Exact Linear Algebra Algorithmic: Theory and Practice

ISSAC'15 Tutorial

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Exact linear algebra

Matrices can be

- Dense: store all coefficients
- Sparse: store the non-zero coefficients only
- Black-box: no access to the storage, only *apply* to a vector

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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 $\approx 100, 200, 1000, 2000, \dots$ bits

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

Polynomials: K$[X]$ for K any of the above

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Need to structure the design.

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.

Content

The scope of this presentation:

- not an exhaustive overview on linear algebra algorithmic and complexity improvements
- a few guidelines, for the use and design of exact linear algebra in practice
- bridging the theoretical algorihmic development and practical efficiency concerns

Outline

1. Choosing the underlying arithmetic
   - Using boolean arithmetic
   - Using machine word arithmetic
   - Larger field sizes
2. Reductions and building blocks
   - In dense linear algebra
   - In blackbox linear algebra
3. Size dimension trade-offs
   - Hermite normal form
   - Frobenius normal form
4. Parallel exact linear algebra
   - Ingredients for the parallelization
   - Parallel dense linear algebra mod p

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
$\mathbb{Z}_{3,5,7}$	2-3 bits
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Available CPU arithmetic

- boolean
- integer (fixed size)
- floating point
- .. and their vectorization

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$\mathbb{Z}_2$	1 bit	$\rightsquigarrow$ bit-packing
$\mathbb{Z}_{3,5,7}$	2-3 bits	$\rightsquigarrow$ bit-slicing, bit-packing
$\mathbb{Z}_p$	4-26 bits	$\rightsquigarrow$ CPU arithmetic
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$\mathbb{Z}_p$	$>$ 32 bits	$\rightsquigarrow$ multiprec. ints, big ints, CRT
GF$(p^k) \equiv \mathbb{Z}_p[X]/(Q)$		$\rightsquigarrow$ Polynomial, Kronecker, Zech log, ...

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Dense linear algebra over $\mathbb{Z}_2$: bit-packing

`uint64_t` $\equiv (\mathbb{Z}_2)^{64}$ $\rightsquigarrow$

^ : bit-wise XOR, (+ mod 2)

& : bit-wise AND, (* mod 2)

dot-product (a,b)

```
uint64_t t = 0;
for (int k=0; k < N/64; ++k)
    t ^= a[k] & b[k];
c = parity(t)
```

parity(x)

```
if (size(x) == 1)
    return x;
else return parity (High(x) ^ Low(x))
```

$\rightsquigarrow$ Can be parallelized on 64 instances.

Tabulation:

- avoid computing parities
- balance computation vs communication
- (slight) complexity improvement possible

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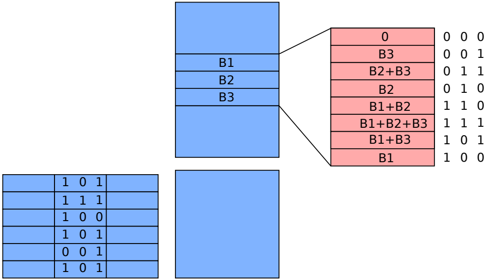
The Four Russian method [Arlazarov, Dinic, Kronrod, Faradzev 70]

1. compute all 2^k linear combinations of k rows of B. **Gray code**: each new line costs 1 vector add (vs $k/2$)
2. multiply chunks of length k of A by table look-up



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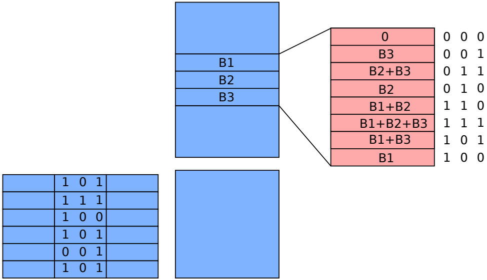

- **For $k = \log n \rightsquigarrow O(n^3/\log n)$.**
- **In pratice: choice of k s.t. the table fits in L2 cache.**

Dense linear algebra over $\mathbb{Z}_2$

The M4RI library [Albrecht Bard Hart 10]

- bit-packing
- Method of the Four Russians
- SIMD vectorization of boolean instructions (128 bits registers)
- Cache optimization
- Strassen's $O(n^{2.81})$ algorithm

n	7000	14 000	28 000
SIMD bool arithmetic	2.109s	15.383s	111.82
SIMD + 4 Russians	0.256s	2.829s	29.28s
SIMD + 4 Russians + Strassen	0.257s	2.001s	15.73

Table : Matrix product $n \times n$ by $n \times n$, on an i5 SandyBridge 2.6Ghz.

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$\mathbb{Z}_3 = \{0, 1, -1\} \quad = \{00, 01, 10\}$

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Bit-slicing

$$(-1, 0, 1, 0, 1, -1, -1, 0) \in \mathbb{Z}_3^8 \to (\texttt{11}, \texttt{00}, \texttt{10}, \texttt{00}, \texttt{10}, \texttt{11}, \texttt{00})$$

Stored as 2 words
(1,0,1,0,1,1,0)
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⇝ $\vec{y} \leftarrow \vec{y} + x\vec{b}$ for $x \in \mathbb{Z}_3, \vec{y}, \vec{b} \in \mathbb{Z}_3^{64}$ in 6 boolean word ops.

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Recipe for $\mathbb{Z}_5$

- Use redundant representations on 3 bits + bit-slicing
- integer add + bool operations
- Pseudo-reduction mod 5 ($4 \rightarrow 3$ bits) in 8 bool ops found by computer assisted search.

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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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addsd   %xmm0, %xmm1
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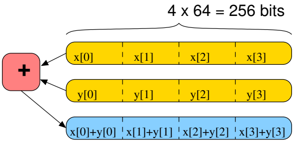
```
vinsertf128   $0x1, 16(%rcx,%rax), %ymm0,
vmulpd        %ymm1, %ymm0, %ymm0
vaddpd        (%rsi,%rax),%ymm0, %ymm0
vmovapd       %ymm0, (%rsi,%rax)
```

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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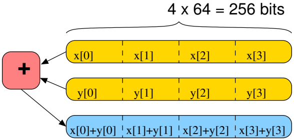

Pipeline: amortize the latency of an operation when used repeatedly

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

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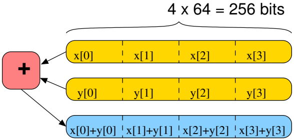

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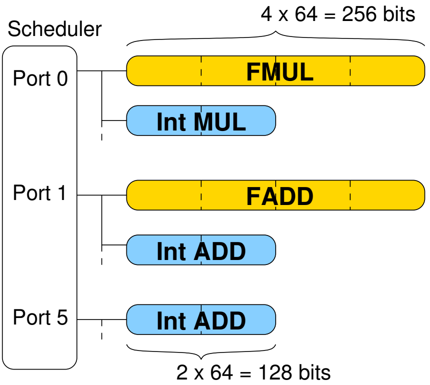
Execution Unit parallelism: multiple arith. units acting simulatneously on distinct registers

SIMD and vectorization

Intel Sandybridge micro-architecture



Performs at every clock cycle:

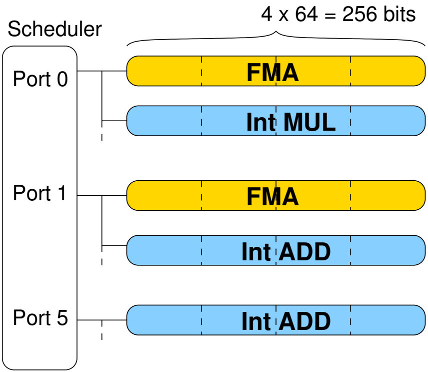
- 1 Floating Pt. Mul $\times 4$
- 1 Floating Pt. Add $\times 4$

Or:

- 1 Integer Mul $\times 2$
- 2 Integer Add $\times 2$

SIMD and vectorization

Intel Haswell micro-architecture



Performs at every clock cycle:

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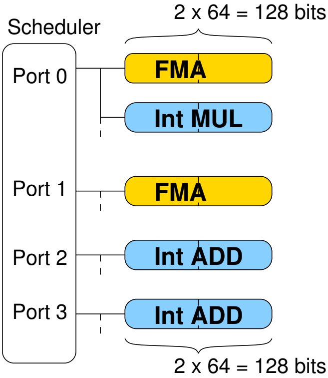
FMA: Fused Multiplying & Accumulate, `c += a * b`

SIMD and vectorization

AMD Bulldozer micro-architecture



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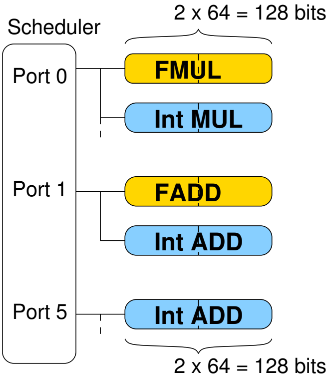

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Summary: 64 bits AXPY throughput

		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**	
AVX2	FP	256			2	8	3.5	**56**	
Intel Sandybridge	INT								
AVX1	FP								
AMD Bulldozer	INT								
FMA4	FP								
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Speed of light: CPU freq $\times$ (# daxpy / Cycle) $\times 2$

Summary: 64 bits AXPY throughput

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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]

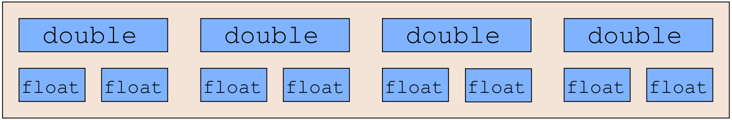
Experiments:

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

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

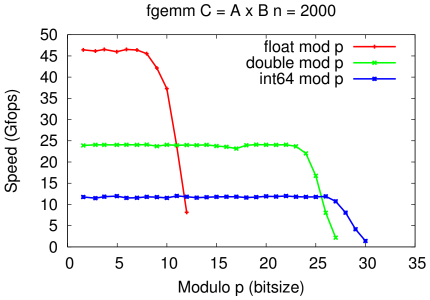
Integer Packing

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

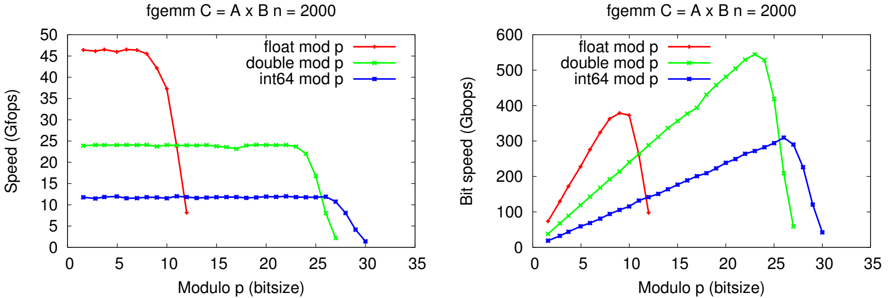


SandyBridge i5-3320M@3.3Ghz. $n = 2000$.

