt{y} \pm \texttt{a} * \texttt{b}$$

- dot-product
- matrix-matrix multiplication
- rank 1 update in Gaussian elimination
- Schur complements, ...

Efficiency relies on

- fast arithmetic
- fast memory accesses

Here: focus on dense linear algebra

Which computer arithmetic ?

Many base fields/rings to support

$\mathbb{Z}_2$	1 bit
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$\mathbb{Z}_p$	$>$ 32 bits	$\rightsquigarrow$ multiprec. ints, big ints, CRT
$\mathsf{GF}(p^k) \equiv \mathbb{Z}_p[X]/(Q)$		$\rightsquigarrow$ Polynomial, Kronecker, Zech log, ...

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Dense linear algebra over $\mathbb{Z}_p$ for word-size p

Delayed modular reductions

1. Compute using integer arithmetic
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When to reduce ?

Bound the values of all intermediate computations.

- A priori:

Representation of $\mathbb{Z}_p$	$\{0 \dots p-1\}$	$\{-\frac{p-1}{2} \dots \frac{p-1}{2}\}$
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- Maintain locally a bounding interval on all matrices computed

Computing over fixed size integers

How to compute with (machine word size) integers efficiently?

1. use CPU's **integer arithmetic units**
   `y += a * b`: correct if $|ab + y| < 2^{63} \rightsquigarrow |a|, |b| < 2^{31}$

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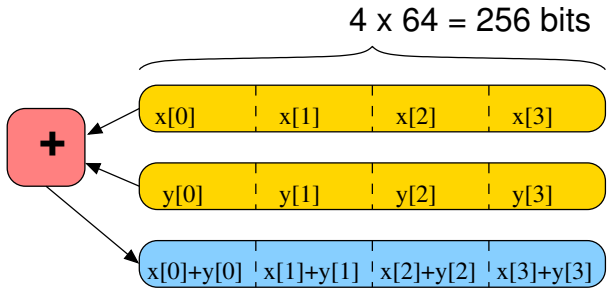
```
vinsertf128   $0x1, 16(%rcx,%rax), %ymm0,
vmulpd        %ymm1, %ymm0, %ymm0
vaddpd        (%rsi,%rax),%ymm0, %ymm0
vmovapd       %ymm0, (%rsi,%rax)
```

Exploiting *in-core* parallelism

Ingredients

SIMD: Single Instruction Multiple Data:
1 arith. unit acting on a vector of data

MMX	64 bits
SSE	128bits
AVX	256 bits
AVX-512	512 bits



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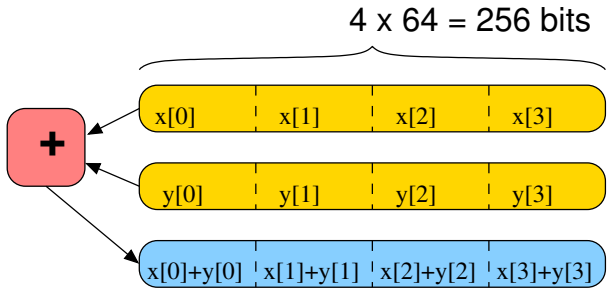

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throughput of 1 op/ Cycle for all arithmetic ops considered here

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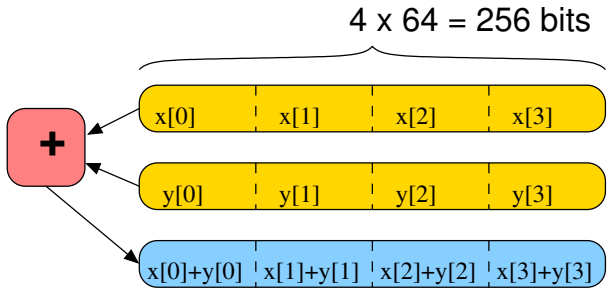

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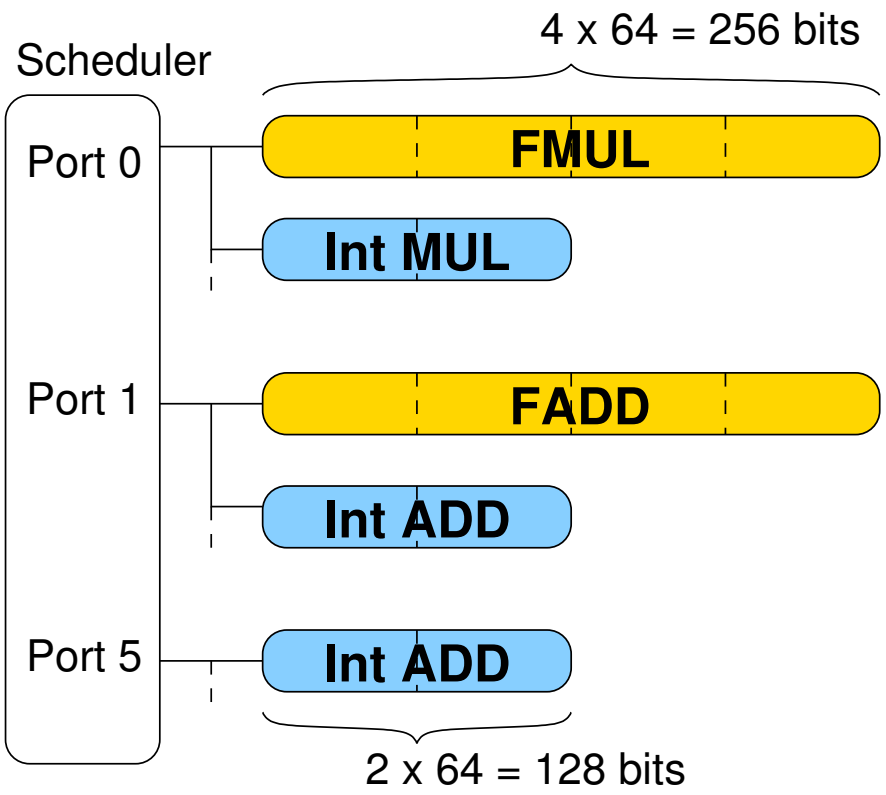
Execution Unit parallelism: multiple arith. units acting simulatneously on distinct registers

SIMD and vectorization

Intel Sandybridge micro-architecture



Performs at every clock cycle:

- 1 Floating Pt. Mul $\times$ 4
- 1 Floating Pt. Add $\times$ 4

Or:

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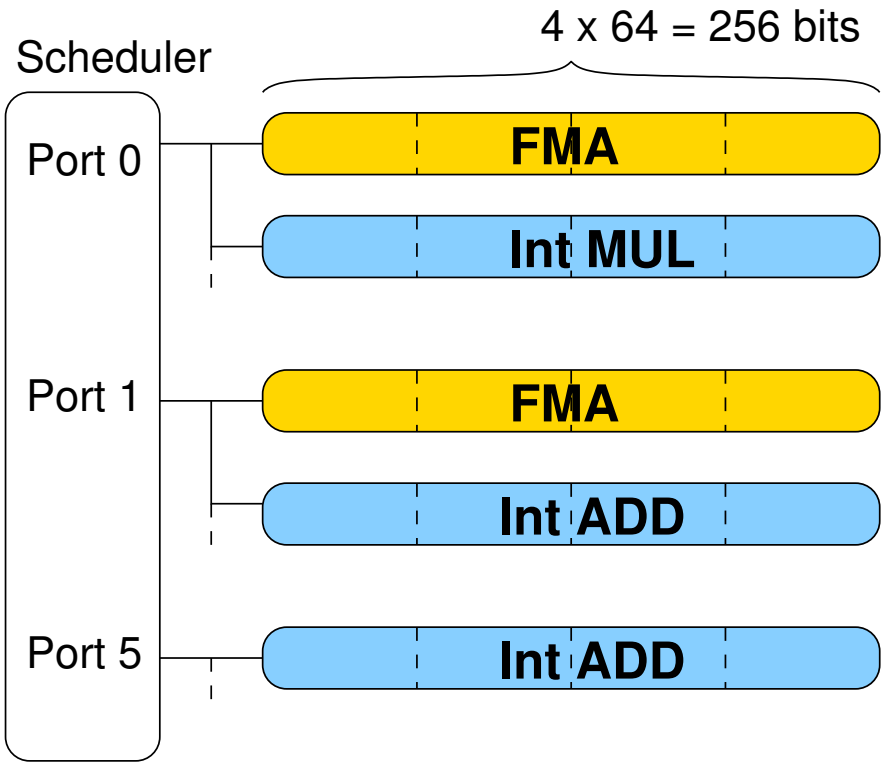
- 2 Integer Add $\times$ 2

SIMD and vectorization

Intel Haswell micro-architecture



Performs at every clock cycle:

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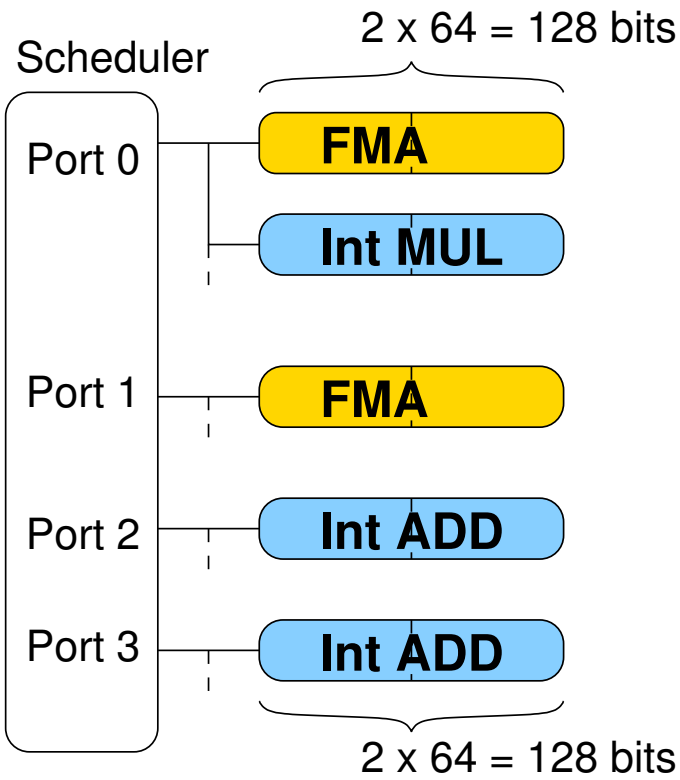
FMA: Fused Multiplying & Accumulate, `c += a * b`

SIMD and vectorization

AMD Bulldozer micro-architecture



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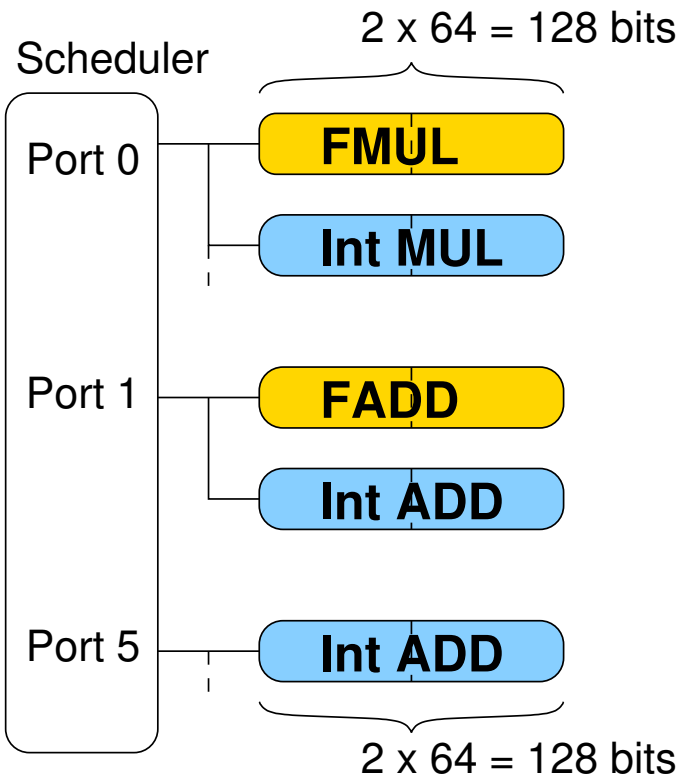

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Intel Haswell	INT	256	2	1		4	3.5	**28**	
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Speed of light: CPU freq $\times$ (# daxpy / Cycle) $\times 2$

Summary: 64 bits AXPY throughput

		Register size	# Adders	# Multipliers	# FMA	# daxpy /Cycle	CPU Freq. (Ghz)	Speed of Light (Gfops)	Speed in practice (Gfops)
Intel Haswell	INT	256	2	1		4	3.5	**28**	**23.3**
AVX2	FP	256			2	8	3.5	**56**	**49.2**
Intel Sandybridge	INT	128	2	1		2	3.3	**13.2**	**12.1**
AVX1	FP	256	1	1		4	3.3	**26.4**	**24.6**
AMD Bulldozer	INT	128	2	1		2	2.1	**8.4**	**6.44**
FMA4	FP	128			2	4	2.1	**16.8**	**13.1**
Intel Nehalem	INT	128	2	1		2	2.66	**10.6**	**4.47**
SSE4	FP	128	1	1		2	2.66	**10.6**	**9.6**
AMD K10	INT	64	2	1		1	2.4	**4.8**	
SSE4a	FP	128	1	1		2	2.4	**9.6**	**8.93**

Speed of light: CPU freq $\times$ (# daxpy / Cycle) $\times 2$

Computing over fixed size integers: ressources

Micro-architecture bible: Agner Fog's software optimization resources [www.agner.org/optimize]

