Adaptive and Generic Parallel Exact Linear Algebra

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PhD Defense

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PhD research context

- Parallel computing



Symmetric Multi-Processors

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Symmetric Multi-Processors

- Effective exact parallel linear alegbra
  - Solve target problems : dedicated codes
  - Widely distributed software : general purpose codes (SAGE, Macauley2)

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Symmetric Multi-Processors

- Effective exact parallel linear alegbra
  - Solve target problems : dedicated codes
  - Widely distributed software : general purpose codes (SAGE, Macauley2)
- Design a software for parallel exact linear algebra

Exact linear algebra

Exact computation

- Computation in computer algebra
  $\rightarrow$ computing exactly : over $\mathbb{Z}$, $\mathbb{Q}$, $\mathbb{Z}[x]$
- In practice, often boils down to computation over prime fields $\mathbb{Z}/p\mathbb{Z}$

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Exact linear algebra applications

- Breaking Discrete Log Pb. in quasi-polynomial time [Barbulescu & al.14]
- Building modular form databases to test the BSD conjecture [Stein 12]
- Exact mixed-integer programming [Steffy et al. 12]
- Formal verification of Hales proof of Kepler conjecture [Hales 05]

Use case example of an application

HPAC on-going Challenge : D.L.P. cryptanalysis over curves over $\mathbb{F}(2^{29})$.

Problem dimensions

- Sparse matrix with 126M var. / 130M eq.
- Modulo a prime number on 114 bits : 20769187434139310549529495610151239
- Matrix has 520M non-zero

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Main steps of block Wiedemann

- First filtering (structured Gauss)
  $\rightarrow$ nRows : 8.7M, nCols : 8.7M.
  $\rightarrow$ Matrix has 810M non-zero with blocs 32×16
- MinPoly coefficients 16×16, degree 545966
  $\rightarrow$ needs efficient PLUQ factorization !
- Evaluation uses M.M. : $(n \times 32)$ times (32×32) $\rightarrow$ n is large !

Dense exact linear algebra

Dense linear algebra : A key building block for :

- dense problems by nature (Hermite-Padé approx, ...)
- Sparse problems degenerate to dense :
  - Sparse Direct :
    Switch to dense after fill-in
  - Sparse Iterative :
    Induce dense elimination on blocks of iterated vectors
    (block-Wiedemann, block Lanczos, ...)

Gaussian elimination in exact dense algebra

Gaussian elimination is a building block in dense linear algebra

Matrix factorization (**LU decomposition**)

- Solving linear systems
- Computing determinant
- Rank.

Linear dependencies (**Echelon structure**)

- Characteristic Polynomial : Finding Krylov basis [Keller Gehrig 85]
- Grobner basis computation : F4 algorithm [FGB]

Design of parallel dense exact linear algebra

	numerical	exact
Sequential	BLAS, LAPACK	FFLAS-FFPACK
Parallel	pBLAS, ScaLAPACK	

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Parallelizing dense linear algebra

- Specificities of exact linear algebra
  - Recursive algorithms
  - Rank deficiencies
- Similarities with numerical linear algebra
  Parallel blocking is constrained by pivoting :

  Numerical : ensuring numerical stability
  Exact : recovering rank profiles and echelon structure

Outline

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1. Pivoting and rank profiles
2. Generic parallel Linear Algebra
3. Parallel exact Gaussian elimination

Linear dependencies and row/column rank profiles

Definition (Row Rank Profile : RowRP)

Given $A \in K^{m \times n}$, $r =$ *rank*(A).

informally : *first* r *linearly independent rows*

formally : *lexico-minimal sub-sequence of* $(1, \ldots, m)$ *of* r *indices of linearly independant rows.*

Example

$$\begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

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Rank = 3
RowRP = $\{$ *1,2,4* $\}$

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Generic RowRP/ColRP : if it equals $\{1,\ldots,r\}$.

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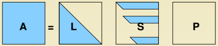
Rank = 3
RowRP = $\{$*1,2,4*$\}$
ColRP = $\{$*1,2,3*$\}$ $\rightarrow$ *Generic ColRP.*

Generic RowRP/ColRP : if it equals $\{1,\ldots,r\}$.

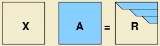
Computing rank profiles

Via Gaussian elimination revealing row echelon forms :

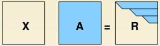
[Ibarra, Moran and Hui 82]



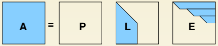
[Keller-Gehrig 85]



[Storjohann 00]



[Jeannerod, Pernet and Storjohann 13]



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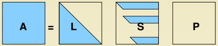

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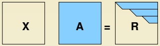

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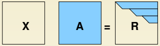

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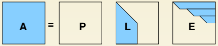
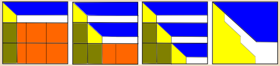


Lessons learned (or what we thought was necessary) :

- treat rows in order
- exhaust all columns before next row
- **slab** block splitting (rec or iter)

$\Rightarrow$ similar to partial pivoting



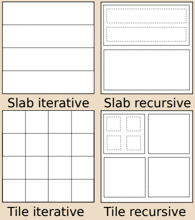
Motivation

Need more flexible blocking

Slab blocking

- can lead to inefficient memory access patterns
- is harder to parallelize

Tile blocking instead ?