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



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
- 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)
   $\leadsto$ using moduli delivering optimum bitspeed

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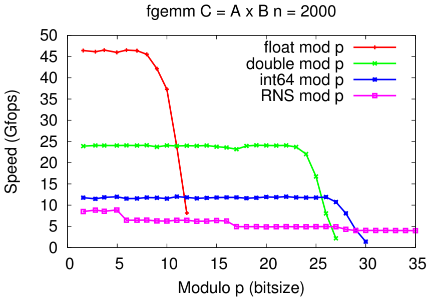
$\log_2 p$	50	100	150
GMP	58.1s	94.6s	140s
RecInt	5.7s	28.6s	837s
RNS	0.785s	1.42s	1.88s

$n = 1000$, 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
0
5
10
15
20
25
30
35
40
45
50
0
5
10
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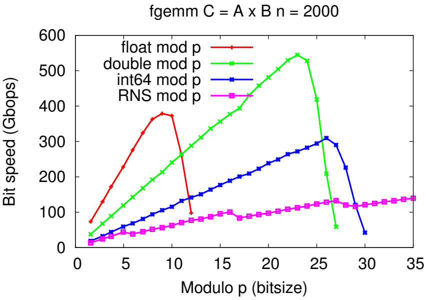
20
25
30
35


fgemm C = A x B n = 2000
Bit speed (Gbops)
Modulo p (bitsize)
float mod p
double mod p
int64 mod p
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0
100
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600
0
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10
15
20
25
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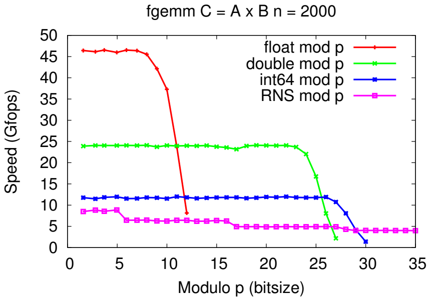
35

In practice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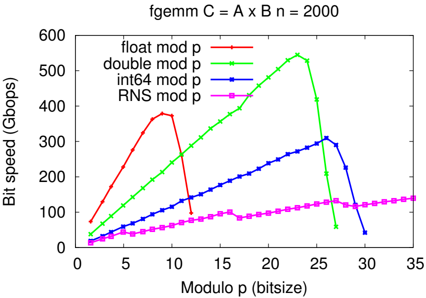
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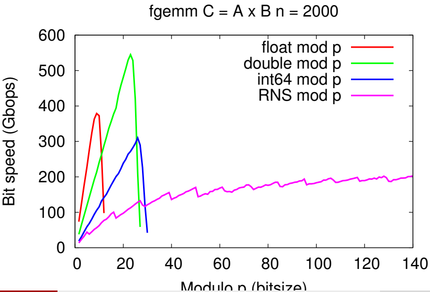
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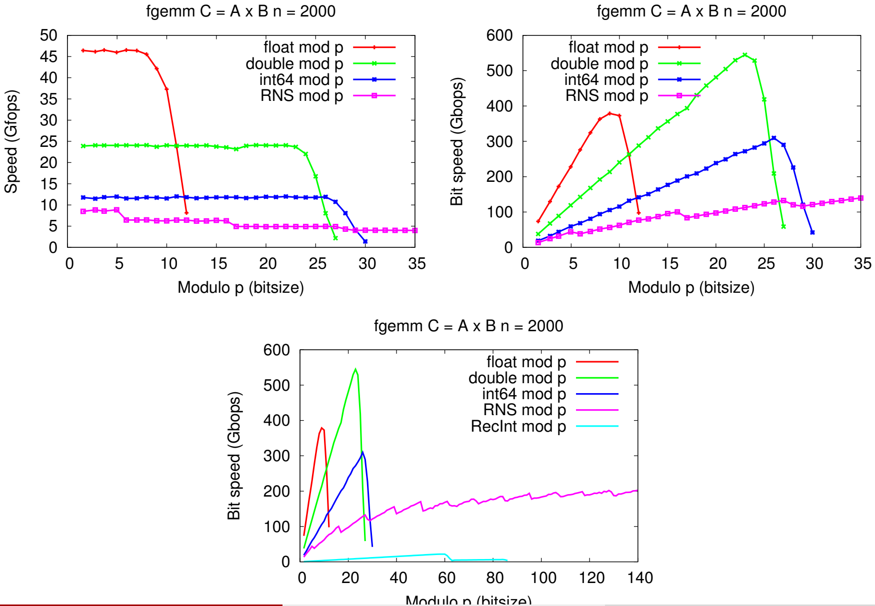
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Outline

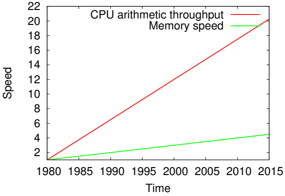
Reductions to building blocks

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

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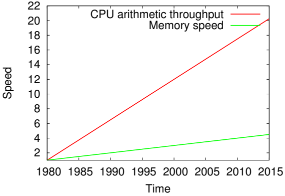

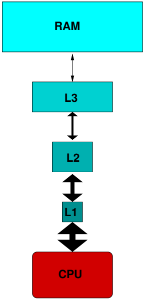

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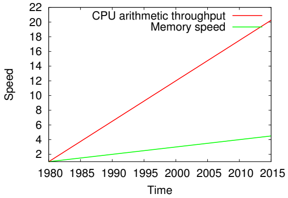
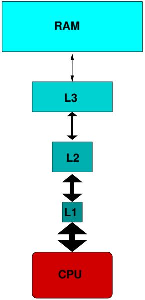
$\rightsquigarrow$ Need to overlap communications by computation





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, Danilevskĭi, etc)

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

[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 $O(n^\omega)$
[Keller-Gehrig 85]:	CharPoly in $O(n^\omega \log n)$

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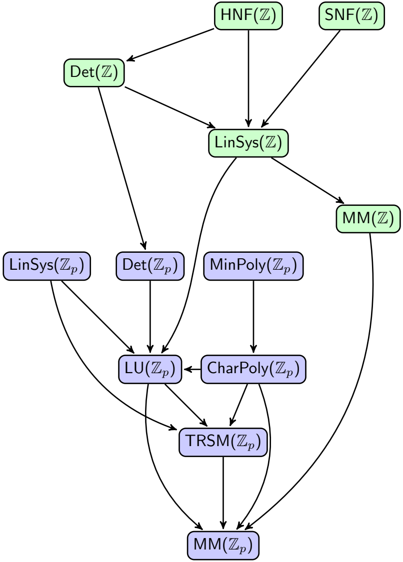
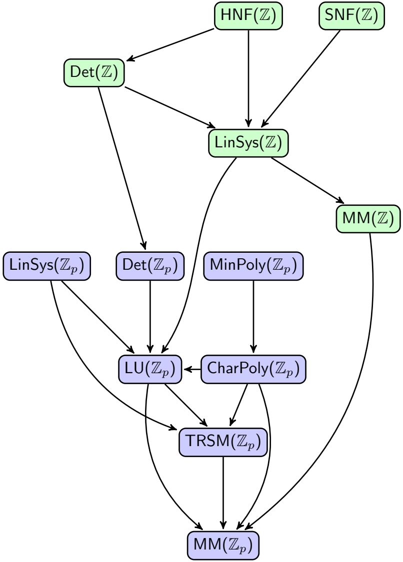
MatMul has become a building block in theoretical reductions

Reductions: theory



Reductions: theory

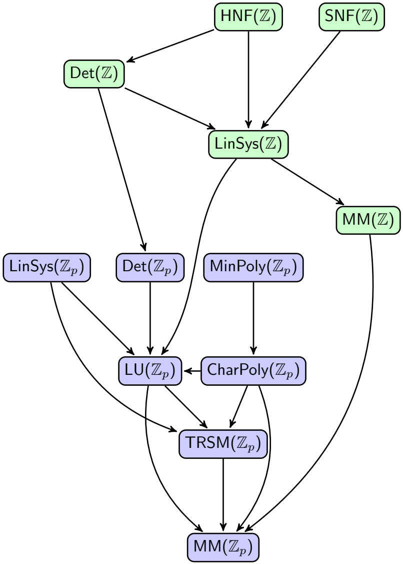


Common mistrust

Fast linear algebra is

- ✗ never faster
- ✗ numerically unstable

Reductions: theory and practice



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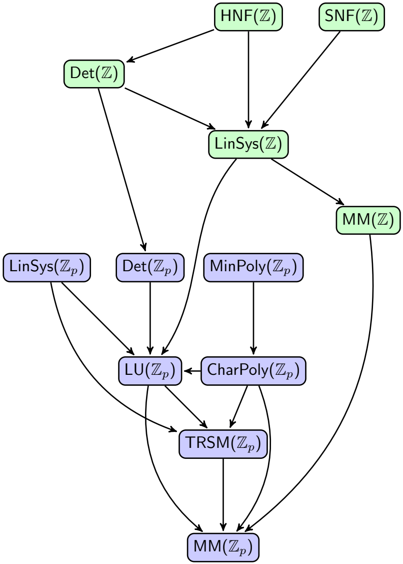
$\rightsquigarrow$ reduction trees are still relevant

Reductions: theory and practice



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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

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

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

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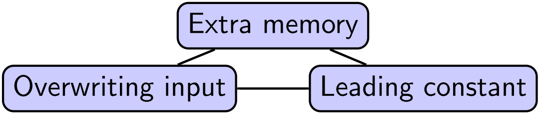
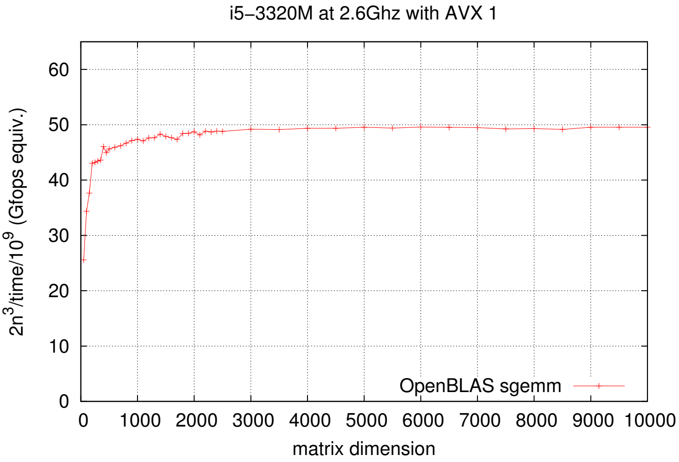
with memory efficient schedules [Boyer, Dumas, P. and Zhou 09]
Tradeoffs:

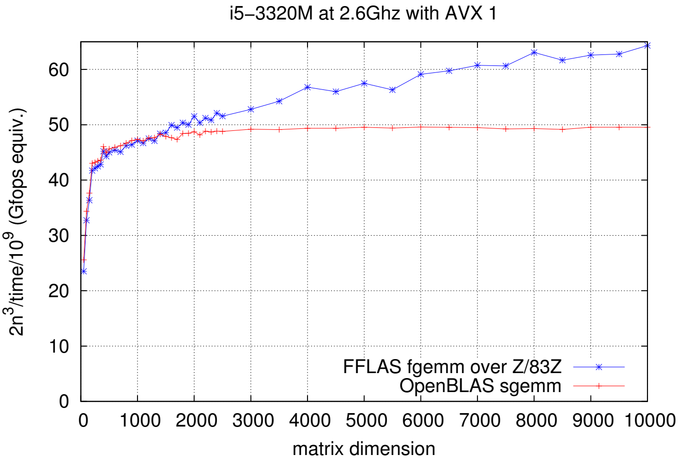


Fully in-place in $7.2n^{2.807} + \ldots$

Sequential Matrix Multiplication

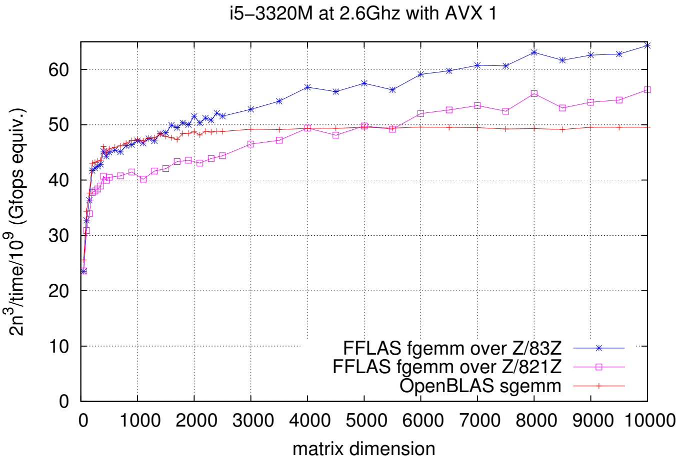


Sequential Matrix Multiplication



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

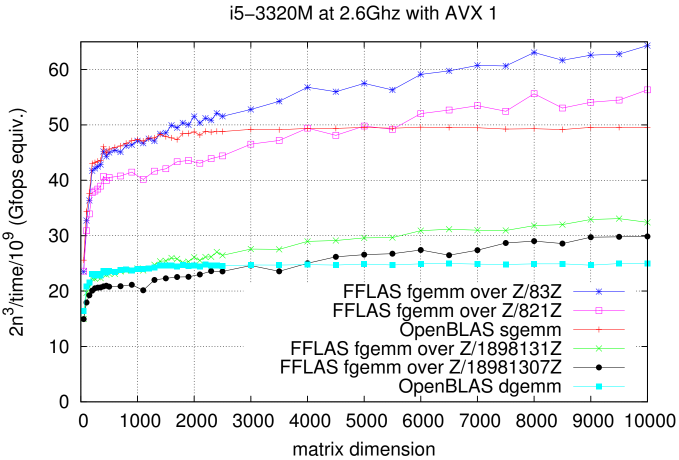
Sequential Matrix Multiplication



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

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

Sequential Matrix Multiplication



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

Intel Ivy-Bridge i5-3320 2.6Ghz using OpenBLAS-0.2.9

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

$\times 7.63$

$\times 6.59$

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**

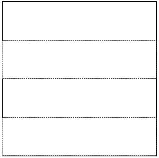
Intel Ivy-Bridge i5-3320 2.6Ghz using OpenBLAS-0.2.9

$\times 7.5$

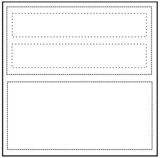
$\times 6.7$

The case of Gaussian elimination

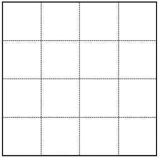
Which reduction to MatMul ?



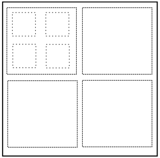
Slab iterative
`LAPACK`



Slab recursive
`FFLAS-FFPACK`



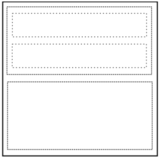
Tile iterative
`PLASMA`



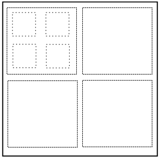
Tile recursive
`FFLAS-FFPACK`

The case of Gaussian elimination

Which reduction to MatMul ?



Slab recursive
FFLAS-FFPACK

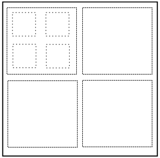


Tile recursive
FFLAS-FFPACK

- Sub-cubic complexity: recursive algorithms

The case of Gaussian elimination

Which reduction to MatMul ?

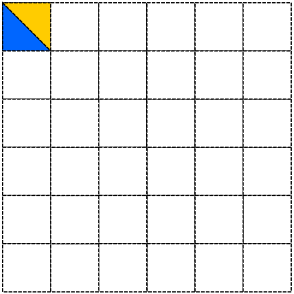


Tile recursive
FFLAS-FFPACK

- Sub-cubic complexity: recursive algorithms
- Data locality

Block algorithms

Tiled Iterative | Slab Recursive | Tiled Recursive



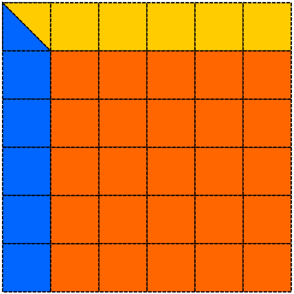
getrf: $A \rightarrow L, U$

Block algorithms

Tiled Iterative

Slab Recursive

Tiled Recursive



trsm: $B \leftarrow BU^{-1}$, $B \leftarrow L^{-1}B$

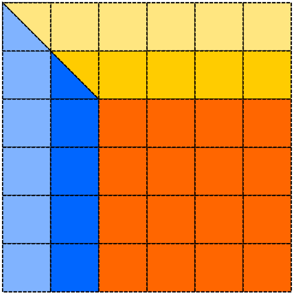
gemm: $C \leftarrow C - A \times B$

Block algorithms

Tiled Iterative

Slab Recursive

Tiled Recursive



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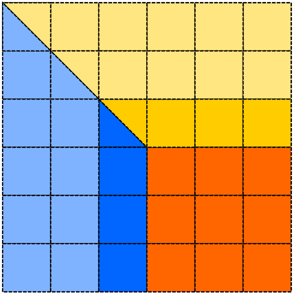

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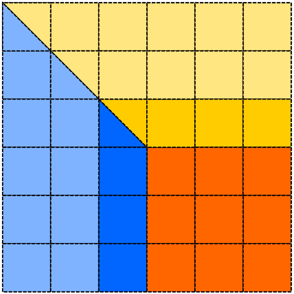
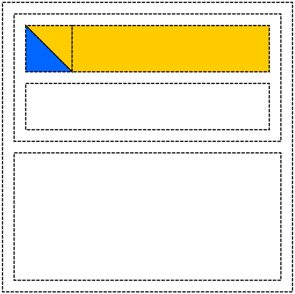
Block algorithms

Tiled Iterative



Slab Recursive

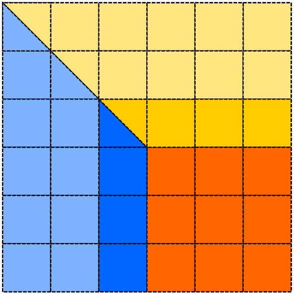


Tiled Recursive

getrf: $A \rightarrow L, U$

Block algorithms

Tiled Iterative



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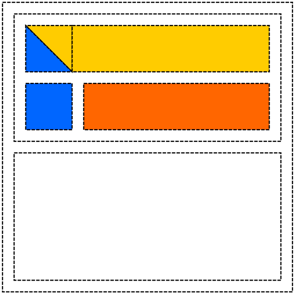

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Block algorithms

Tiled Iterative

Slab Recursive

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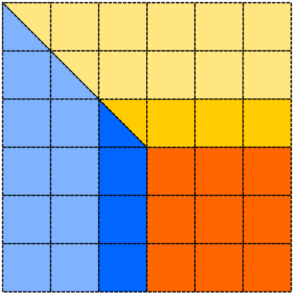
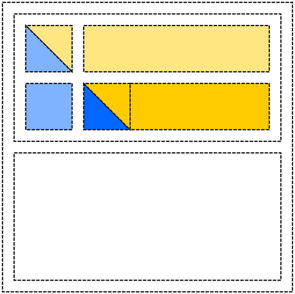
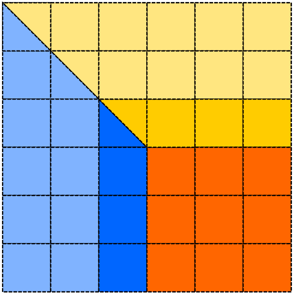




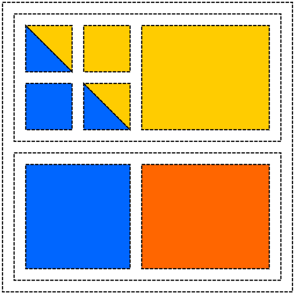
getrf: $A \rightarrow L, U$

Block algorithms

Tiled Iterative



Slab Recursive



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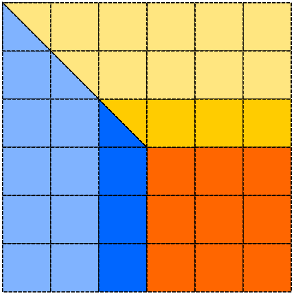
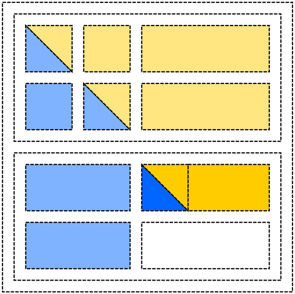
Block algorithms

Tiled Iterative



Slab Recursive

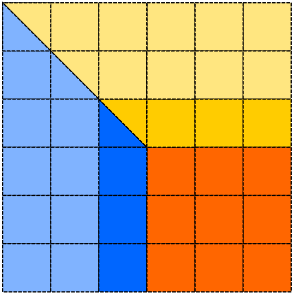


Tiled Recursive

getrf: $A \to L, U$

Block algorithms

Tiled Iterative



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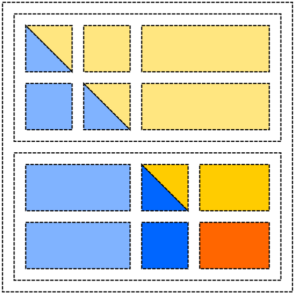

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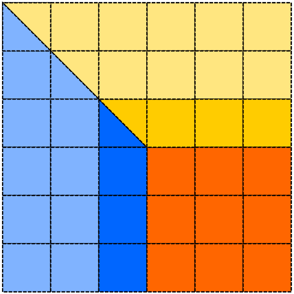

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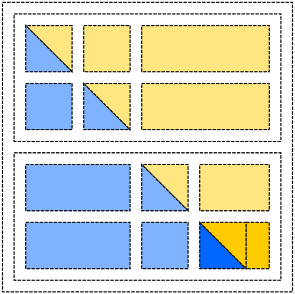

Tiled Recursive

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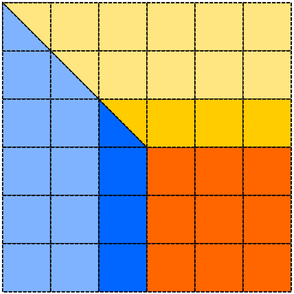
Block algorithms

Tiled Iterative



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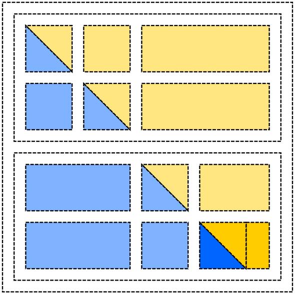

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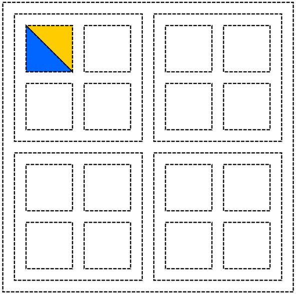
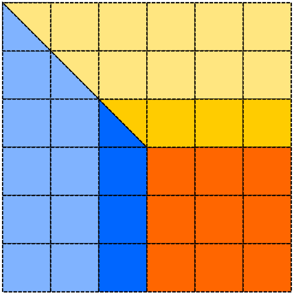


getrf: $A \to L, U$

Block algorithms

Tiled Iterative



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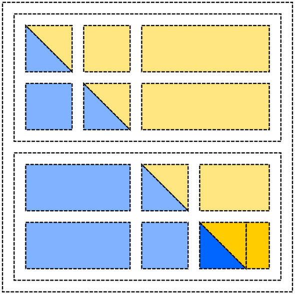