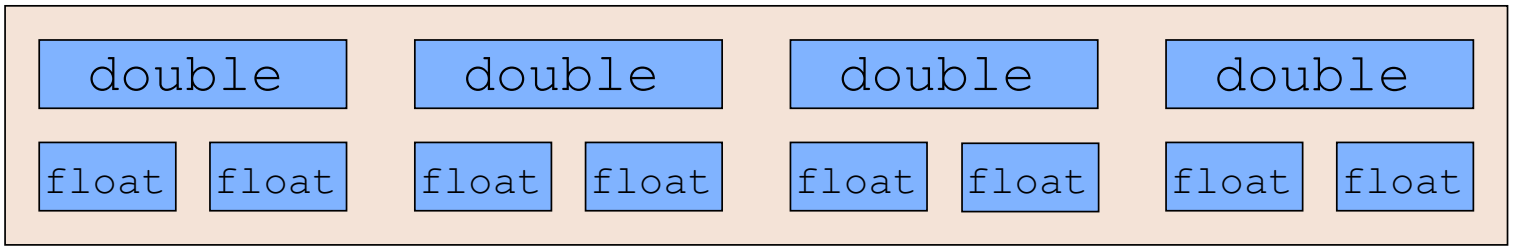
Experiments:

dgemm (double): OpenBLAS [http://www.openblas.net/]

igemm (int64_t): Eigen [http://eigen.tuxfamily.org/] & FFLAS-FFPACK [linalg.org/projects/fflas-ffpack]

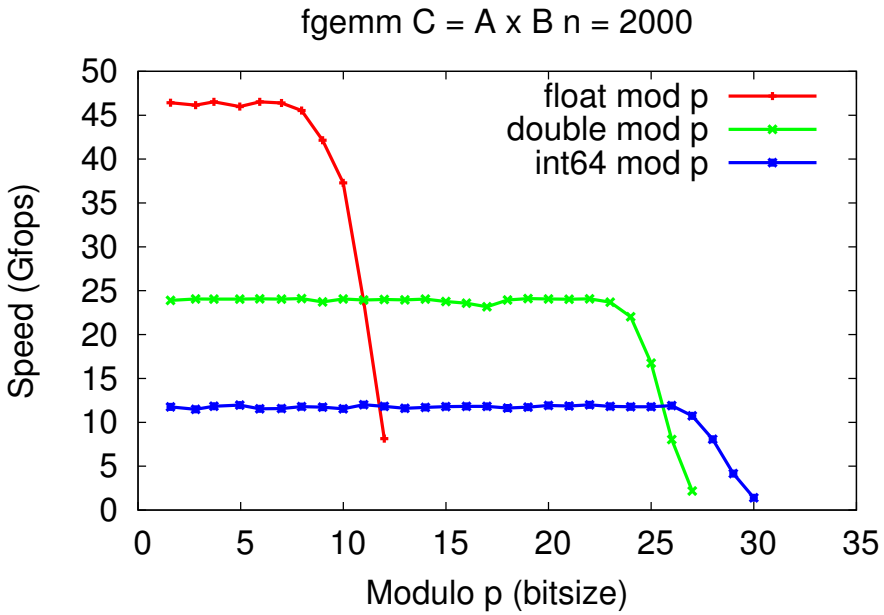
Integer Packing

32 bits: half the precision twice the speed



Gfops	`double`	`float`	`int64_t`	`int32_t`
Intel SandyBridge	24.7	49.1	12.1	24.7
Intel Haswell	49.2	77.6	23.3	27.4
AMD Bulldozer	13.0	20.7	6.63	11.8

Computing over fixed size integers

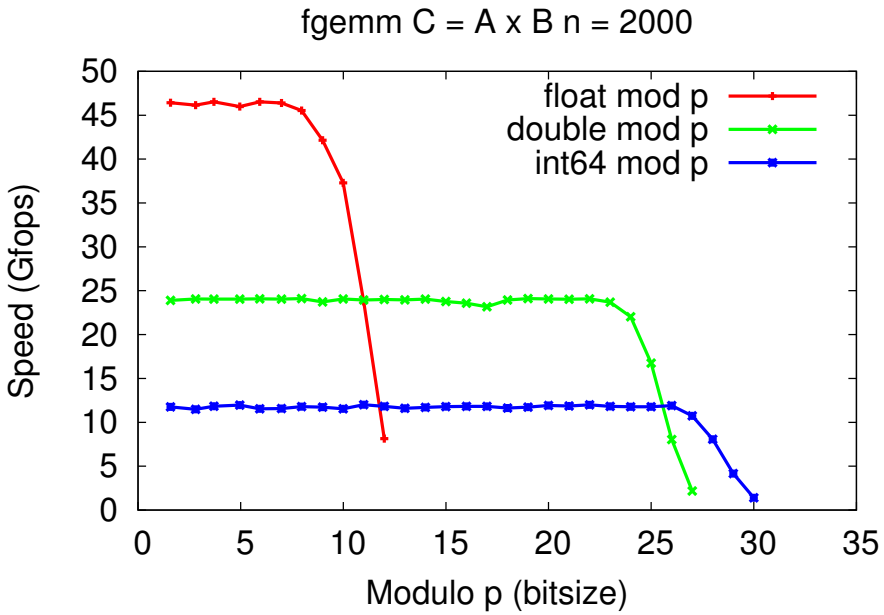


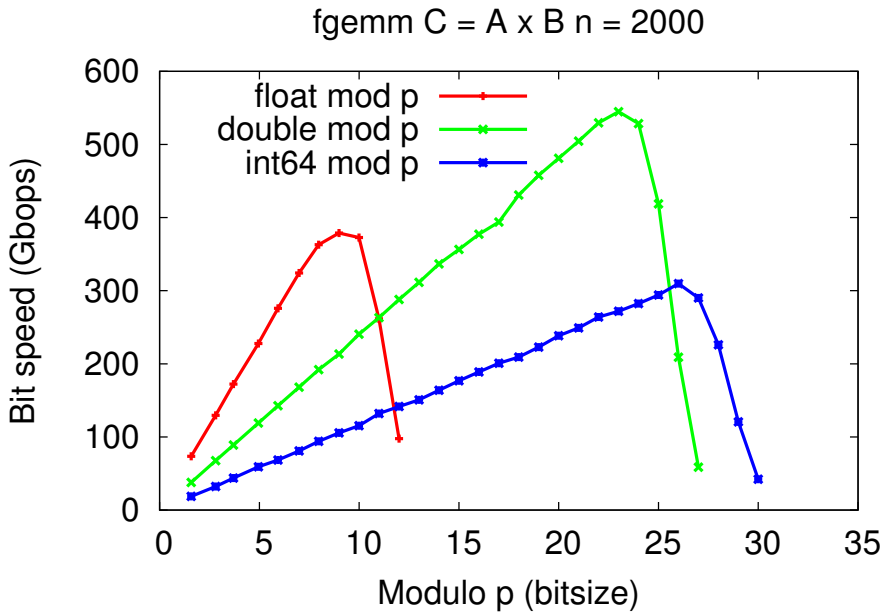
SandyBridge i5-3320M@3.3Ghz. $n = 2000$.

Take home message

- Floating pt. arith. delivers the highest speed (except in corner cases)
- 32 bits twice as fast as 64 bits

Computing over fixed size integers





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Take home message

- Floating pt. arith. delivers the highest speed (except in corner cases)
- 32 bits twice as fast as 64 bits
- best bit computation throughput for double precision floating points.

Larger finite fields: $\log_2 p \geq 32$

As before:

1. Use adequate integer arithmetic
2. reduce modulo p only when necessary

Which integer arithmetic?

1. big integers (GMP)
2. fixed size multiprecision (Givaro-RecInt)
3. Residue Number Systems (Chinese Remainder theorem)
   $\rightsquigarrow$ using moduli delivering optimum bitspeed

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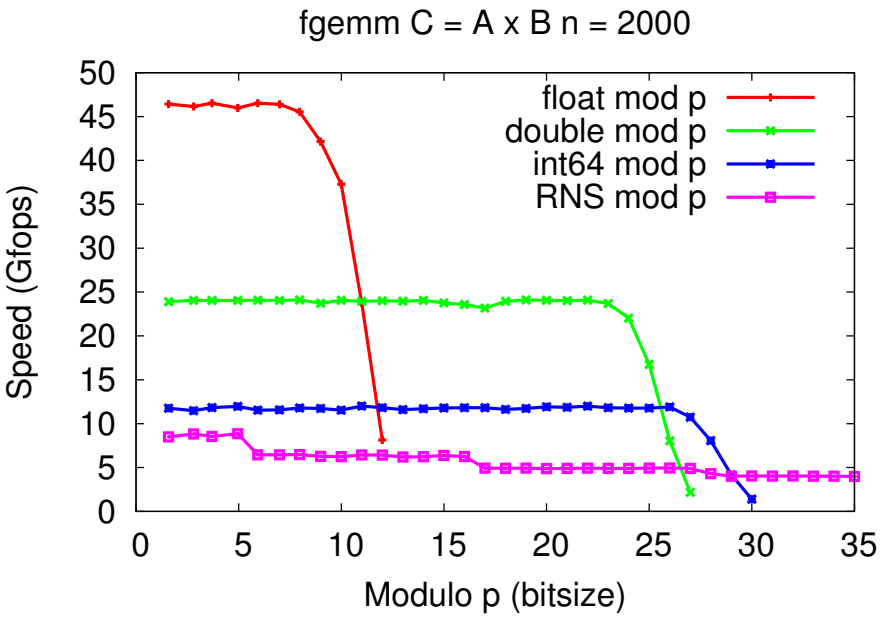
$\log_2 p$	50	100	150
GMP	58.1s	94.6s	140s
RecInt	5.7s	28.6s	837s
RNS	0.785s	1.42s	1.88s

$n = 1000$, on an Intel SandyBridge.