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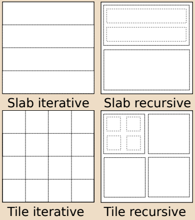


Gathering linear independence invariants

Two ways to look at a matrix (looking left or right) :

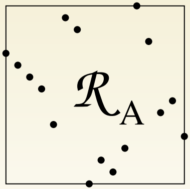
- Row rank profile, column echelon form
- Column rank profile, row echelon form

Unique invariant ?

The rank profile Matrix

Theorem

Let $A \in \mathrm{F}^{m \times n}$.
There exists a unique, $m \times n$, *rank*(A)*-sub-permutation matrix* $\mathcal{R}_A$ *of which every leading sub-matrix has the same rank as the corresponding leading sub-matrix of* A.



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Example

$$\begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 1 & 3 & 2 & 0 \\ 2 & 5 & 4 & 7 \end{bmatrix} \qquad \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

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Properties of the rank profile matrix

Particular cases

- A invertible $\Leftrightarrow \mathcal{R}_A$ is a permutation
- A is square with generic rank profile $\Leftrightarrow \mathcal{R}_A = I_n$

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Properties

- $\mathcal{R}_A$ encodes the $RowRP(A)$ and the $ColRP(A)$
- All leading rank profiles
- $\mathcal{R}_A$ is unique $\implies$ new normal form.

When does a PLUQ decomposition reveal the rank profile matrix ?

Focus on the pivoting strategy :

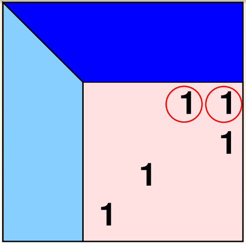
- Pivot search :
  - finding a pivot with minimal coordinates
- Permutation to bring the pivot to the main diagonal

Pivoting and permutation strategies

Pivot Search

Pivot's (i, j) position minimizes some pre-order :

Row order : any non-zero on the first non-zero row



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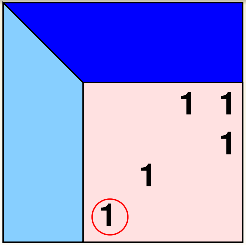

Pivoting and permutation strategies

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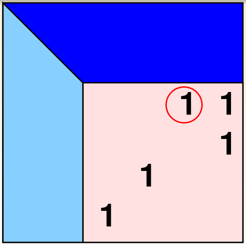
Lex order : first non-zero on the first non-zero row



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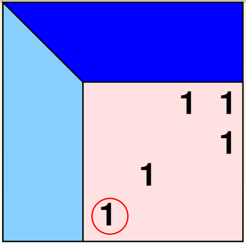

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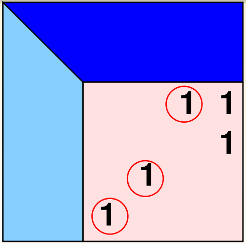

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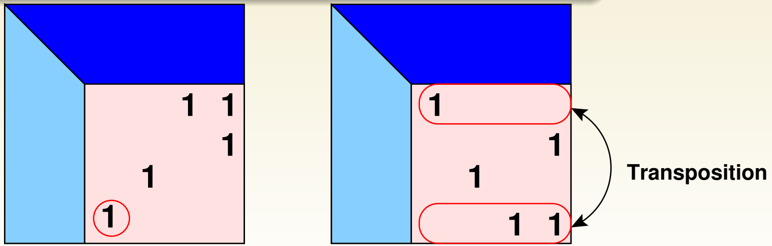
Permutation

- Transpositions



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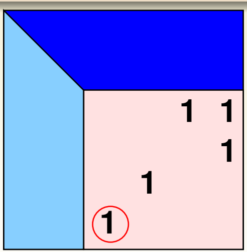
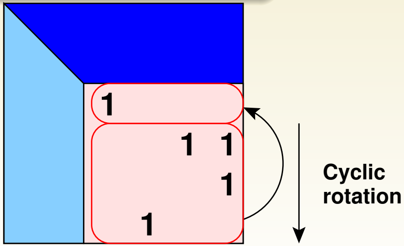
Permutation