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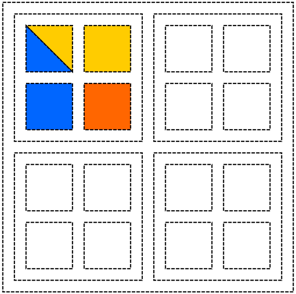

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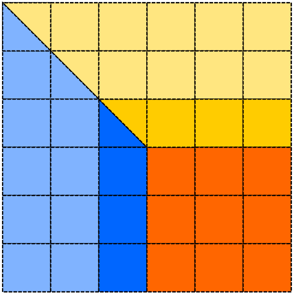
Block algorithms

Tiled Iterative



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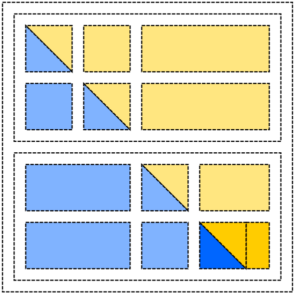

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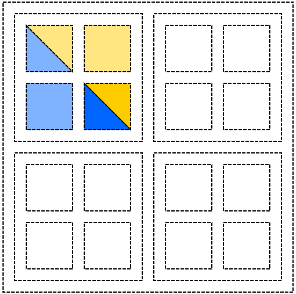

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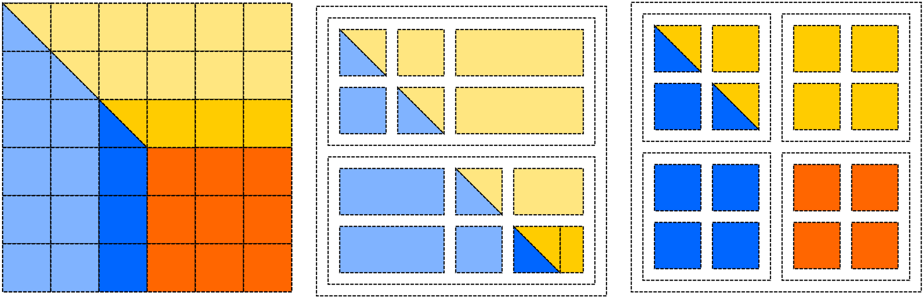
Block algorithms

Tiled Iterative

Slab Recursive

Tiled Recursive



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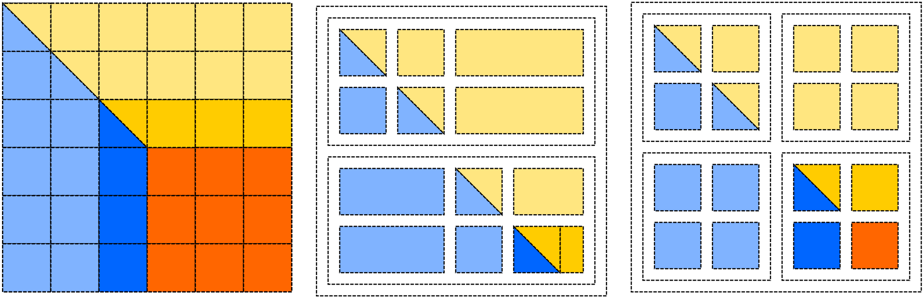
Tiled Iterative | Slab Recursive | Tiled Recursive



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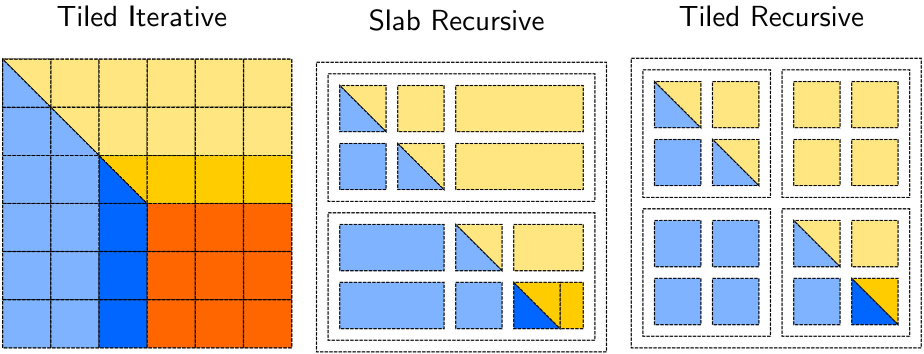


getrf: $A \to L, U$

Counting Modular Reductions

$k \geq 1$	Tiled Iter. Right looking	$\mathbf{\frac{1}{3k} n^3} + \left(1 - \frac{1}{k}\right) n^2 + \left(\frac{1}{6}k - \frac{5}{2} + \frac{3}{k}\right) n$
	Tiled Iter. Left looking	$\mathbf{\left(2 - \frac{1}{2k}\right) n^2} + \left(-\frac{5}{2}k - 1 + \frac{2}{k}\right) n + 2k^2 - 2k + 1$
	Tiled Iter. Crout	$\mathbf{\left(\frac{5}{2} - \frac{1}{k}\right) n^2} + \left(-2k - \frac{5}{2} + \frac{3}{k}\right) n + k^2$

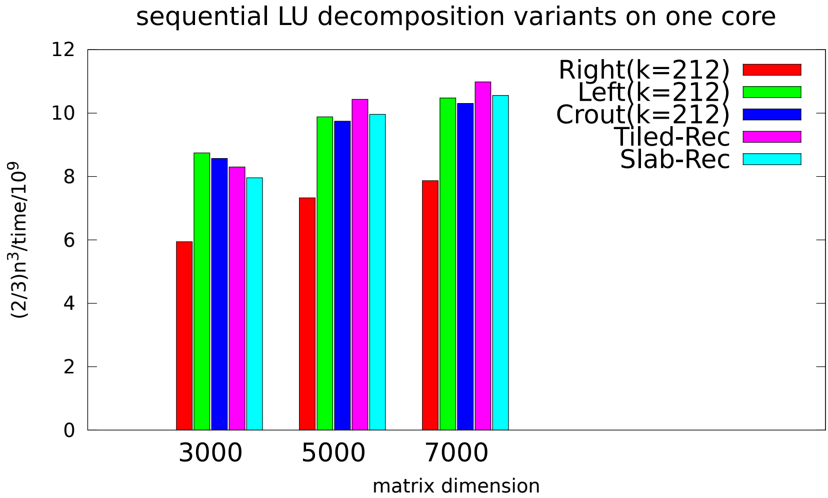
Counting Modular Reductions

$k \geq 1$	Tiled Iter. Right looking	$\mathbf{\frac{1}{3k}n^3} + \left(1 - \frac{1}{k}\right)n^2 + \left(\frac{1}{6}k - \frac{5}{2} + \frac{3}{k}\right)n$
	Tiled Iter. Left looking	$\left(\mathbf{2} - \mathbf{\frac{1}{2k}}\right)\mathbf{n^2} + \left(-\frac{5}{2}k - 1 + \frac{2}{k}\right)n + 2k^2 - 2k + 1$
	Tiled Iter. Crout	$\left(\mathbf{\frac{5}{2}} - \mathbf{\frac{1}{k}}\right)\mathbf{n^2} + \left(-2k - \frac{5}{2} + \frac{3}{k}\right)n + k^2$
$k = 1$	Iter. Right looking	$\mathbf{\frac{1}{3}n^3} - \frac{1}{3}n$
	Iter. Left Looking	$\mathbf{\frac{3}{2}n^2} - \frac{3}{2}n + 1$
	Iter. Crout	$\mathbf{\frac{3}{2}n^2} - \frac{7}{2}n + 3$

Counting Modular Reductions

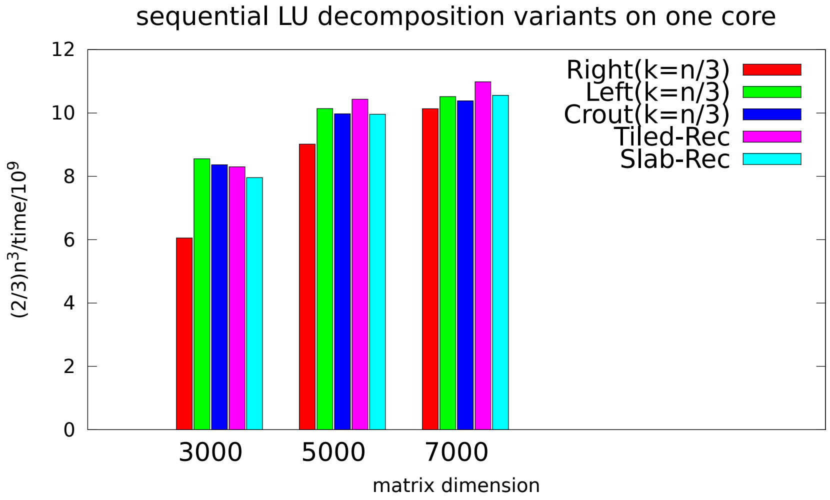
$k \geq 1$	Tiled Iter. Right looking	$\frac{\mathbf{1}}{\mathbf{3k}}\mathbf{n^3} + \left(1-\frac{1}{k}\right)n^2 + \left(\frac{1}{6}k - \frac{5}{2} + \frac{3}{k}\right)n$
	Tiled Iter. Left looking	$\left(\mathbf{2} - \frac{\mathbf{1}}{\mathbf{2k}}\right)\mathbf{n^2} + \left(-\frac{5}{2}k - 1 + \frac{2}{k}\right)n + 2k^2 - 2k + 1$
	Tiled Iter. Crout	$\left(\frac{\mathbf{5}}{\mathbf{2}} - \frac{\mathbf{1}}{\mathbf{k}}\right)\mathbf{n^2} + \left(-2k - \frac{5}{2} + \frac{3}{k}\right)n + k^2$
$k = 1$	Iter. Right looking	$\frac{\mathbf{1}}{\mathbf{3}}\mathbf{n^3} - \frac{1}{3}n$
	Iter. Left Looking	$\frac{\mathbf{3}}{\mathbf{2}}\mathbf{n^2} - \frac{3}{2}n + 1$
	Iter. Crout	$\frac{\mathbf{3}}{\mathbf{2}}\mathbf{n^2} - \frac{7}{2}n + 3$
	Tiled Recursive	$\mathbf{2n^2} - n\log_2 n - n$
	Slab Recursive	$(\mathbf{1} + \frac{\mathbf{1}}{\mathbf{4}}\log_{\mathbf{2}}\mathbf{n})\mathbf{n^2} - \frac{1}{2}n\log_2 n - n$

Impact in practice



- As anticipated : Right-looking < Crout < Left-looking

Impact in practice

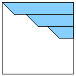


- As anticipated : Right-looking < Crout < Left-looking

Dealing with rank deficiencies and computing rank profiles

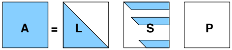
Rank profiles: first linearly independent columns

- Major invariant of a matrix (echelon form)
- Gröbner basis computations (Macaulay matrix)
- Krylov methods

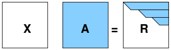


Gaussian elimination revealing echelon forms:

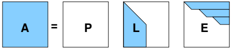
[Ibarra, Moran and Hui 82]



[Keller-Gehrig 85]



[Jeannerod, P. and Storjohann 13]



Computing rank profiles

Lessons learned (or what we thought was necessary):

- treat rows in order
- exhaust all columns before considering the next row
- **slab** block splitting required (recursive or iterative)
  $\rightsquigarrow$ similar to partial pivoting

Computing rank profiles

Lessons learned (or what we thought was necessary):