In practice


fgemm C = A x B n = 2000
Speed (Gfops)
Modulo p (bitsize)
float mod p
double mod p
int64 mod p
RNS mod p
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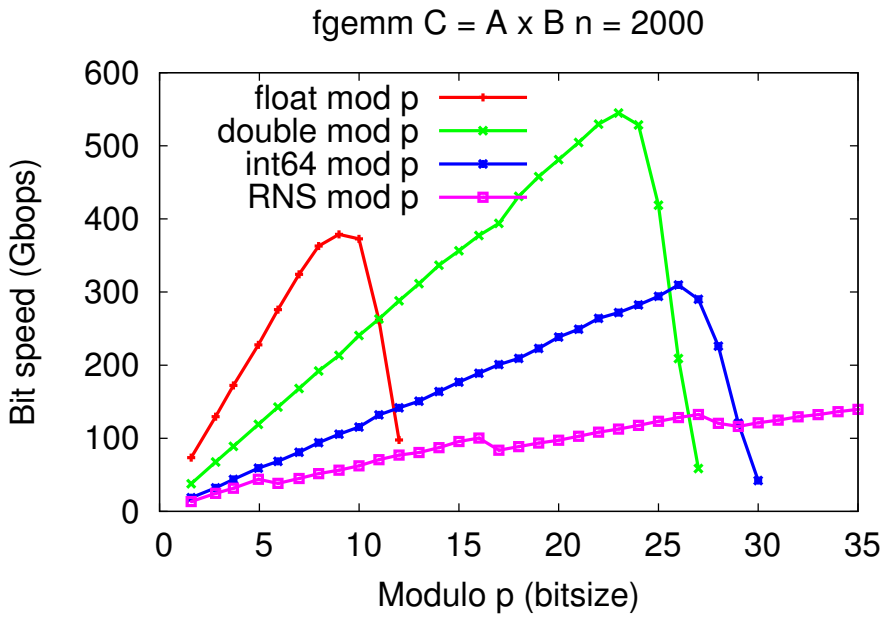
fgemm C = A x B n = 2000
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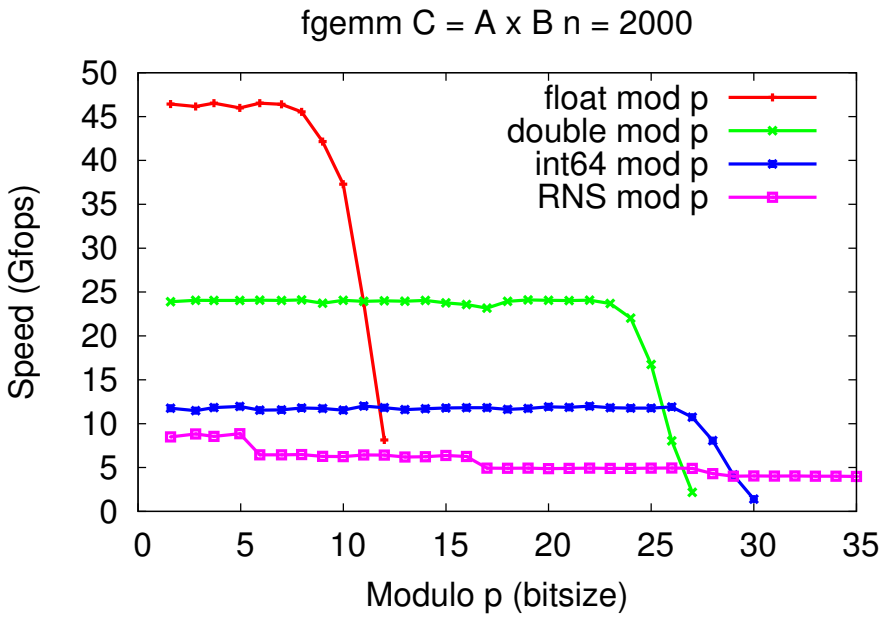
In practice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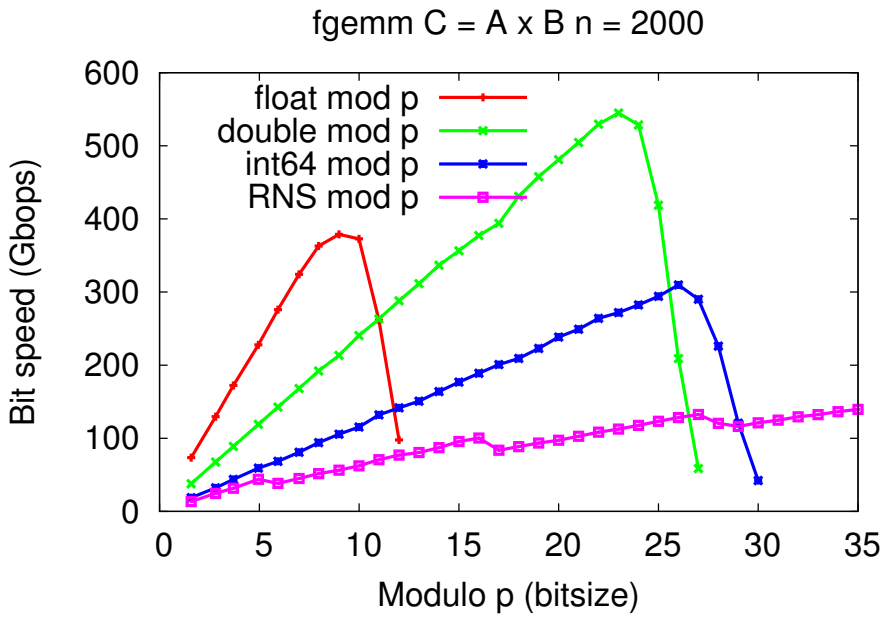
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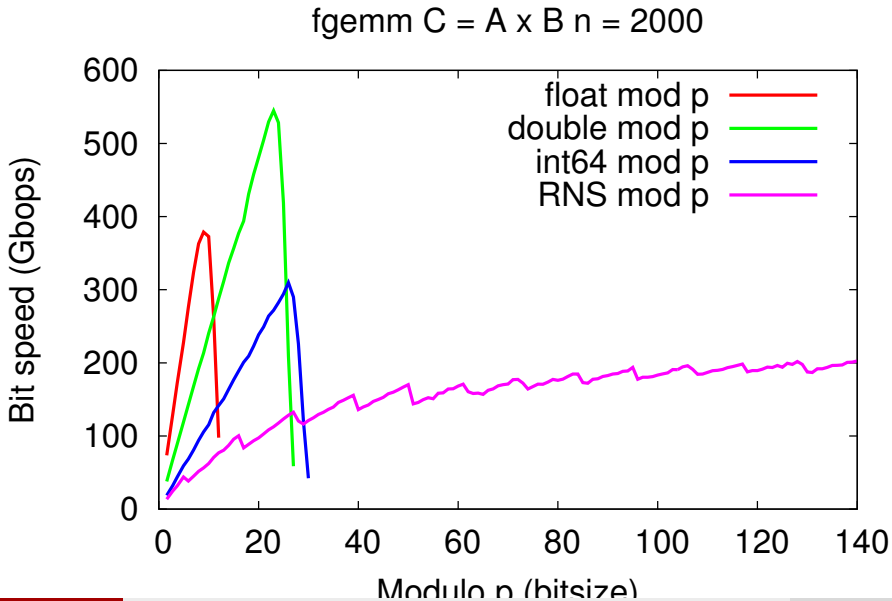
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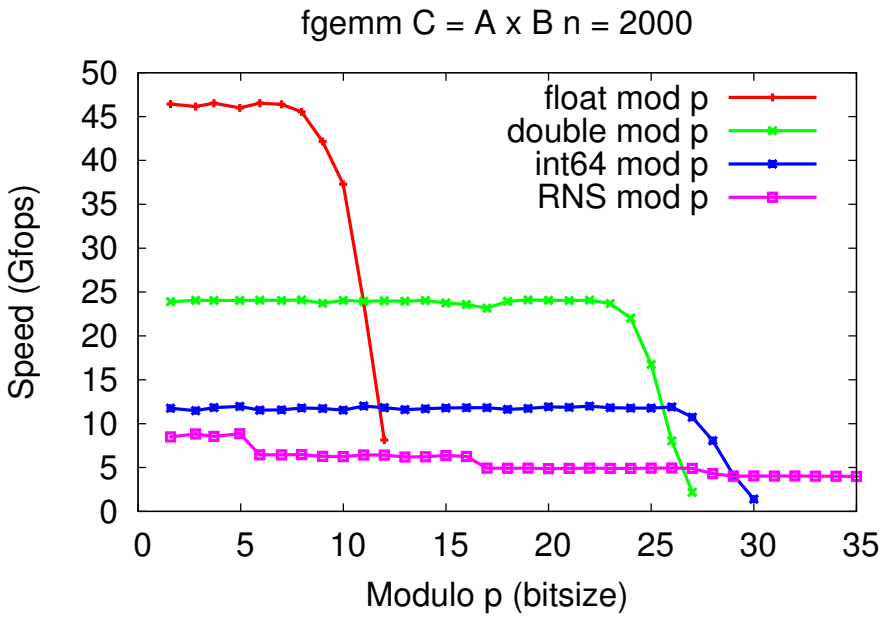
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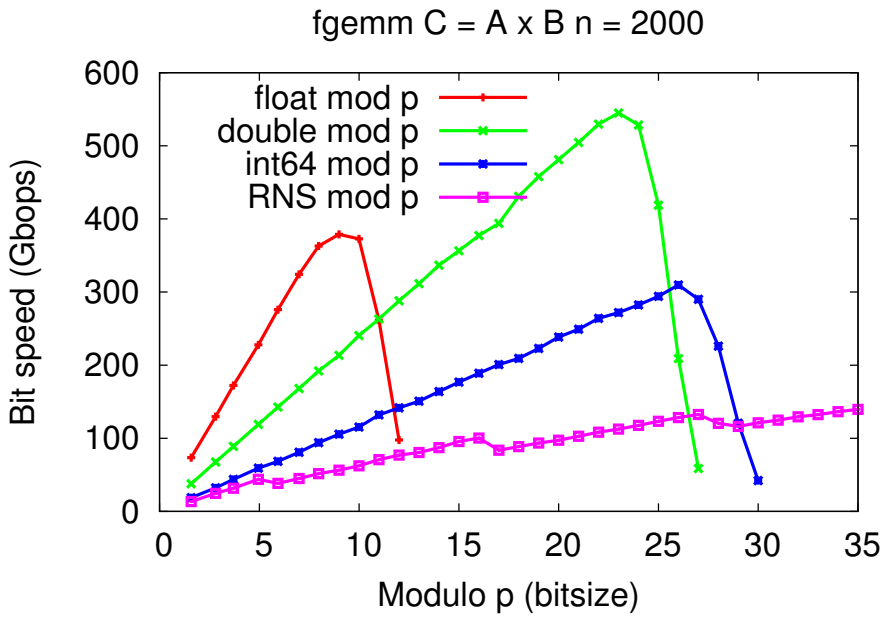
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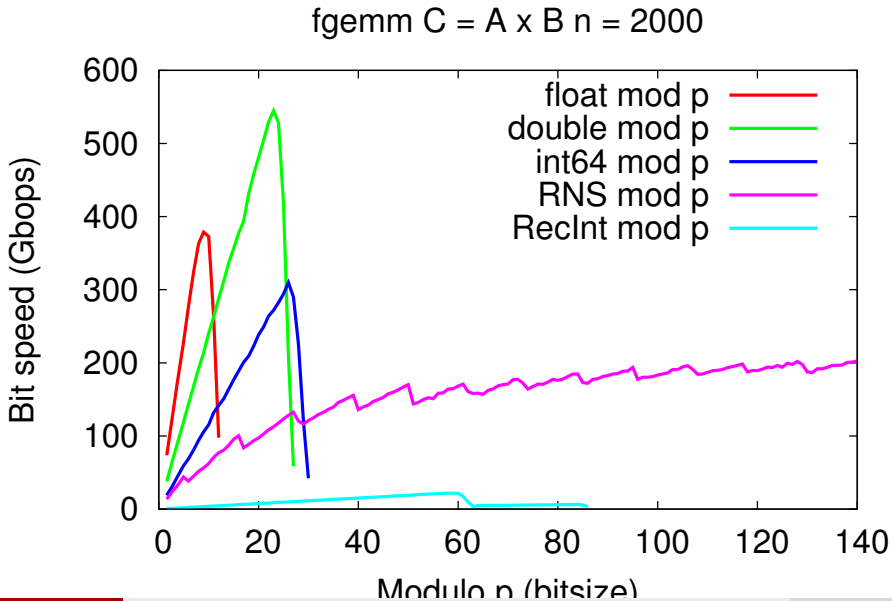
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Outline

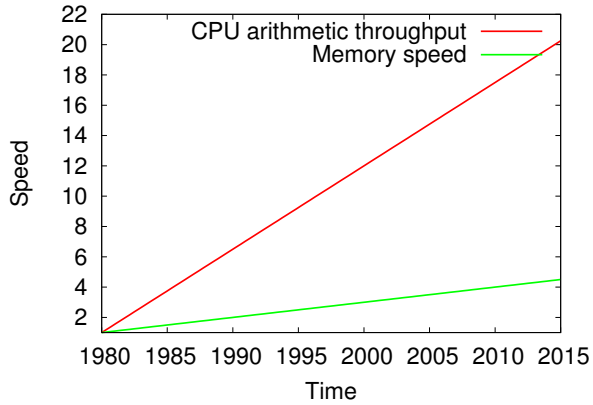
Reductions to building blocks

Huge number of algorithmic variants for a given computation in $O(n^3)$.
Need to structure the design of set of routines :

- Focus tuning effort on a single routine
- Some operations deliver better efficiency:
  - in practice: memory access pattern
  - in theory: better algorithms

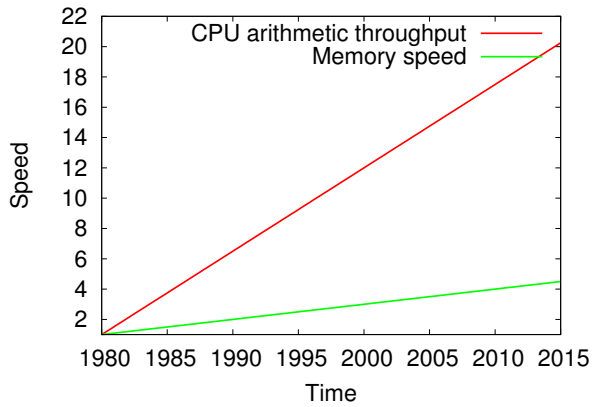
Memory access pattern

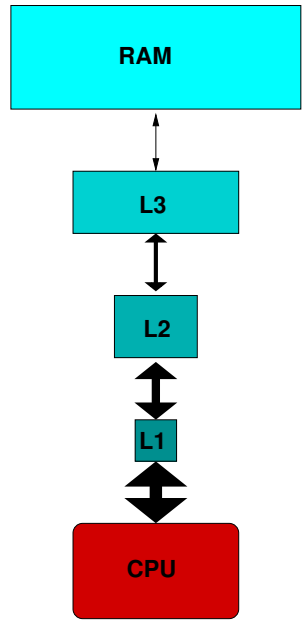
- **The memory wall:** communication speed improves slower than arithmetic



Memory access pattern

- **The memory wall:** communication speed improves slower than arithmetic
- Deep memory hierarchy





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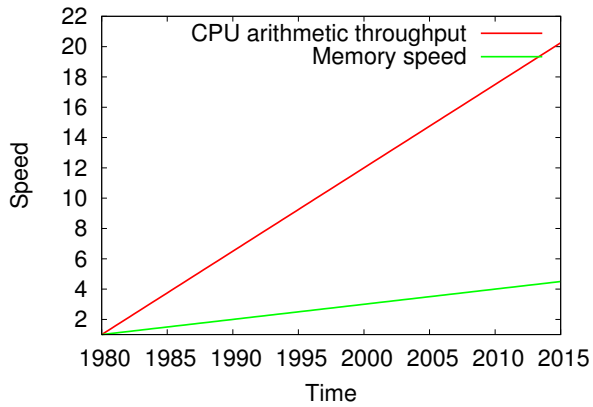
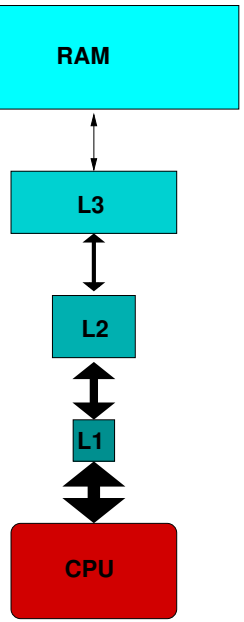
$\rightsquigarrow$ Need to overlap communications by computation





Design of BLAS 3 [Dongarra & Al. 87]

- Group all ops in Matrix products `gemm`:
  Work $O(n^3)$ >> Data $O(n^2)$

MatMul has become a building block in practice

Sub-cubic linear algebra

< 1969: $O(n^3)$ for everyone (Gauss, Householder, Danilevskǐi, etc)

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Matrix Multiplication $\rightsquigarrow O(n^\omega)$

[Strassen 69]:	$O(n^{2.807})$
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[Schönhage 81]	$O(n^{2.52})$
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[Coppersmith, Winograd 90]	$O(n^{2.375})$
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[Schönhage 72]:	QR in $O(n^\omega)$
[Bunch, Hopcroft 74]:	LU in $O(n^\omega)$
[Ibarra & *al.* 82]:	Rank in $O(n^\omega)$
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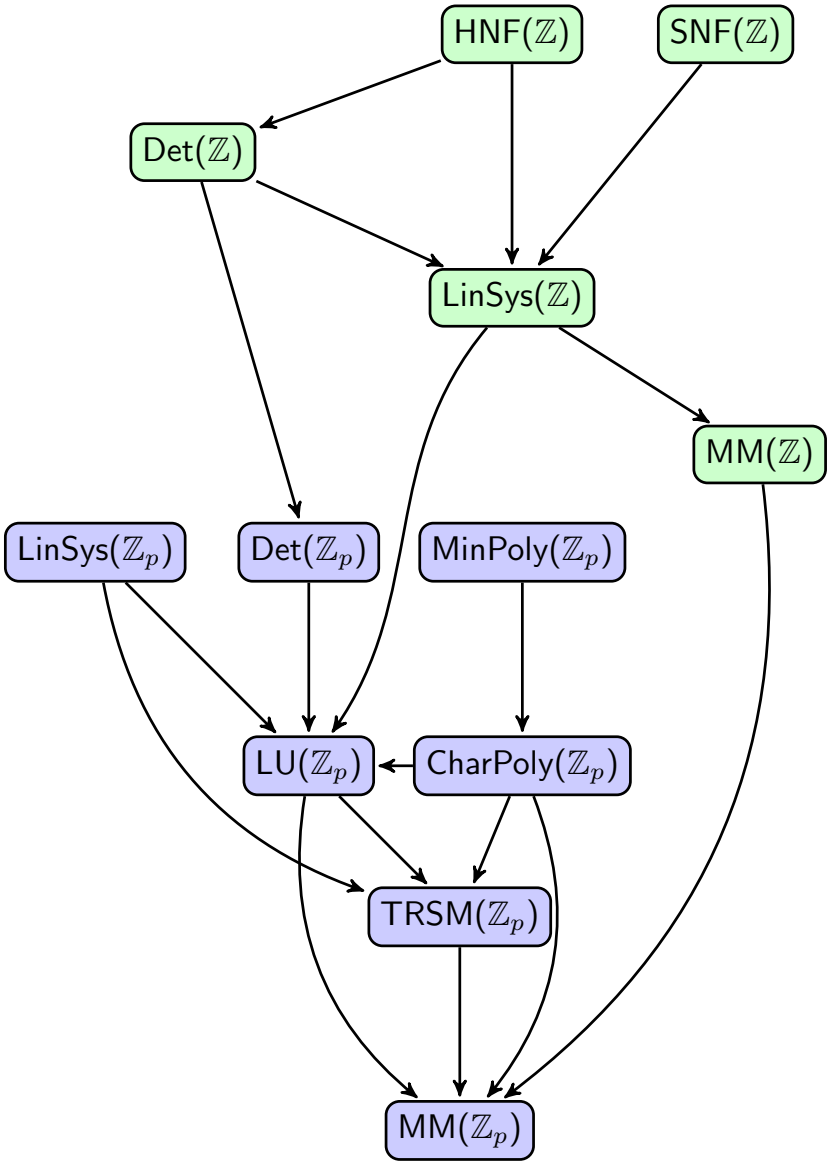
MatMul has become a building block in theoretical reductions

Reductions: theory



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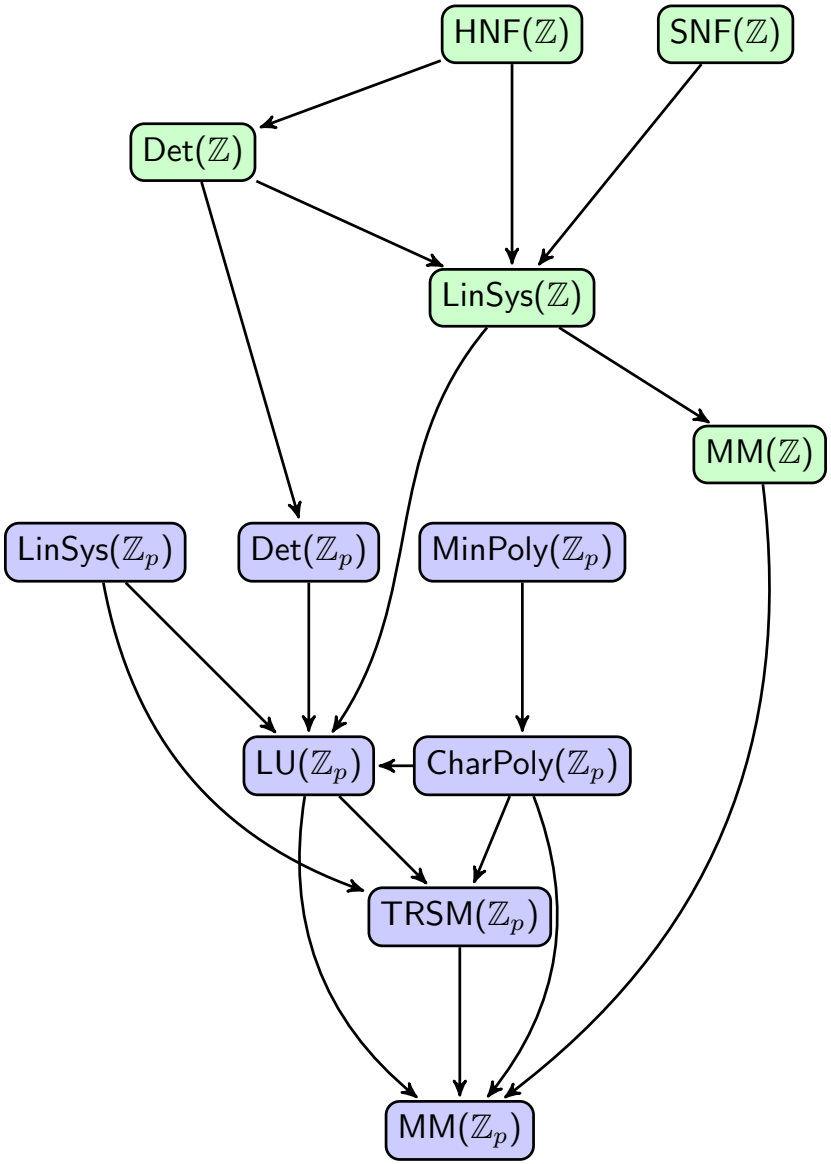
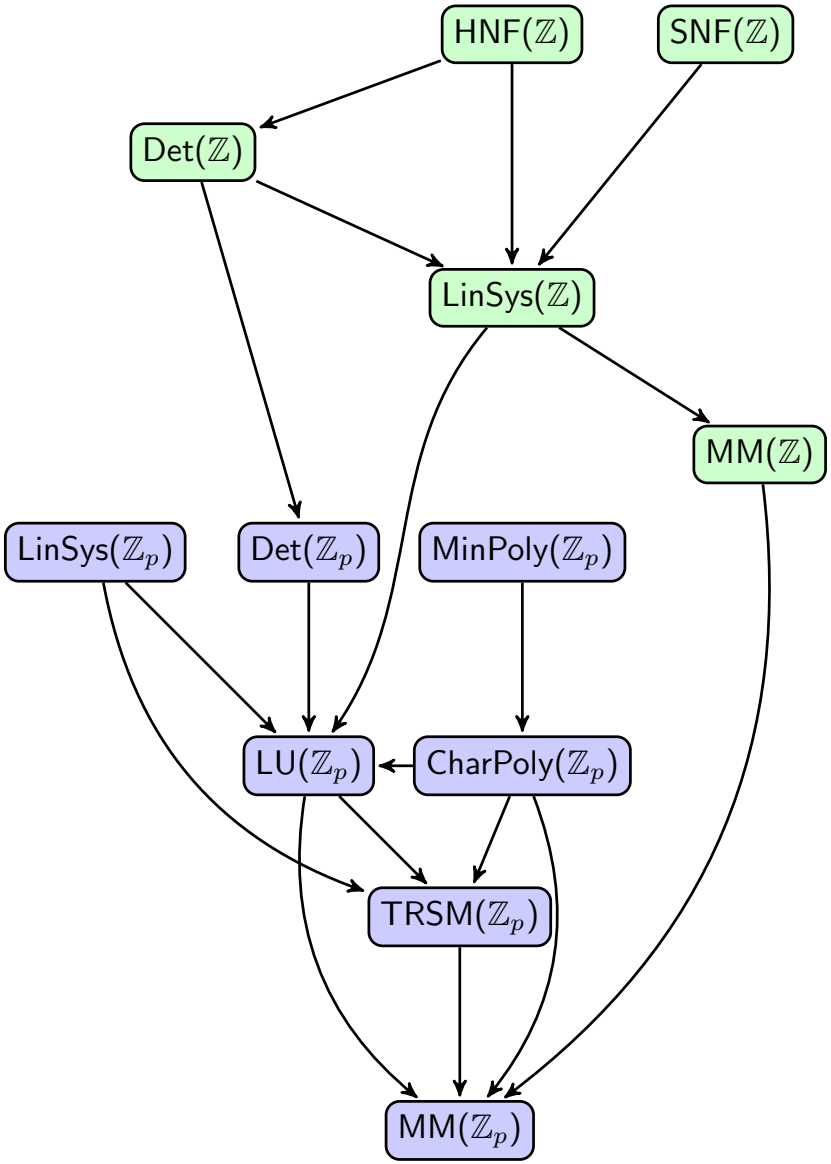


Common mistrust

Fast linear algebra is

- ✗ never faster
- ✗ numerically unstable

Reductions: theory and practice



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⇝ reduction trees are still relevant

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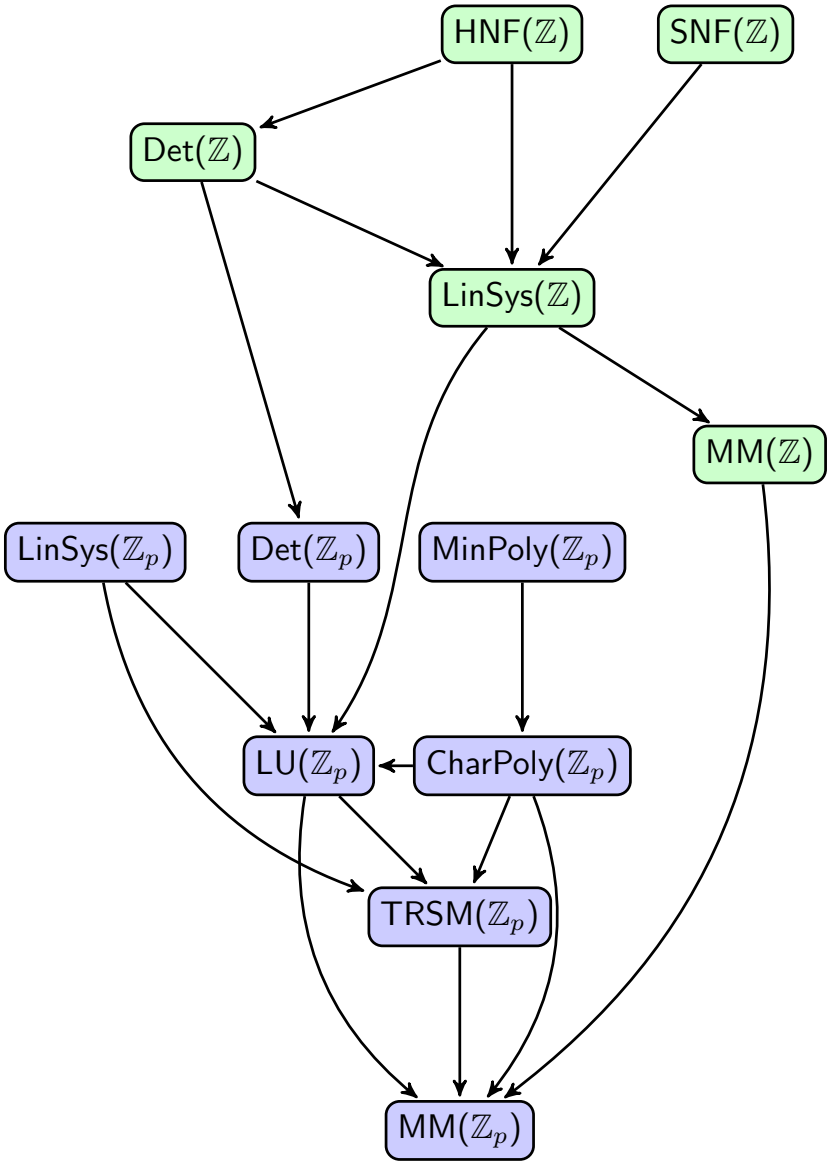

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$\rightsquigarrow$ reduction trees are still relevant

Road map towards efficiency in practice

1. Tune the MatMul building block.
2. Tune the reductions.

Putting it together: MatMul building block over $\mathbb{Z}/p\mathbb{Z}$

Ingedients [FFLAS-FFPACK library]

- Compute over $\mathbb{Z}$ and delay modular reductions

$$\rightsquigarrow \quad k\left(\frac{p-1}{2}\right)^2 < 2^{\text{mantissa}}$$

Putting it together: MatMul building block over $\mathbb{Z}/p\mathbb{Z}$

Ingedients [FFLAS-FFPACK library]

- Compute over $\mathbb{Z}$ and delay modular reductions

$\rightsquigarrow$ $k\left(\frac{p-1}{2}\right)^2 < 2^{53}$

- Fastest integer arithmetic: `double`
- Cache optimizations

$\rightsquigarrow$ numerical BLAS

Putting it together: MatMul building block over $\mathbb{Z}/p\mathbb{Z}$

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- Compute over $\mathbb{Z}$ and delay modular reductions

$$\rightsquigarrow \quad 9^\ell \left\lfloor \frac{k}{2^\ell} \right\rfloor \left(\frac{p-1}{2}\right)^2 < 2^{53}$$