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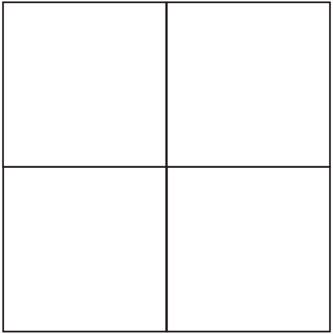
- **slab** block splitting required (recursive or iterative)
  $\rightsquigarrow$ similar to partial pivoting

Tiled recursive PLUQ [Dumas P. Sultan 13,15]

1. Generalized to handle rank deficiency
   - 4 recursive calls necessary
   - in-place computation
2. Pivoting strategies exist to recover rank profile and echelon forms

A tiled recursive algorithm

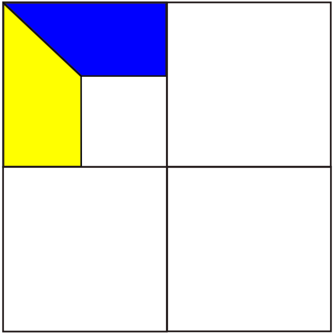
[Dumas, P. and Sultan 13]



2×2 block splitting

A tiled recursive algorithm

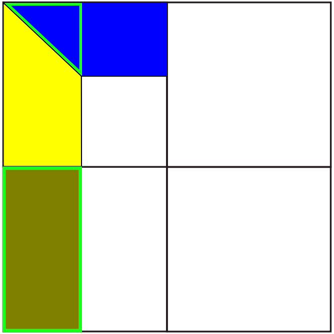
[Dumas, P. and Sultan 13]



Recursive call

A tiled recursive algorithm

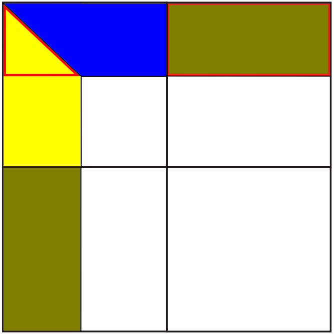
[Dumas, P. and Sultan 13]



TRSM: $B \leftarrow BU^{-1}$

A tiled recursive algorithm

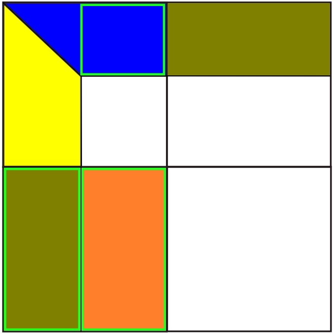
[Dumas, P. and Sultan 13]



TRSM: $B \leftarrow L^{-1}B$

A tiled recursive algorithm

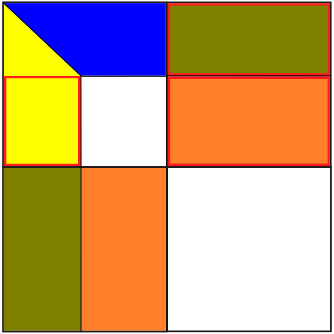
[Dumas, P. and Sultan 13]



`MatMul`: $C \leftarrow C - A \times B$

A tiled recursive algorithm

[Dumas, P. and Sultan 13]



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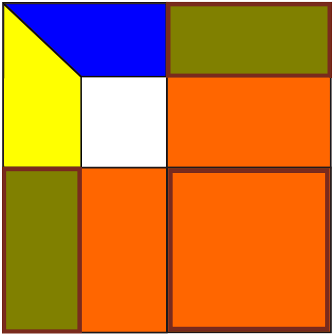
[Dumas, P. and Sultan 13]



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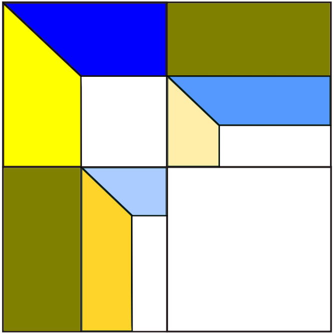
A tiled recursive algorithm

[Dumas, P. and Sultan 13]



2 independent recursive calls

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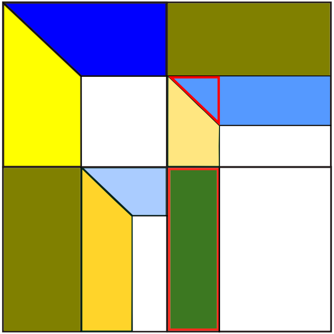

TRSM: $B \leftarrow BU^{-1}$

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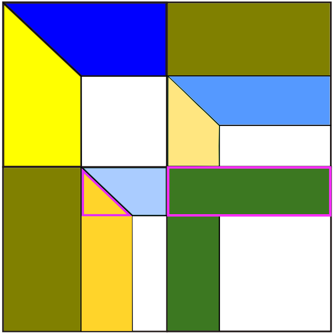

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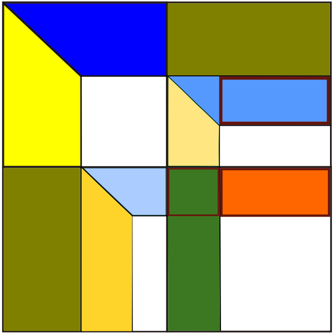

`MatMul`: $C \leftarrow C - A \times B$

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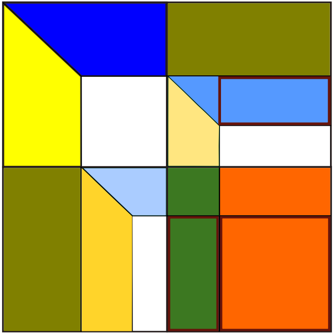

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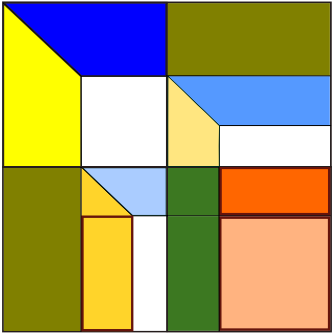

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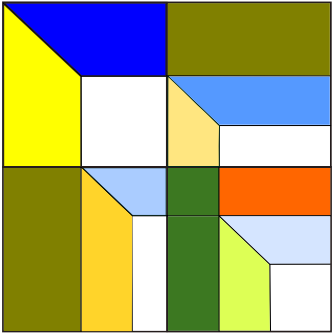

Recursive call

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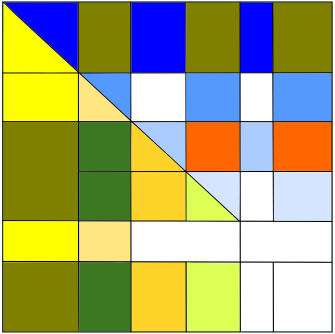
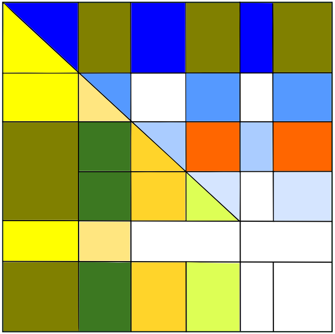
[Dumas, P. and Sultan 13]



Puzzle game (block cyclic rotations)

A tiled recursive algorithm

[Dumas, P. and Sultan 13]



- $O(mnr^{\omega-2})$ (degenerating to $2/3n^3$)
- computing col. and row rank profiles of all leading sub-matrices
- fewer modular reductions than slab algorithms
- rank deficiency introduces parallelism

Computing all rank profiles at once

Dumas, P. and Sultan ISSAC'15 (Thursday 9 @ 3PM)

Definition (Rank Profile matrix)

The unique $\mathcal{R}_A \in \{0,1\}^{m\times n}$ such that any pair of (i,j)-leading sub-matrix of $\mathcal{R}_A$ and of A have the same rank.

$$A = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 2 & 4 & 5 & 8 \\ 1 & 2 & 3 & 4 \\ 3 & 5 & 9 & 12 \end{bmatrix} \longrightarrow \mathcal{R} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}$$

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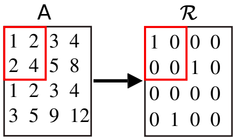

RowRP $= \{1\}$
ColRP $= \{1\}$

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ColRP = {1,3}

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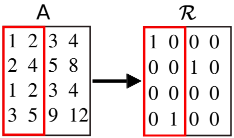

RowRP = {1,4}
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A

1	2	3	4
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1	2	3	4
3	5	9	12

→

$\mathcal{R}$

1	0	0	0
0	0	1	0
0	0	0	0
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With appropriate pivoting: $\Pi_{P,Q} = \mathcal{R}(A)$

Reductions in black box linear algebra

Matrix-Vector Product: building block,
$\rightsquigarrow$ costs $E(n)$

Minimal polynomial: [Wiedemann 86]
$\rightsquigarrow$ iterative Krylov/Lanczos methods
$\rightsquigarrow O(nE(n) + n^2)$

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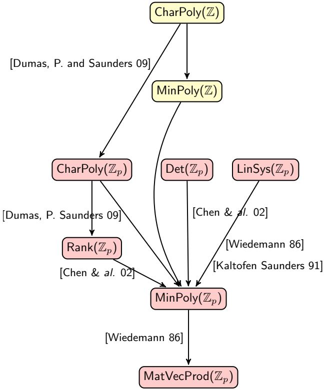

Outline

Size Dimension trade-offs

Computing with coefficients of varying size: $\mathbb{Z}, \mathbb{Q}, K[X], \ldots$

Multimodular methods

over K[X]: evaluation-interpolation

over $\mathbb{Z}$,$\mathbb{Q}$: Chinese Remainder Theorem

$$\text{Cost} = \text{Algebraic Cost} \times \text{Size(Output)}$$

✓ avoids coefficient blow-up

✗ uniform (worst case) cost for all arithmetic ops

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Example

Hadamard's bound: $|\det(A)| \leq (\|A\|_\infty \sqrt{n})^n$.