- Fastest integer arithmetic: `double`
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$$\rightsquigarrow \quad \text{numerical BLAS}$$

- Strassen-Winograd $6n^{2.807} + \ldots$

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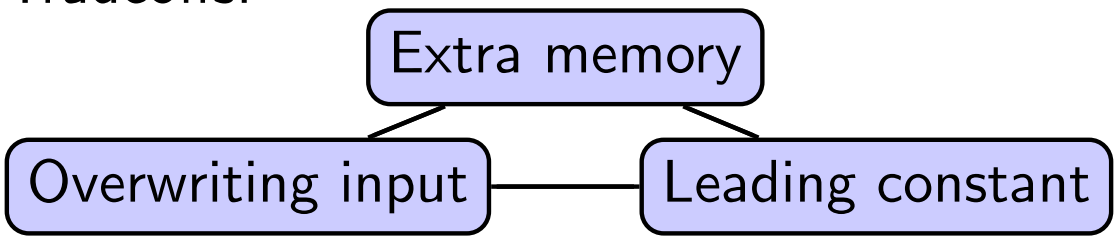
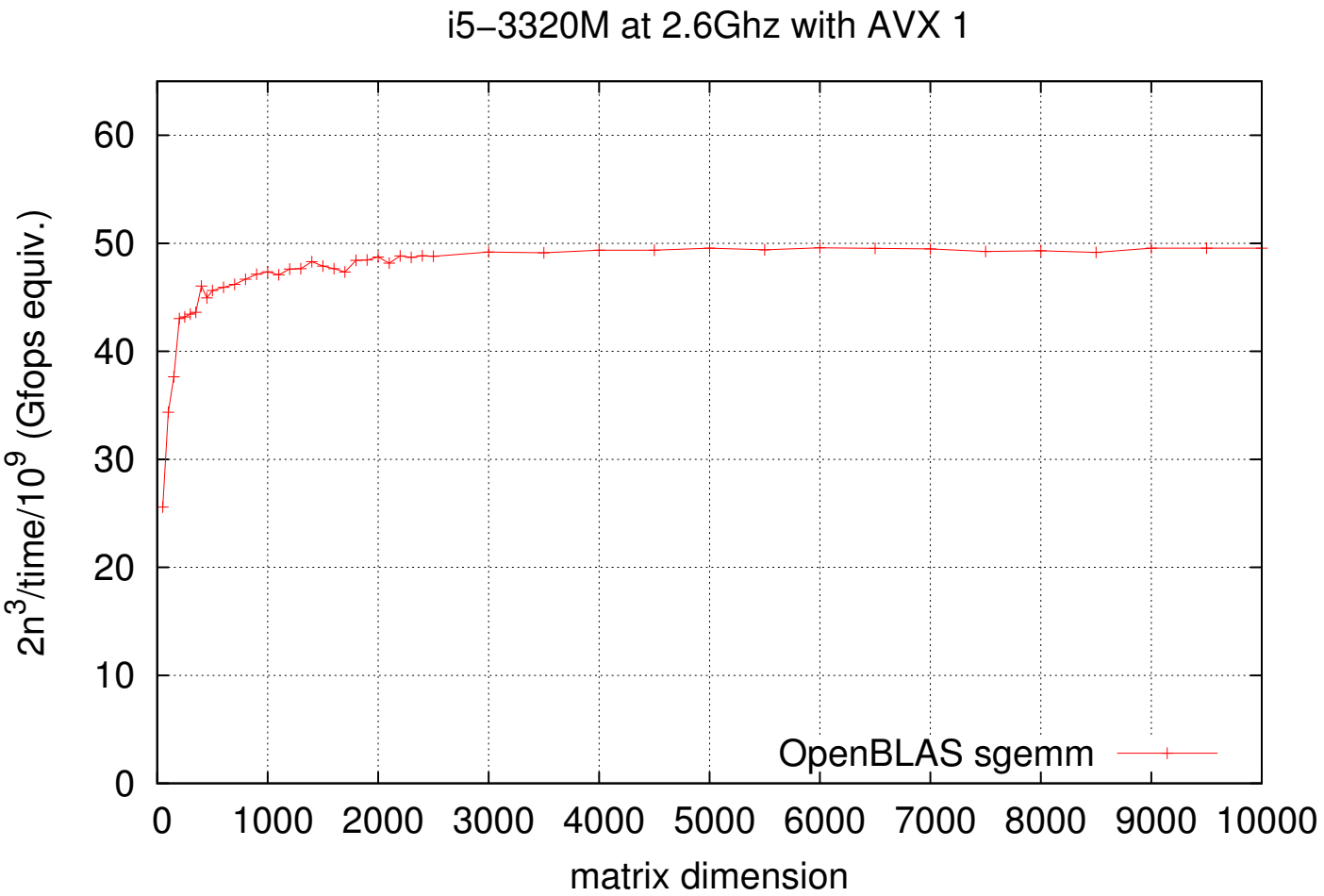
with memory efficient schedules [Boyer, Dumas, P. and Zhou 09]
Tradeoffs:



Fully in-place in

$$7.2n^{2.807} + \ldots$$

Sequential Matrix Multiplication



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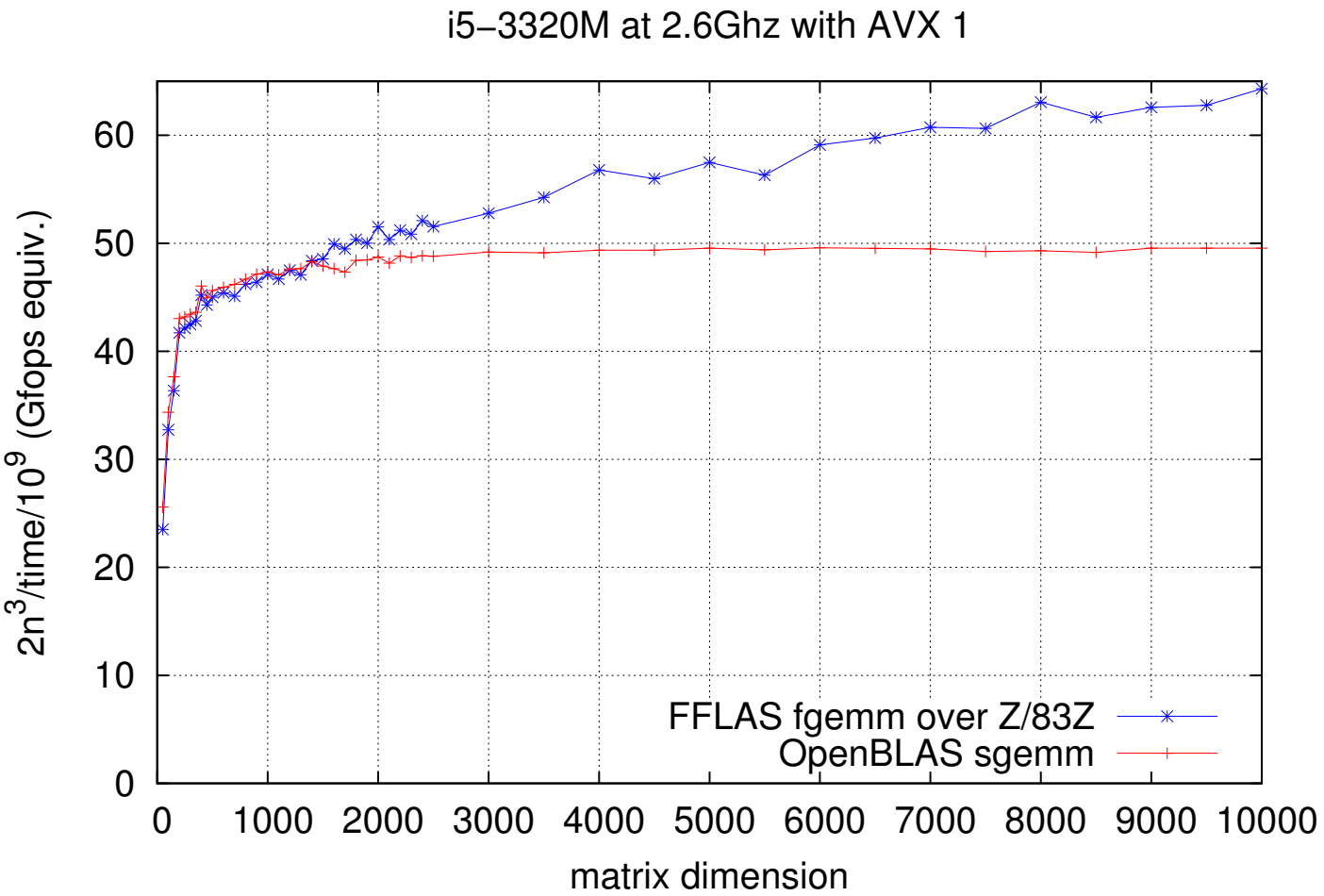
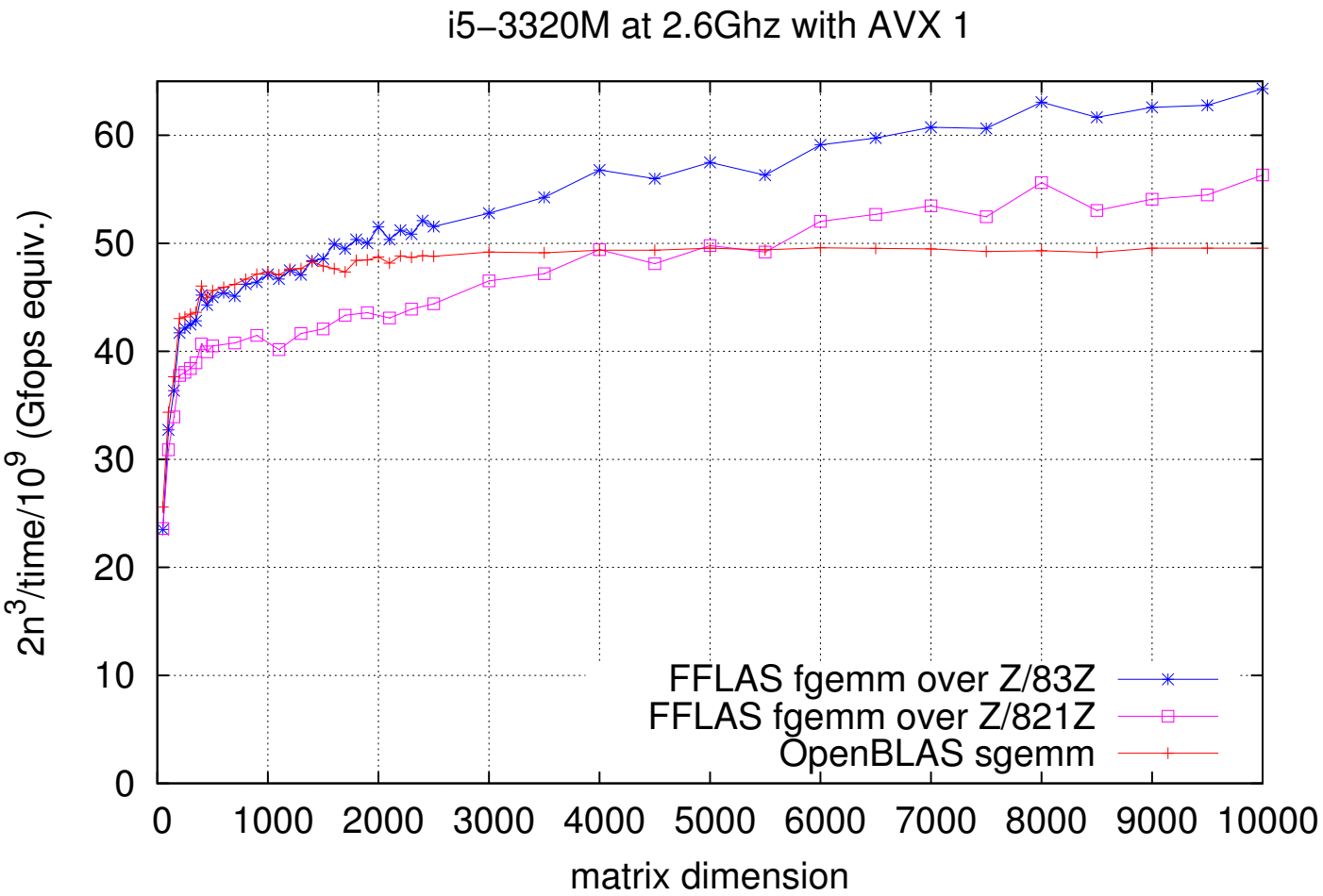


$p = 83$, $\rightsquigarrow$ 1 mod / 10000 mul.

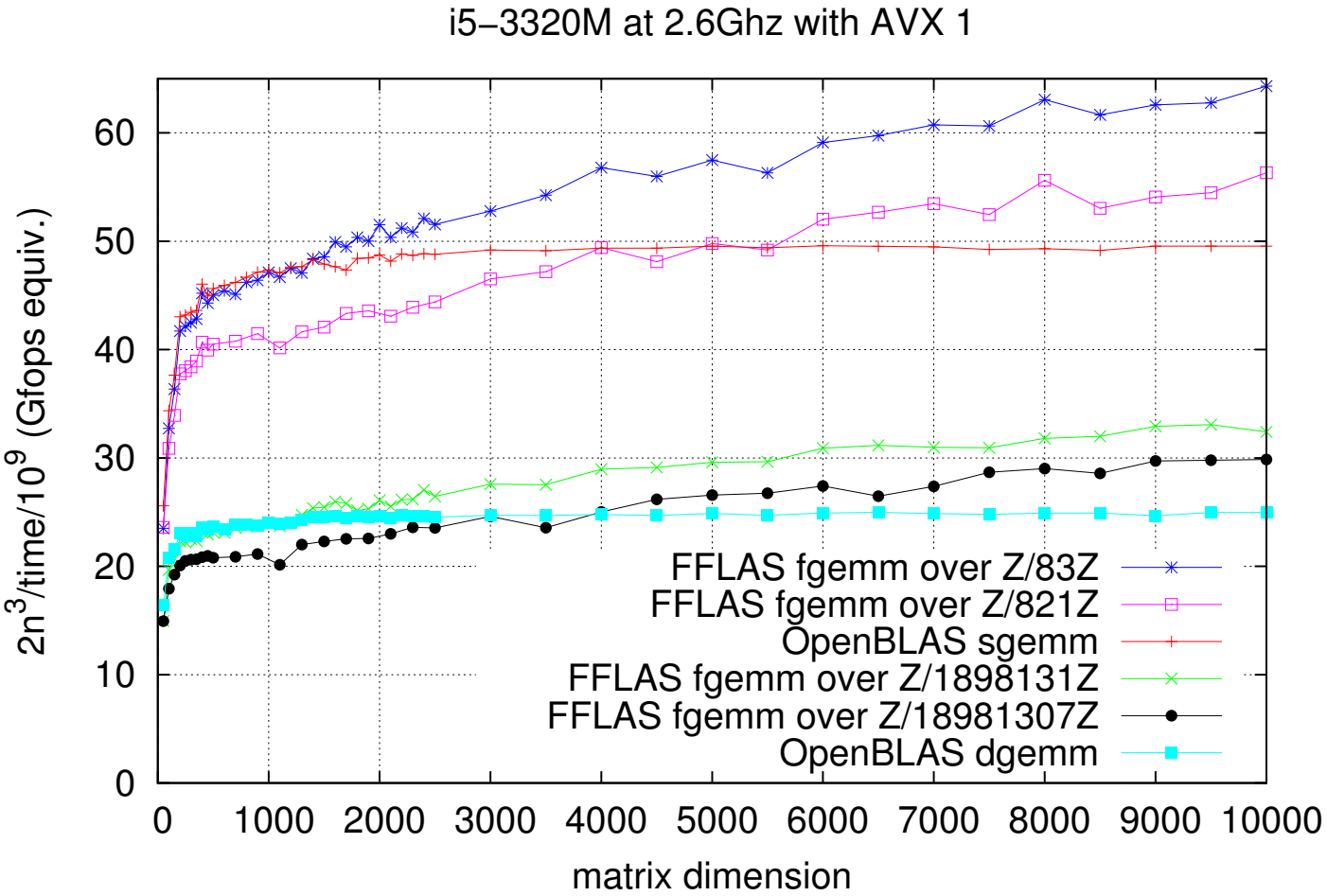
Sequential Matrix Multiplication



$p = 83$, $\rightsquigarrow$ 1 mod / 10000 mul.

$p = 821$, $\rightsquigarrow$ 1 mod / 100 mul.

Sequential Matrix Multiplication



$p = 83$, $\rightsquigarrow$ 1 mod / 10000 mul.
$p = 821$, $\rightsquigarrow$ 1 mod / 100 mul.
$p = 1898131$, $\rightsquigarrow$ 1 mod / 10000 mul.
$p = 18981307$, $\rightsquigarrow$ 1 mod / 100 mul.

Reductions in dense linear algebra

LU decomposition

- Block recursive algorithm $\rightsquigarrow$ reduces to MatMul $\rightsquigarrow$ $O(n^\omega)$

n	1000	5000	10000	15000	20000
`LAPACK-dgetrf`	**0.024s**	**2.01s**	**14.88s**	48.78s	113.66
`fflas-ffpack`	0.058s	2.46s	16.08s	**47.47s**	**105.96s**

Intel Haswell E3-1270 3.0Ghz using OpenBLAS-0.2.9

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Characteristic Polynomial

- A new reduction to matrix multiplication in $O(n^\omega)$.

n	1000	2000	5000	10000
`magma-v2.19-9`	1.38s	24.28s	332.7s	2497s
`fflas-ffpack`	**0.532s**	**2.936s**	**32.71s**	**219.2s**

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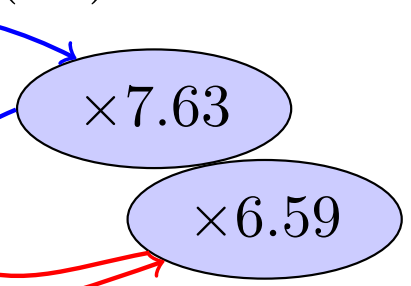

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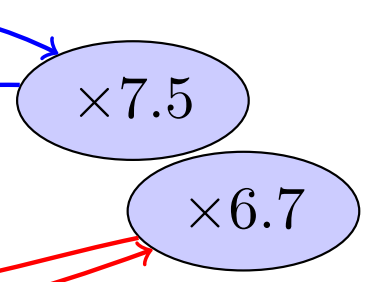


Outline

Parallelization

Parallel numerical linear algebra

- cost invariant wrt. splitting
  - $O(n^3)$

  $\rightsquigarrow$ fine grain

  $\rightsquigarrow$ block iterative algorithms
- regular task load
- Numerical stability constraints

Parallelization

Parallel numerical linear algebra

- cost invariant wrt. splitting
  - $O(n^3)$

  $\rightsquigarrow$ fine grain

  $\rightsquigarrow$ block iterative algorithms
- regular task load
- Numerical stability constraints

Exact linear algebra specificities

- cost affected by the splitting
  - $O(n^\omega)$ for $\omega < 3$
  - modular reductions

  $\rightsquigarrow$ coarse grain

  $\rightsquigarrow$ recursive algorithms
- rank deficiencies

  $\rightsquigarrow$ unbalanced task loads

Ingredients for the parallelization

Criteria

- good performances
- portability across architectures
- abstraction for simplicity

Challenging key point: scheduling as a plugin

Program: only describes where the parallelism lies

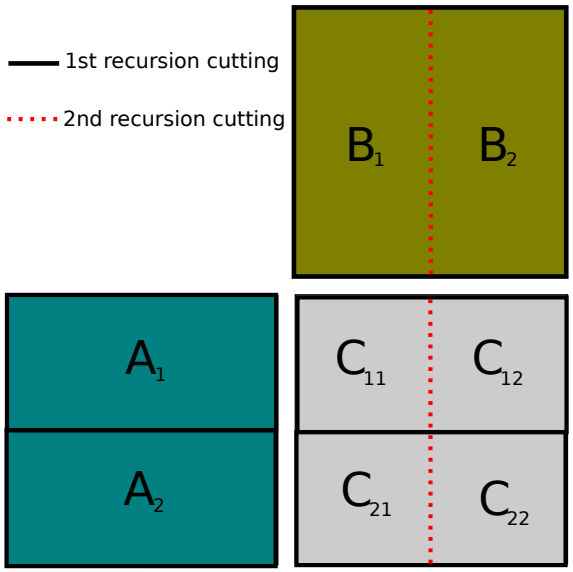
Runtime: scheduling & mapping, depending on the context of execution

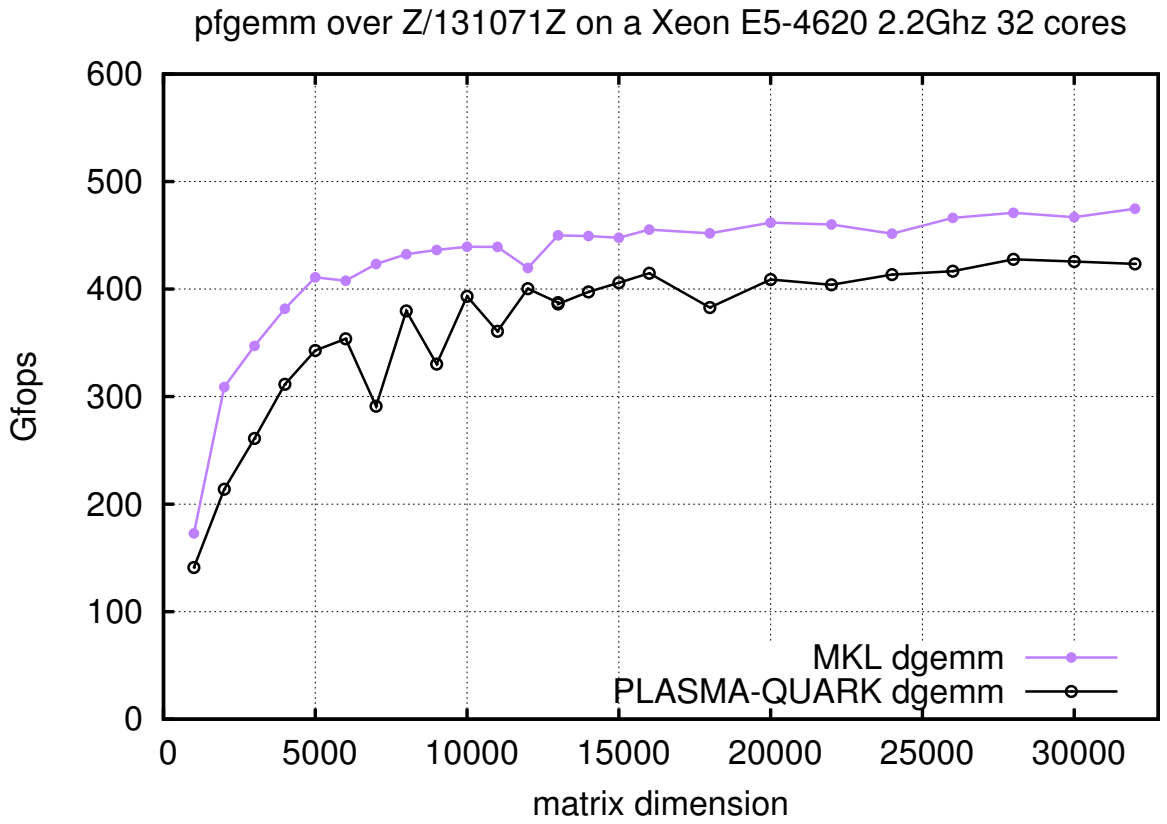
3 main models:

1. Parallel loop [data parallelism]
2. Fork-Join (independent tasks) [task parallelism]
3. Dependent tasks with data flow dependencies [task parallelism]

Parallel matrix multiplication

[Dumas, Gautier, P. & Sultan 14]





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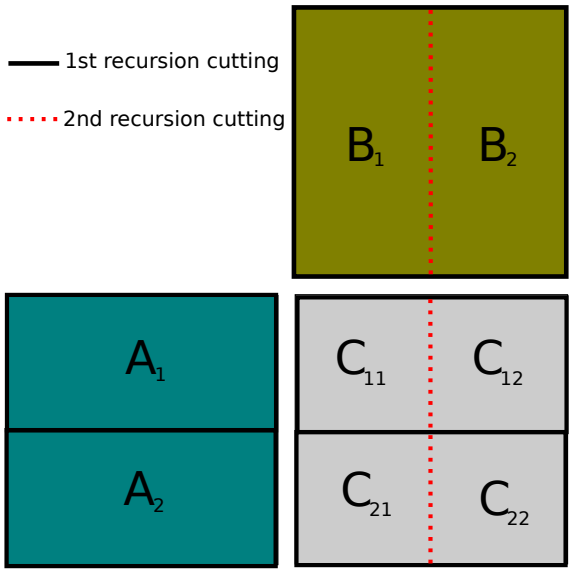