$\texttt{LinSys}_\mathbb{Z}(n) = O(n^\omega \times n(\log n + \log \|A\|_\infty))$

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Lifting techniques

p-adic lifting: [Moenck & Carter 79, Dixon 82]

- One computation over $\mathbb{Z}_p$
- Iterative lifting of the solution to $\mathbb{Z}, \mathbb{Q}$

Example

$\texttt{LinSys}_{\mathbb{Z}}(n) = O(n^3 \log \|A\|_\infty^{1+\epsilon})$

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High order lifting : [Storjohann 02,03]

- Fewer iteration steps
- larger dimension in the lifting

Example

$\texttt{LinSys}_{\mathbb{Z}}(n) = O\tilde{~}(n^\omega \log \|A\|_\infty)$

Improving time Complexities

Matrix multiplication: door to fast linear algebra

- over $\mathbb{Z}$: $O(n^\omega M(\log \|A\|)) = O\tilde{}(n^\omega \log \|A\|)$

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Equivalence over $\mathbb{Z}$ or K[X]: Hermite normal form

- [Kannan & Bachem 79]: $\in P$
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- [Storjohann 00]: $O\tilde{}(n^\omega)$ deterministic
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Building blocks and reductions

In brief

Reductions to a building block

Matrix Mult: block rec. $\sum_{i=1}^{\log n} n \left(\frac{n}{2^i}\right)^{\omega-1} = O(n^\omega)$ (Gauss, REF)

Matrix Mult: Iterative $\sum_{k=1}^{n} k \left(\frac{n}{k}\right)^{\omega} = O(n^\omega)$ (Frobenius)

Linear Sys: over $\mathbb{Z}$ (Hermite Normal Form)

Size/dimension compromises

- Hermite normal form : rank 1 updates reducing the determinant
- Frobenius normal form : degree k, dimension n/k for $k = 1 \dots n$

Hermite normal form: naive algorithm

Reduced Echelon form over a ring: $\begin{bmatrix} p_1 & * & x_{1,2} & * & * & x_{1,3} & * \\ & & p_2 & * & * & x_{2,3} & * \\ & & & & & p_3 & * \\ & & & & & & \end{bmatrix}$ with

$$0 \leq x_{*,j} < p_j.$$

for $i = 1 \dots n$ **do**
- $(g, t_i, \dots, t_n) = \text{xgcd}(A_{i,i}, A_{i+1,i}, \dots, A_{n,i})$
- $L_i \leftarrow \sum_{j=i+1}^{n} t_j L_j$
- **for** $j = i+1 \dots n$ **do**
  - $L_j \leftarrow L_j - \frac{A_{j,i}}{g} L_i$ ▷ eliminate
- **end for**
- **for** $j = 1 \dots i-1$ **do**
  - $L_j \leftarrow L_j - \lfloor \frac{A_{j,i}}{g} \rfloor L_i$ ▷ reduce
- **end for**

end for

Computing modulo the determinant [Domich & Al. 87]

Property

- *For A non-singular:* $\max_i \sum_j H_{ij} \leq \det H = \det A$

Example

$$A = \begin{bmatrix} -5 & 8 & -3 & -9 & 5 & 5 \\ -2 & 8 & -2 & -2 & 8 & 5 \\ 7 & -5 & -8 & 4 & 3 & -4 \\ 1 & -1 & 6 & 0 & 8 & -3 \end{bmatrix}, H = \begin{bmatrix} 1 & 0 & 3 & 237 & -299 & 90 \\ 0 & 1 & 1 & 103 & -130 & 40 \\ 0 & 0 & 4 & 352 & -450 & 135 \\ 0 & 0 & 0 & 486 & -627 & 188 \end{bmatrix}$$

$$\det A = 1944$$

Computing modulo the determinant [Domich & Al. 87]

Property

- *For* A *non-singular:* $\max_i \sum_j H_{ij} \leq \det H = \det A$
- *Every computation can be done modulo* $d = \det A$*:*

$$U' \begin{bmatrix} A & \\ dI_n & I_n \end{bmatrix} = \begin{bmatrix} H & \\ & I_n \end{bmatrix}$$

Example

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$$\det A = 1944$$

$\rightsquigarrow O(n^3) \times M(n(\log n + \log \|A\|)) = O\tilde{}(n^5 \log \|A\|^2)$

Computing modulo the determinant

- Pessimistic estimate on the arithmetic size
- d large but most coefficients of H are small
- *On average* : only the last few columns are *large*

$\rightsquigarrow$ Compute H' *close* to H but with small determinant

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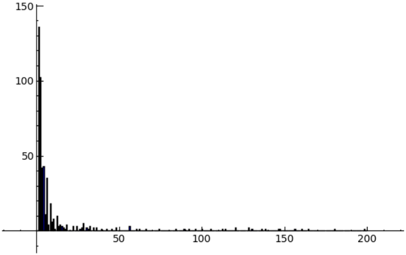
[Micciancio & Warinschi 01]

$$A = \begin{bmatrix} B & b \\ c^T & a_{n-1,n} \\ d^T & a_{n,n} \end{bmatrix}$$

$$d_1 = \det\left(\begin{bmatrix} B \\ c^T \end{bmatrix}\right), d_2 = \det\left(\begin{bmatrix} B \\ d^T \end{bmatrix}\right)$$

$g = \text{gcd}(d_1, d_2) = sd_1 + td_2$ Then

$$\det\left(\begin{bmatrix} B \\ sc^T + td^T \end{bmatrix}\right) = g$$



Micciancio & Warinschi algorithm

Compute $d_1 = \det\left(\begin{bmatrix} B \\ c^T \end{bmatrix}\right), d_2 = \det\left(\begin{bmatrix} B \\ d^T \end{bmatrix}\right)$ ▷ Double Det

$(g, s, t) = \mathsf{xgcd}(d_1, d_2)$

Compute H_1 the HNF of $\begin{bmatrix} B \\ sc^T + td^T \end{bmatrix} \mod g$ ▷ Modular HNF

Recover H_2 the HNF of $\begin{bmatrix} B & b \\ sc^T + td^T & sa_{n-1,n} + ta_{n,n} \end{bmatrix}$ ▷ AddCol

Recover H_3 the HNF of $\begin{bmatrix} B & b \\ c^T & a_{n-1,n} \\ d^T & a_{n,n} \end{bmatrix}$ ▷ AddRow

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Double Determinant

First approach: LU mod $p_1, \ldots, p_k$ + CRT

- Only one elimination for the $n-2$ first rows
- 2 updates for the last rows (triangular back substitution)
- k *large* such that $\prod_{i=1}^{k} p_i > n^n \log \|A\|^{n/2}$

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Second approach: [Abbott Bronstein Mulders 99]

- Solve $Ax = b$.
- $\delta = \text{lcm}(q_1, \ldots, q_n)$ s.t. $x_i = p_i/q_i$

Then δ is a *large* divisor of $D = \det A$.

- Compute D/δ by LU mod $p_1, \ldots, p_k$ + CRT
- k *small*, such that $\prod_{i=1}^{k} p_i > n^n \log \|A\|^{n/2}/\delta$

Double Determinant : improved

Property

Let $x = [x_1, \ldots, x_n]$ *be the solution of* $\left[\begin{array}{c|c} A & c \end{array}\right] x = d$*. Then* $y = [-\frac{x_1}{x_n}, \ldots, -\frac{x_{n-1}}{x_n}, \frac{1}{x_n}]$ *is the solution of* $\left[\begin{array}{c|c} A & d \end{array}\right] y = c$*.*

- 1 system solve
- 1 LU for each p_i

$\rightsquigarrow d_1, d_2$ computed at about the cost of 1 déterminant

AddCol

Problem

Find a vector e *such that*

$$\begin{bmatrix} H_1 & | & e \end{bmatrix} = U \begin{bmatrix} B & b \\ sc^T + td^T & sa_{n-1,n} + ta_{n,n} \end{bmatrix}$$

$$\begin{aligned} e &= U \begin{bmatrix} b \\ sa_{n-1,n} + ta_{n,n} \end{bmatrix} \\ &= H_1 \begin{bmatrix} B \\ sc^T + td^T \end{bmatrix}^{-1} \begin{bmatrix} b \\ sa_{n-1,n} + ta_{n,n} \end{bmatrix} \end{aligned}$$

⇝ Solve a system.

- $n-1$ first rows are *small*
- last row is *large*

AddCol

Idea:

replace the last row by a random *small* one w^T.

$$\begin{bmatrix} B \\ w^T \end{bmatrix} y = \begin{bmatrix} b \\ a_{n-1,n-1} \end{bmatrix}$$

Let $\{k\}$ be a basis of the kernel of B. Then

$$x = y + \alpha k.$$

where

$$\alpha = \frac{a_{n-1,n-1} - (sc^T + td^T) \cdot y}{(sc^T + td^T) \cdot k}$$

$\rightsquigarrow$ limits the *expensive* arithmetic to a few dot products

Computing the Frobenius normal form

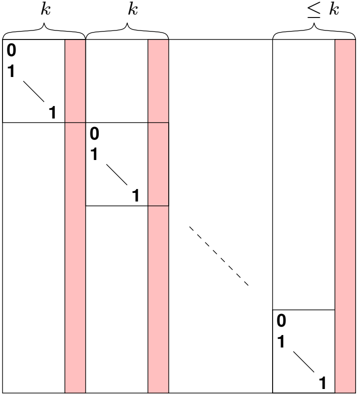
Definition

Unique $F = U^{-1}AU = \mathrm{Diag}(C_{f_0}, \ldots, C_{f_k})$ with $f_k | f_{k-1} | \ldots | f_0$.

Computing the Frobenius normal form

[P. & Storjohann 07]

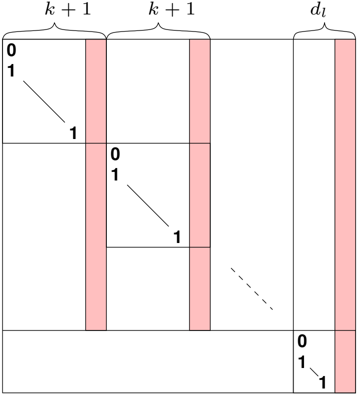
k-shifted form:



Computing the Frobenius normal form

[P. & Storjohann 07]

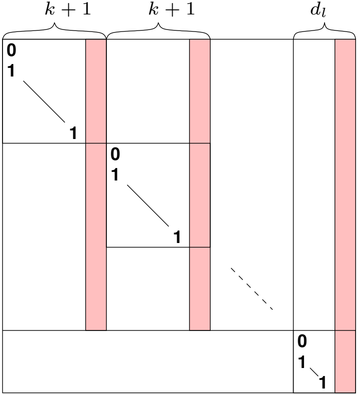
$k+1$-shifted form:



Computing the Frobenius normal form

[P. & Storjohann 07]

$k+1$-shifted form:

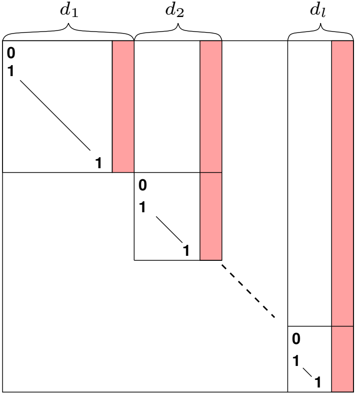


- From k to $k+1$-shifted in $O(k(\frac{n}{k})^\omega)$
- Compute iteratively from a 1-shifted form
- Invariant factors appear by increasing degree

Computing the Frobenius normal form

[P. & Storjohann 07]

Hessenberg polycyclic:

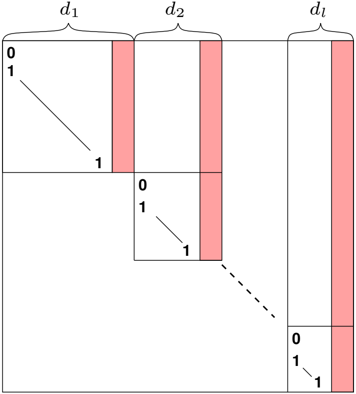


- From k to $k+1$-shifted in $O(k(\frac{n}{k})^{\omega})$
- Compute iteratively from a 1-shifted form
- Invariant factors appear by increasing degree
- Until the Hessenberg polycyclic form

Computing the Frobenius normal form

[P. & Storjohann 07]

Hessenberg polycyclic:



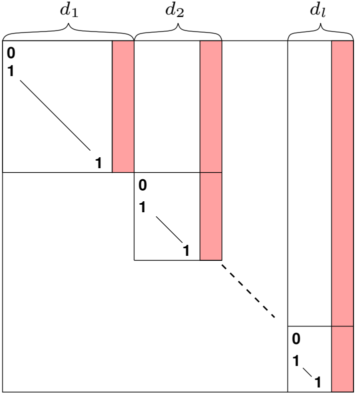
- From k to $k+1$-shifted in $O(k(\frac{n}{k})^\omega)$
- Compute iteratively from a 1-shifted form
- Invariant factors appear by increasing degree
- Until the Hessenberg polycyclic form

$$n^\omega \sum_{k=1}^{n} \left(\frac{1}{k}\right)^{\omega-1} \leq \zeta(\omega-1)n^\omega = O(n^\omega)$$