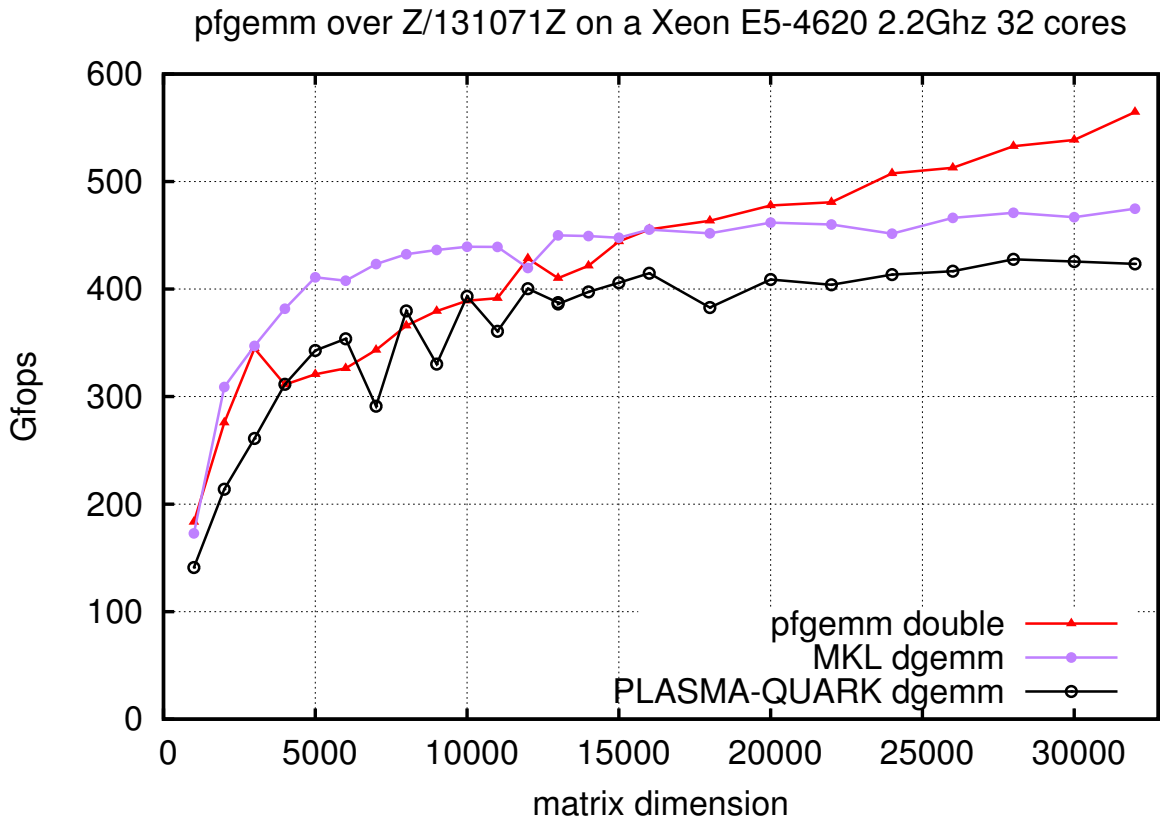

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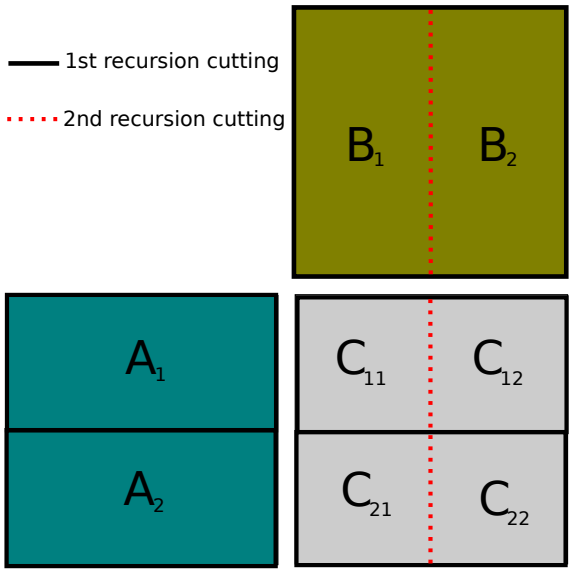
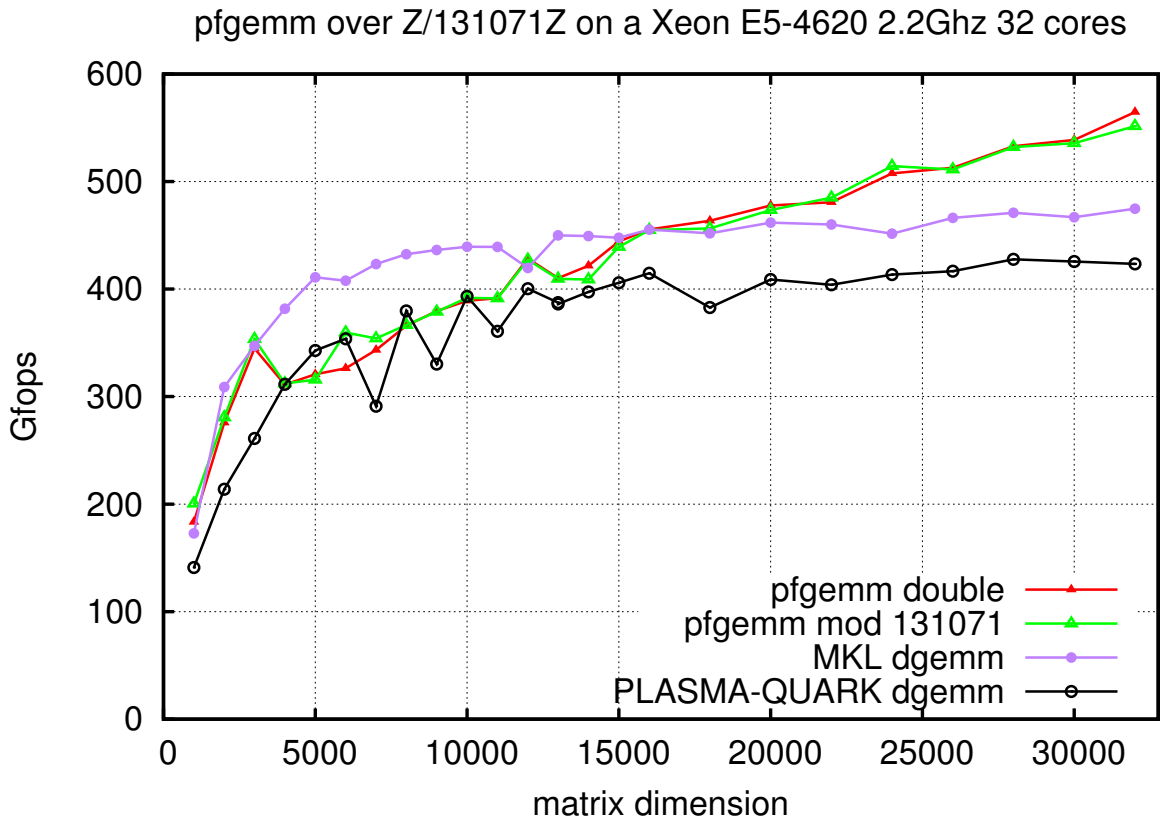
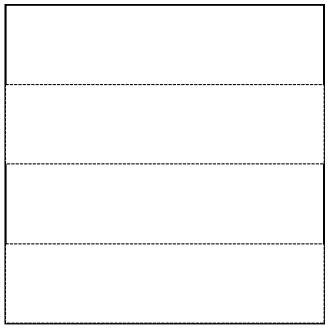


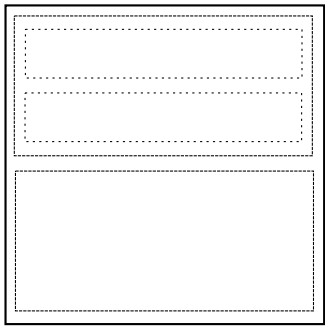


Gaussian elimination



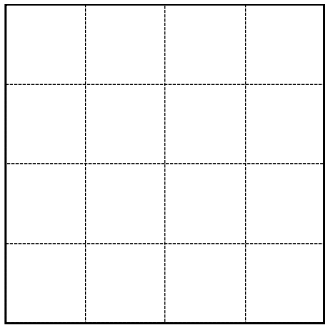
Slab iterative

`LAPACK`



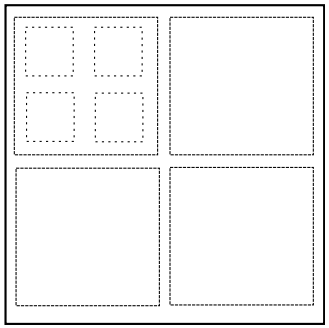
Slab recursive

`FFLAS-FFPACK`



Tile iterative

`PLASMA`



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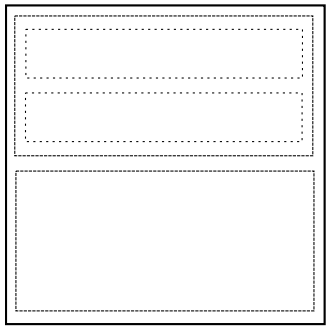

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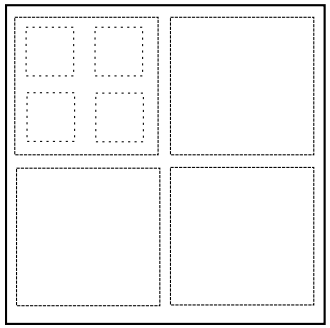

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- Prefer recursive algorithms

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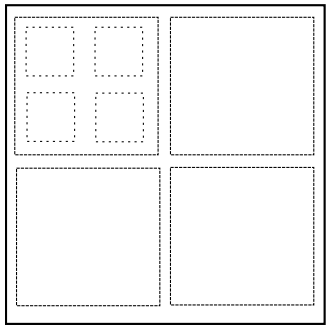

Tile recursive

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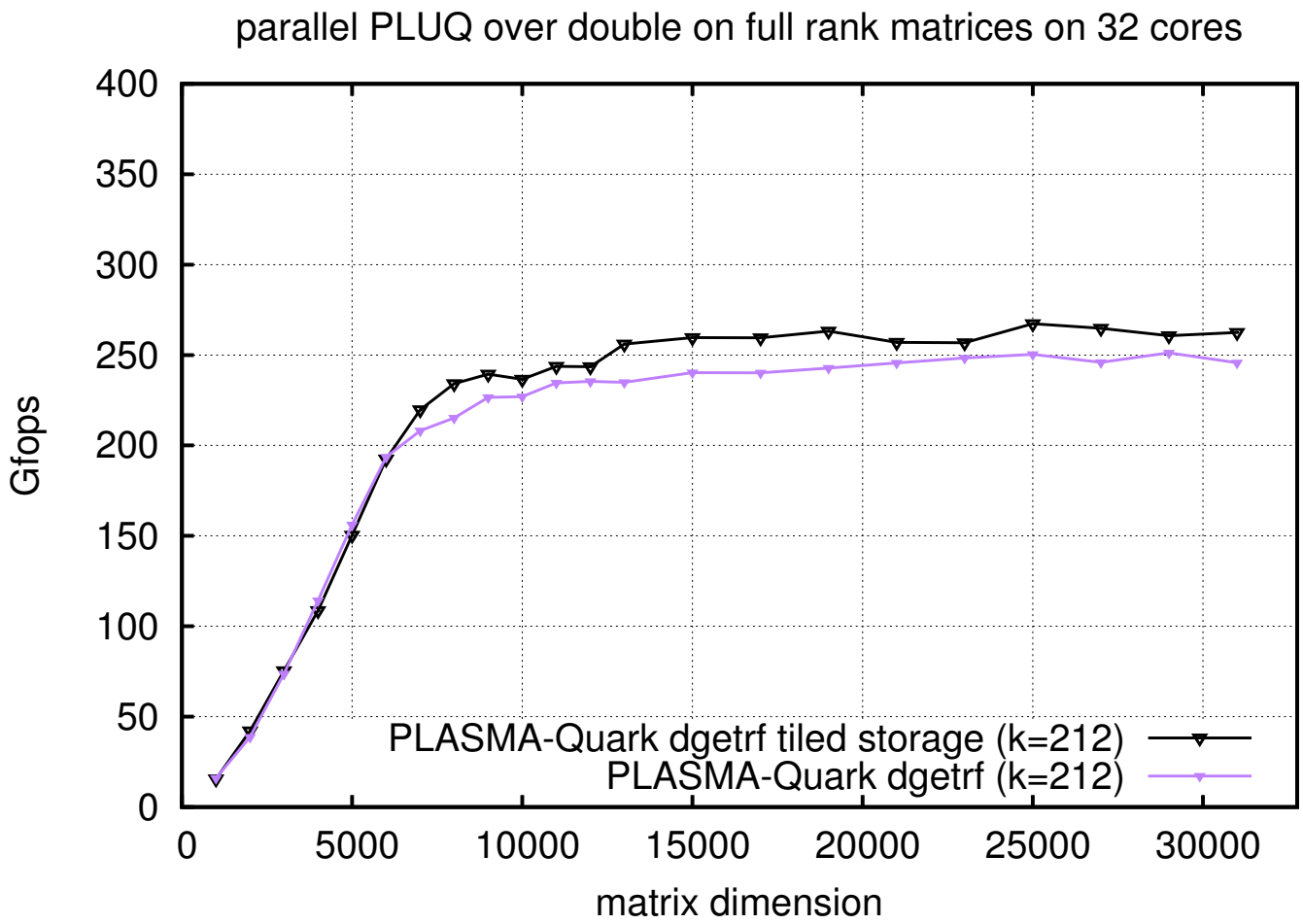
- Prefer recursive algorithms
- Better data locality

Full rank Gaussian elimination

[Dumas, Gautier, P. and Sultan 14] Over $\mathbb{R}$ (no modulo)



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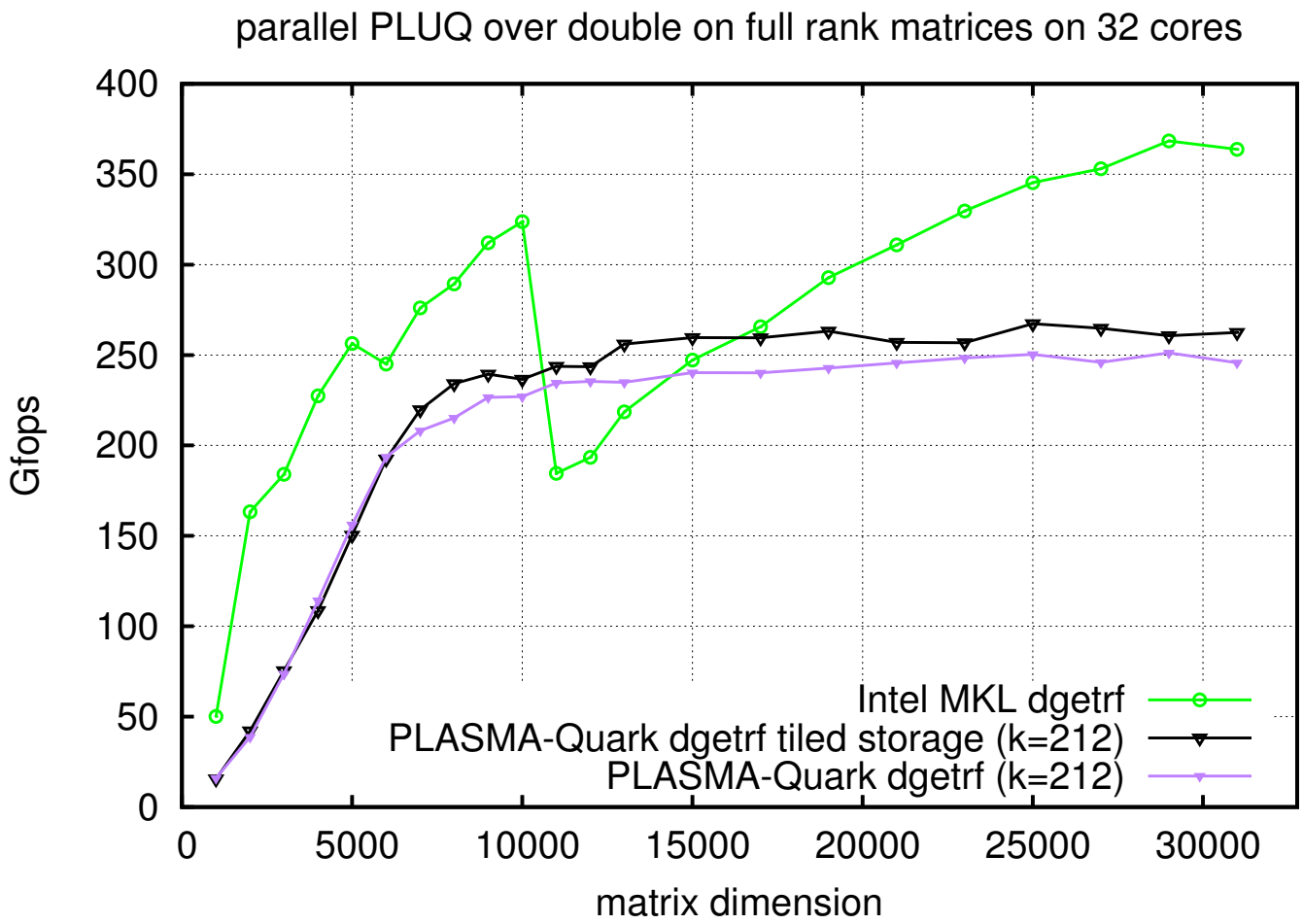

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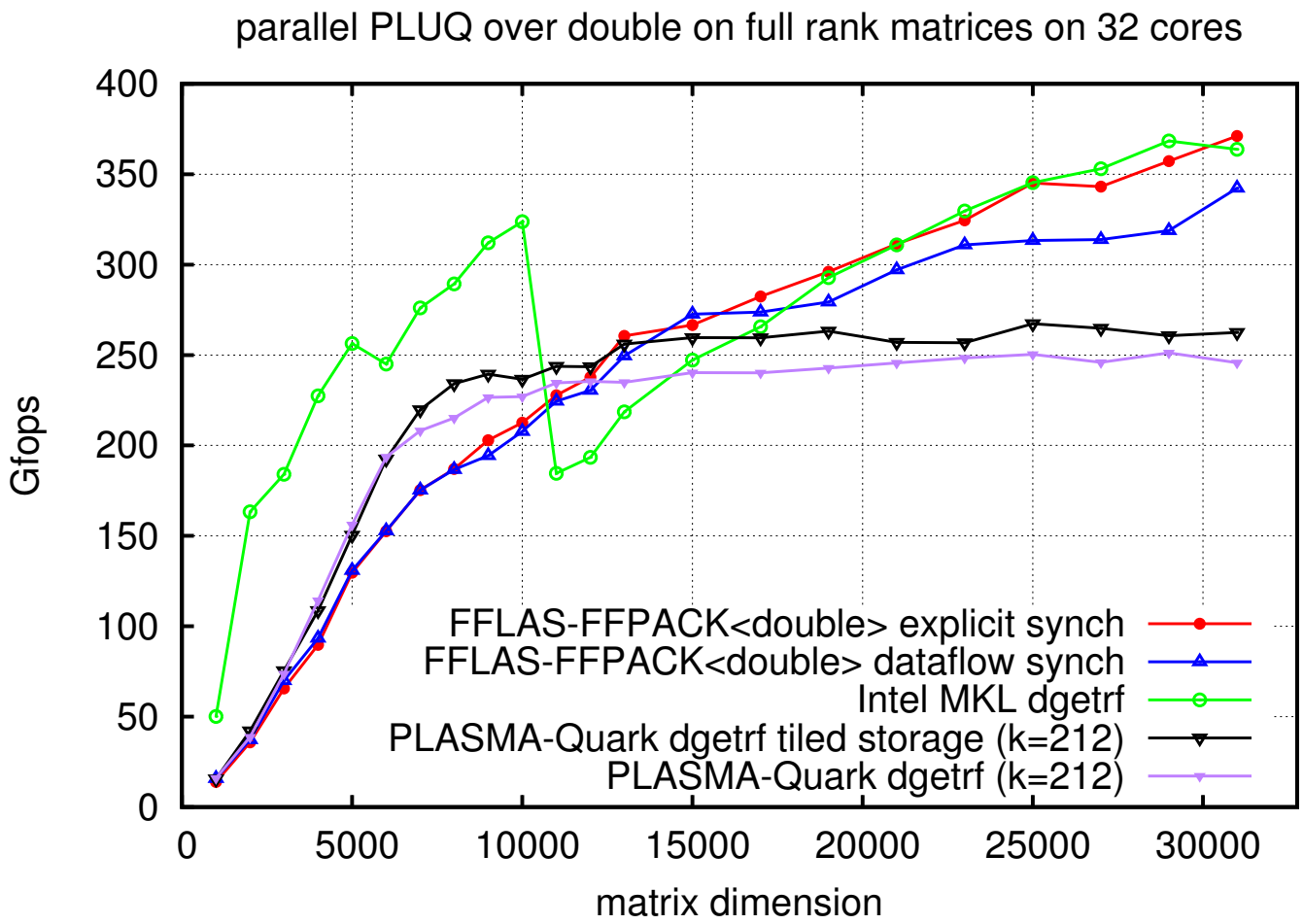

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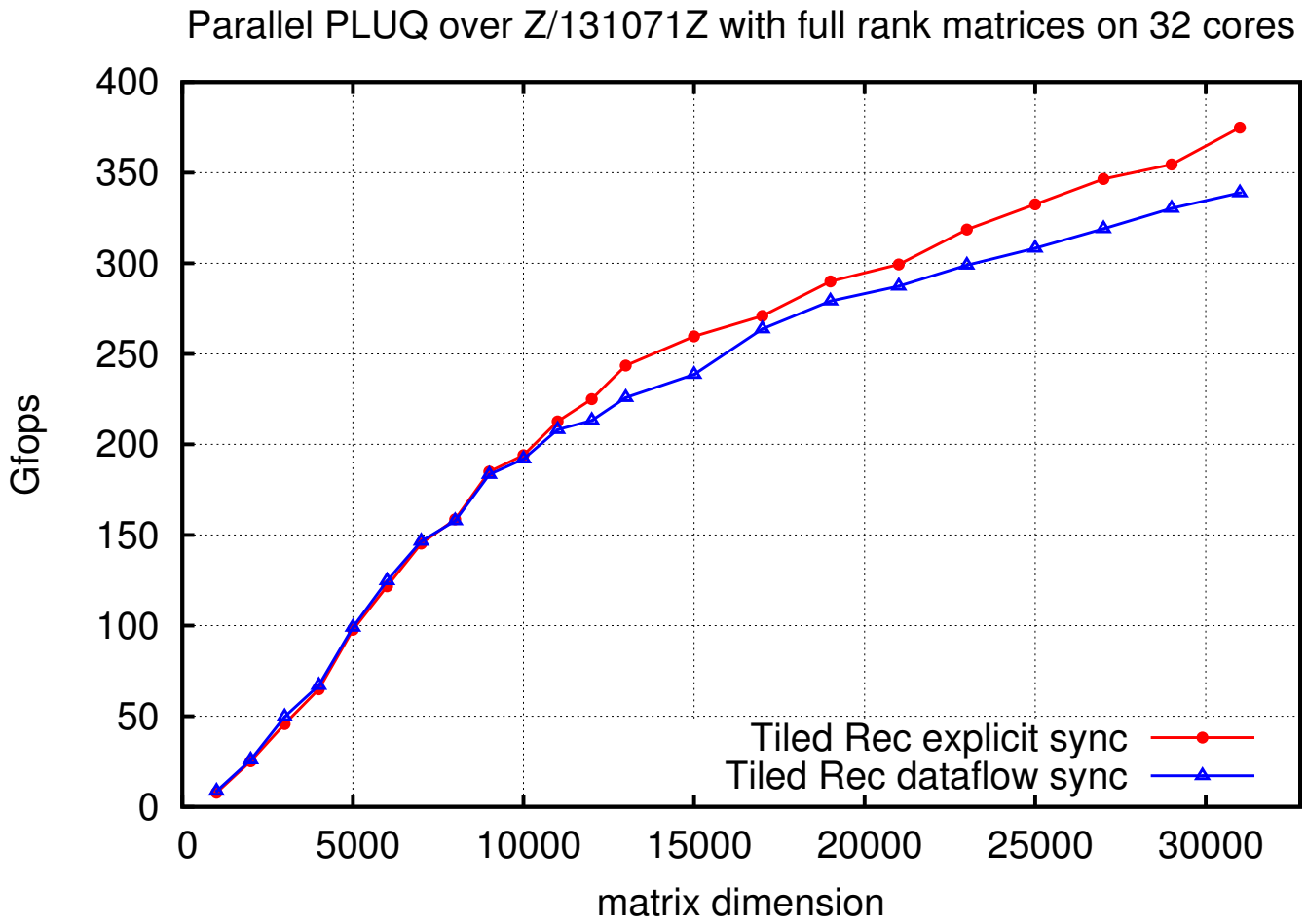

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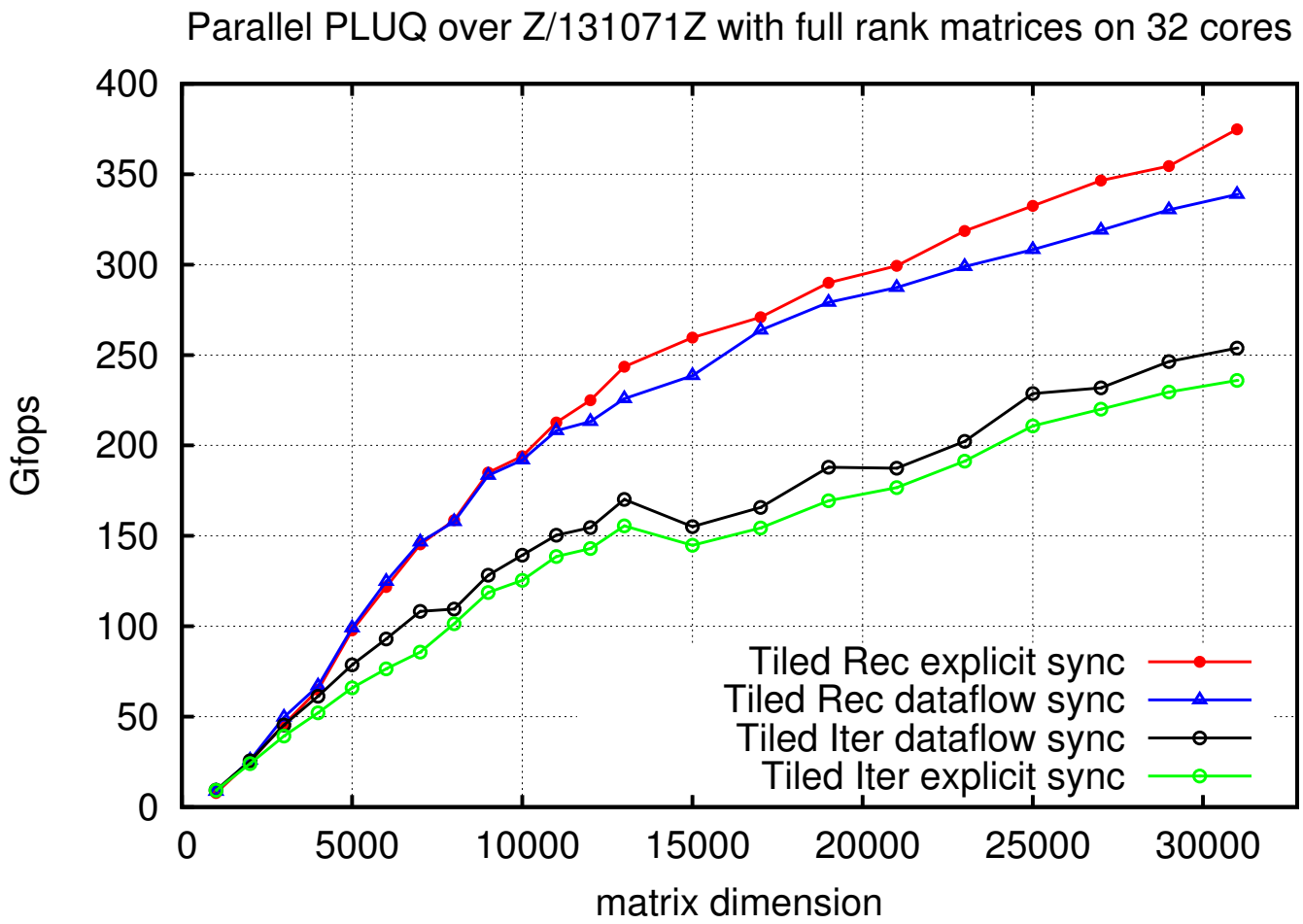

Perspectives

Large scale distributed exact linear algebra

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Thank you