Computing the Frobenius normal form

[P. & Storjohann 07]

Hessenberg polycyclic:

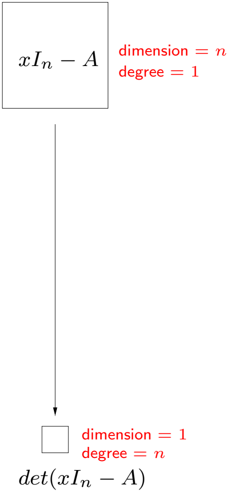


- From k to $k+1$-shifted in $O(k(\frac{n}{k})^\omega)$
- Compute iteratively from a 1-shifted form
- Invariant factors appear by increasing degree
- Until the Hessenberg polycyclic form

$$n^\omega \sum_{k=1}^{n} \left(\frac{1}{k}\right)^{\omega-1} \leq \zeta(\omega-1)n^\omega = O(n^\omega)$$

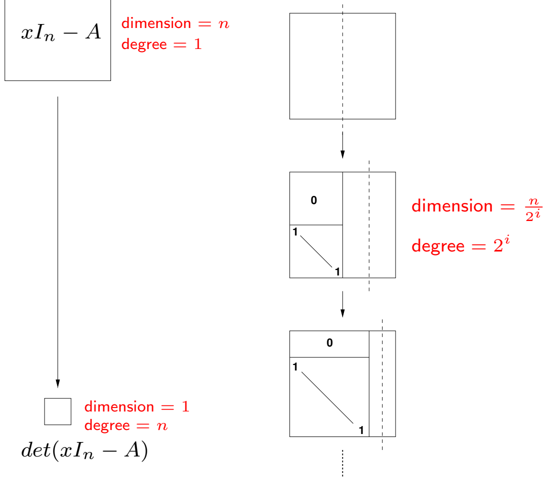
- Generalized to the Frobenius form as well
- Transformation matrix in $O(n^\omega \log\log n)$

A new type size dimension trade-off

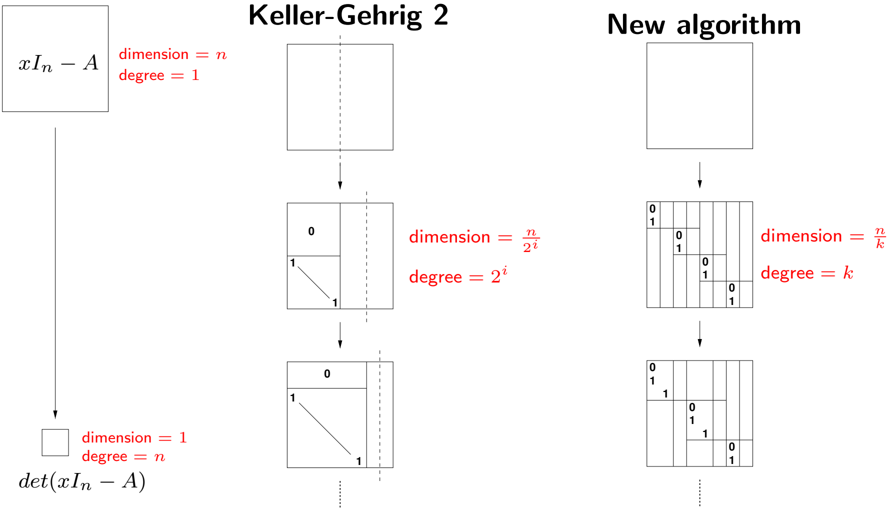


A new type size dimension trade-off

Keller-Gehrig 2



A new type size dimension trade-off



Outline

1. Choosing the underlying arithmetic
   - Using boolean arithmetic
   - Using machine word arithmetic
   - Larger field sizes
2. Reductions and building blocks
   - In dense linear algebra
   - In blackbox linear algebra
3. Size dimension trade-offs
   - Hermite normal form
   - Frobenius normal form
4. Parallel exact linear algebra
   - Ingredients for the parallelization
   - Parallel dense linear algebra mod p

Parallelization

Parallel numerical linear algebra

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

  ⇝ fine grain

  ⇝ 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

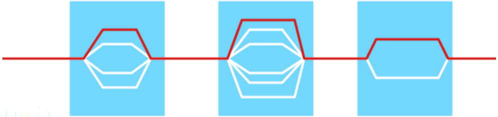
3 main models:

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

Data Parallelism

OMP

```
for (int step = 0; step < 2; ++step){
#pragma omp parallel for
    for (int i = 0; i < count; ++i)
        A[i] = (B[i+1] + B[i-1] + 2.0*B[i])*0.25;
}
```



Limitation: very un-efficient with recursive parallel regions

- Limited to iterative algorithms
- No composition of routines

Task parallelism with fork-Join

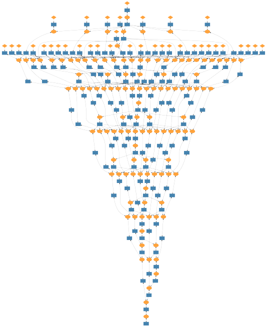
- Task based program: **spawn** + **sync**
- Especially suited for recursive programs

OMP (since v3)

```
void fibonacci(long* result, long n) {
  if (n < 2)
    *result = n;
  else {
    long x,y;
#pragma omp task
    fibonacci( &x, n-1 );
    fibonacci( &y, n-2 );
#pragma omp taskwait
    *result = x + y;
  }
}
```

Tasks with dataflow dependencies

- Task based model avoiding synchronizations
- Infer synchronizations from the read/write specifications
  - A task is ready for execution when all its inputs variables are ready
  - A variable is ready when it has been written
- Recently supported: Athapascan [96], Kaapi [06], StarSs [07], StarPU [08], Quark [10], OMP since v4 [14]...



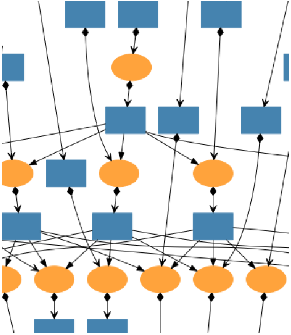
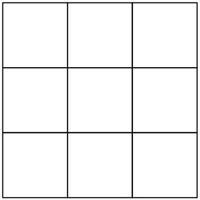


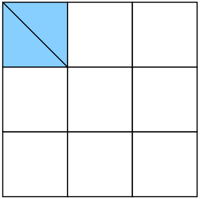
Illustration: Cholesky factorization

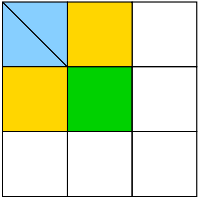
```
void Cholesky( double* A, int N, size_t NB ) {

  for (size_t k=0; k < N; k += NB)
  {
    clapack_dpotrf( CblasRowMajor, CblasLower, NB, &A[k*N+k], N );

    for (size_t m=k+ NB; m < N; m += NB)
    {

      cblas_dtrsm ( CblasRowMajor, CblasLeft, CblasLower, CblasNoTrans, CblasUnit,
        NB, NB, 1., &A[k*N+k], N, &A[m*N+k], N );
    }

    for (size_t m=k+ NB; m < N; m += NB)
    {

      cblas_dsyrk ( CblasRowMajor, CblasLower, CblasNoTrans,
        NB, NB, -1.0, &A[m*N+k], N, 1.0, &A[m*N+m], N );

      for (size_t n=k+NB; n < m; n += NB)
      {

        cblas_dgemm ( CblasRowMajor, CblasNoTrans, CblasTrans,
          NB, NB, NB, -1.0, &A[m*N+k], N, &A[n*N+k], N, 1.0, &A[m*N+n], N );
      }
    }

  }
}
```

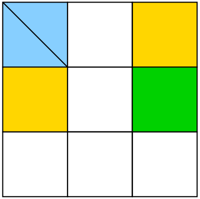
Illustration: Cholesky factorization

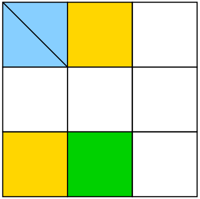
```
void Cholesky( double* A, int N, size_t NB ) {
#pragma omp parallel
#pragma omp single nowait
  for (size_t k=0; k < N; k += NB)
  {
    clapack_dpotrf( CblasRowMajor, CblasLower, NB, &A[k*N+k], N );

    for (size_t m=k+ NB; m < N; m += NB)
    {
#pragma omp task firstprivate(k, m) shared(A)
      cblas_dtrsm ( CblasRowMajor, CblasLeft, CblasLower, CblasNoTrans, CblasUnit,
        NB, NB, 1., &A[k*N+k], N, &A[m*N+k], N );
    }
#pragma omp taskwait // Barrier: no concurrency with next tasks
    for (size_t m=k+ NB; m < N; m += NB)
    {
#pragma omp task firstprivate(k, m) shared(A)
      cblas_dsyrk ( CblasRowMajor, CblasLower, CblasNoTrans,
        NB, NB, -1.0, &A[m*N+k], N, 1.0, &A[m*N+m], N );

      for (size_t n=k+NB; n < m; n += NB)
      {
#pragma omp task firstprivate(k, m) shared(A)
        cblas_dgemm ( CblasRowMajor, CblasNoTrans, CblasTrans,
          NB, NB, NB, -1.0, &A[m*N+k], N, &A[n*N+k], N, 1.0, &A[m*N+n], N );
      }
    }
#pragma omp taskwait // Barrier: no concurrency with tasks at iteration k+1
  }
}
```

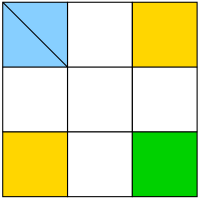












SYNC.

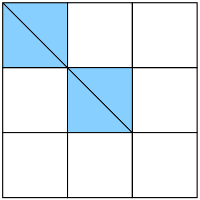
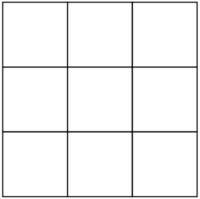
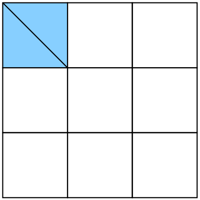
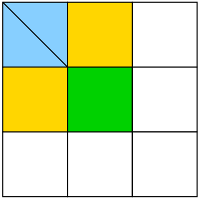


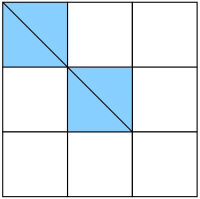
Illustration: Cholesky factorization

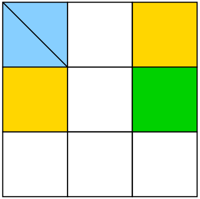
```
void Cholesky( double* A, int N, size_t NB ){
#pragma kaapi parallel
  for (size_t k=0; k < N; k += NB)
  {
#pragma kaapi task readwrite(&A[k*N+k]{ld=N; [NB][NB]})
    clapack_dpotrf( CblasRowMajor, CblasLower, NB, &A[k*N+k], N );

    for (size_t m=k+ NB; m < N; m += NB)
    {
#pragma kaapi task read(&A[k*N+k]{ld=N;[NB][NB]}) readwrite(&A[m*N+k]{ld=N; [NB][NB]})
      cblas_dtrsm ( CblasRowMajor, CblasLeft, CblasLower, CblasNoTrans, CblasUnit,
        NB, NB, 1., &A[k*N+k], N, &A[m*N+k], N );
    }

    for (size_t m=k+ NB; m < N; m += NB)
    {
#pragma kaapi task read(&A[m*N+k]{ld=N;[NB][NB]}) readwrite(&A[m*N+m]{ld=N; [NB][NB]})
      cblas_dsyrk ( CblasRowMajor, CblasLower, CblasNoTrans,
        NB, NB, -1.0, &A[m*N+k], N, 1.0, &A[m*N+m], N );

      for (size_t n=k+NB; n < m; n += NB)
      {
#pragma kaapi task read(&A[m*N+k]{ld=N; [NB][NB]}, &A[n*N+k]{ld=N; [NB][NB]})\
                   readwrite(&A[m*N+n]{ld=N; [NB][NB]})
        cblas_dgemm ( CblasRowMajor, CblasNoTrans, CblasTrans,
          NB, NB, NB, -1.0, &A[m*N+k], N, &A[n*N+k], N, 1.0, &A[m*N+n], N );
      }
    }
  }
  // Implicit barrier only at the end of Kaapi parallel region
}
```

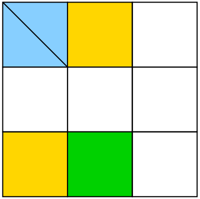


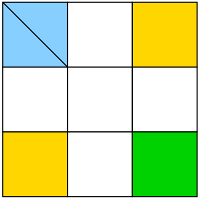






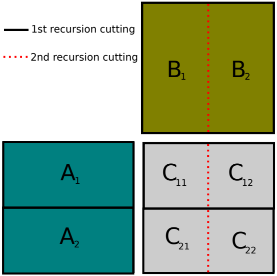


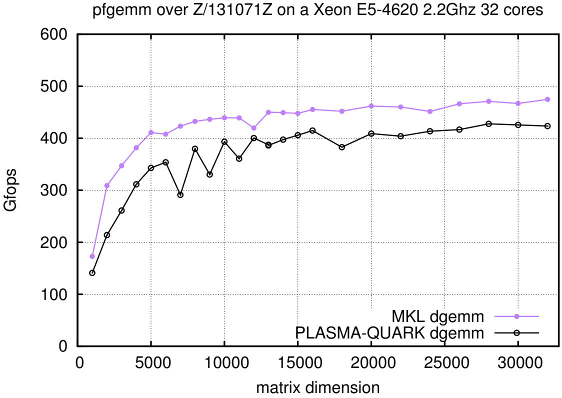




Parallel matrix multiplication

[Dumas, Gautier, P. & Sultan 14]





Parallel matrix multiplication

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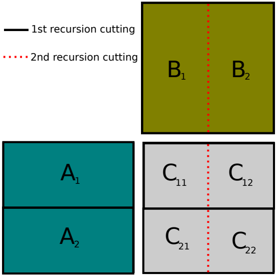
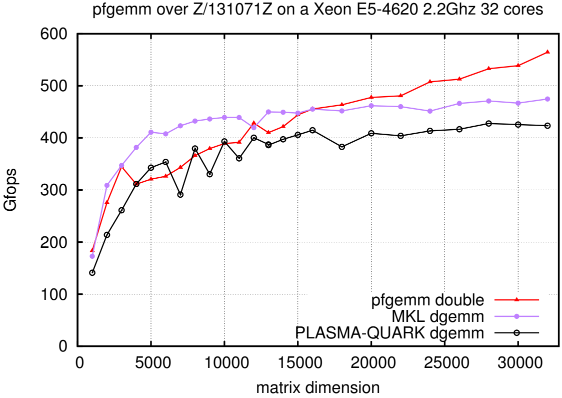
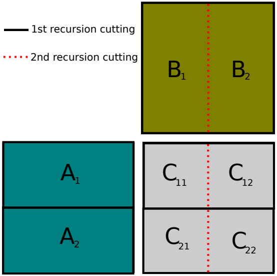
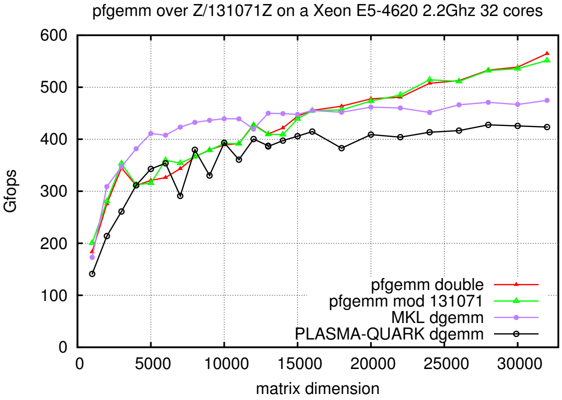




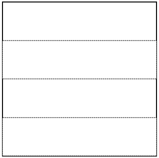
Parallel matrix multiplication

[Dumas, Gautier, P. & Sultan 14]

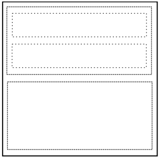




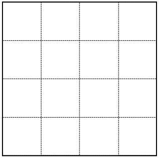
Gaussian elimination



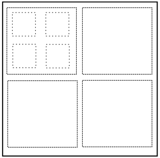
Slab iterative
`LAPACK`



Slab recursive
`FFLAS-FFPACK`

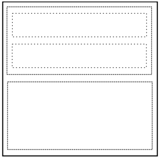


Tile iterative
`PLASMA`

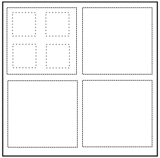


Tile recursive
`FFLAS-FFPACK`

Gaussian elimination



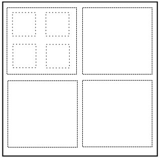
Slab recursive
FFLAS-FFPACK



Tile recursive
FFLAS-FFPACK

- Prefer recursive algorithms

Gaussian elimination

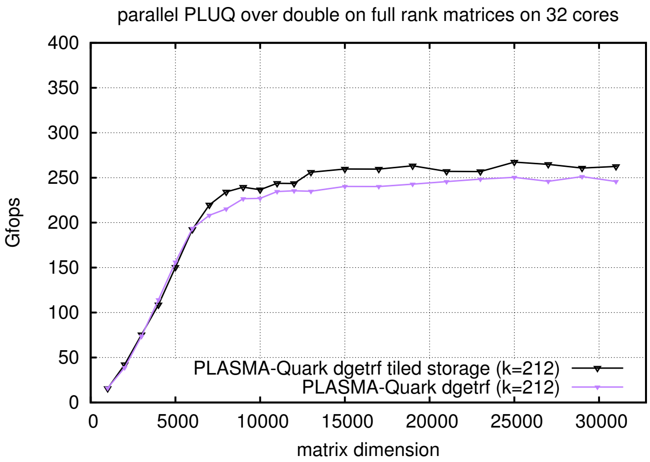


Tile recursive
FFLAS-FFPACK

- Prefer recursive algorithms
- Better data locality

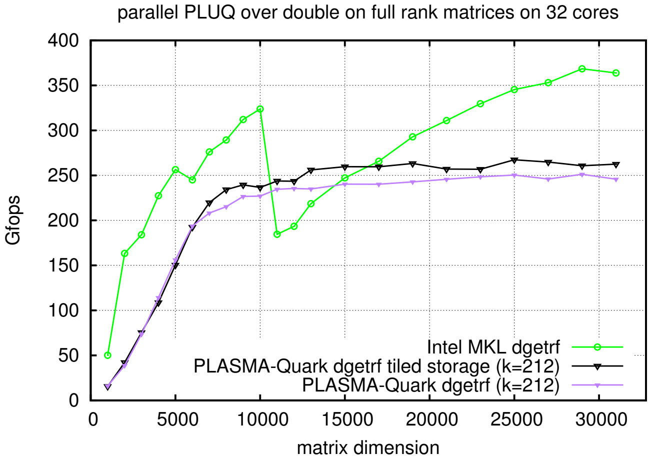
Full rank Gaussian elimination

[Dumas, Gautier, P. and Sultan 14] Comparing numerical efficiency (no modulo)



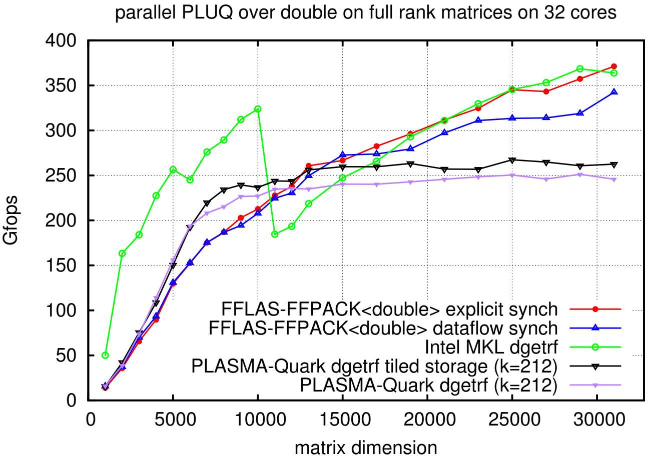
Full rank Gaussian elimination

[Dumas, Gautier, P. and Sultan 14] Comparing numerical efficiency (no modulo)



Full rank Gaussian elimination

[Dumas, Gautier, P. and Sultan 14] Comparing numerical efficiency (no modulo)



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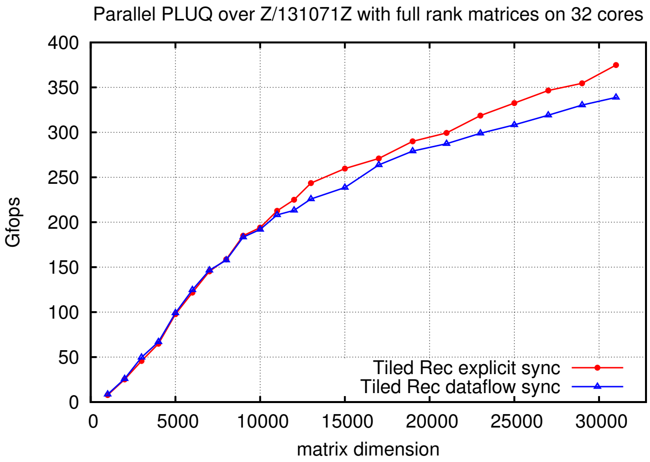
[Dumas, Gautier, P. and Sultan 14] Over the finite field $\mathbb{Z}/131071\mathbb{Z}$



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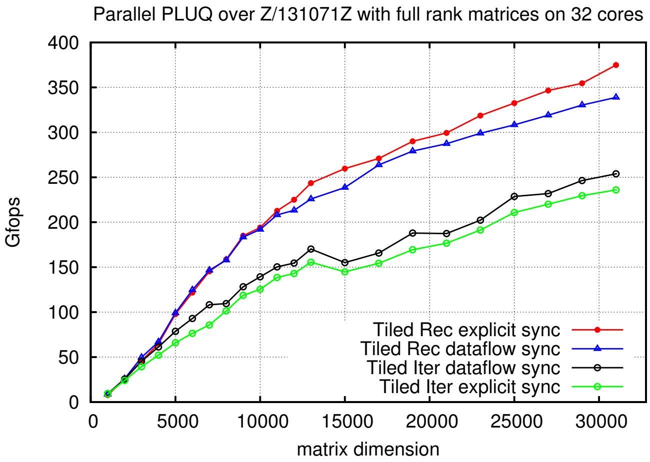

Conclusion

Design framework for high performance exact linear algebra

Asymptotic reduction > algorithm tuning > building block implementation

- So far, **floating point** arithmetic delivers best speed

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Perspectives

Large scale distributed exact linear algebra

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Thank you