- Transpositions
- Cyclic Rotations





Pivoting strategies revealing rank profiles

Search	**Row perm.**	**Col. perm.**	RowRP	ColRP	**Instance**
Row order Col. order					
Lexico.					
Rev. lex.					
Product					

Pivoting strategies revealing rank profiles

Search	**Row perm.**	**Col. perm.**	RowRP	ColRP	**Instance**
Row order Col. order	Transposition	Transposition	✓		[IMH82] [JPS13]
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Pivoting strategies revealing rank profiles

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Lexico.	Transposition	Transposition	✓		[Sto00]
Rev. lex.	Transposition	Transposition		✓	[Sto00]
Product					

Pivoting strategies revealing rank profiles

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Rev. lex.	Transposition	Transposition		✓		[Sto00]
Product	Rotation	Rotation	✓	✓	✓	[DPS13]

$P, L, U, Q \leftarrow PLUQ(A)$ and $P \begin{bmatrix} I_r & \\ & 0 \end{bmatrix} Q = \mathcal{R}_A$.

Pivoting strategies revealing rank profiles

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Product	Rotation	Transposition	✓			[DPS15]
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Product	Rotation	Rotation	✓	✓	✓	[DPS13]

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Lexico.	Transposition	Rotation	✓	✓	✓	[DPS15]
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Rev. lex.	Rotation	Transposition	✓	✓	✓	[DPS15]
Rev. lex.	Rotation	Rotation	✓	✓	✓	[DPS15]
Product	Rotation	Transposition	✓			[DPS15]
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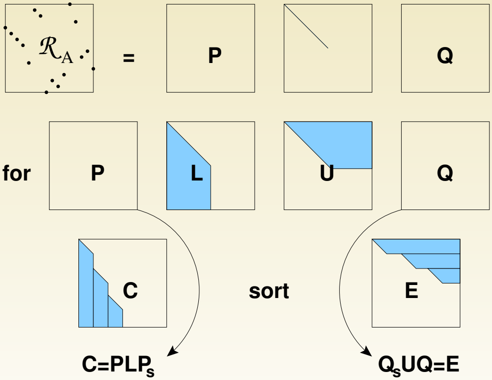
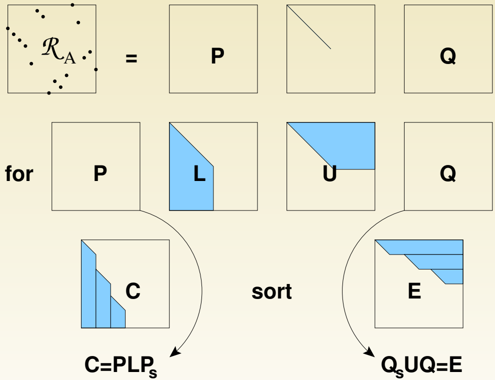
Echelon forms



$$C = P \left[L.P_s \;\; 0_{m\times(n-r)} \right] \qquad E = \begin{bmatrix} Q_s.U \\ 0_{(n-r)\times n} \end{bmatrix} Q$$

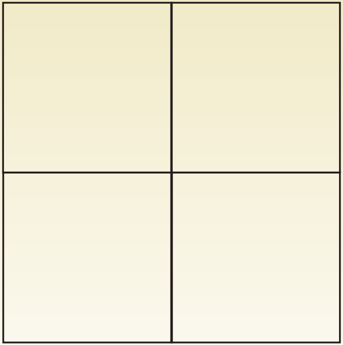
Echelon forms



$$C = P\left[\begin{smallmatrix} L.P_s & 0_{m\times(n-r)}\end{smallmatrix}\right],\ F = P_s^T Q_s^T,\ E = \left[\begin{smallmatrix} Q_s.U \\ 0_{(n-r)\times n}\end{smallmatrix}\right] Q$$

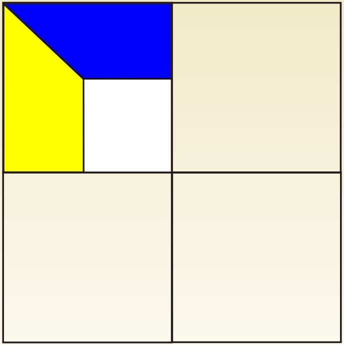
Bonus : Generalized Bruhat *CFE*.

Tile recursive PLUQ algorithm



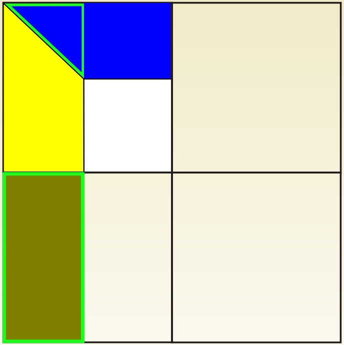
2×2 block splitting

Tile recursive PLUQ algorithm



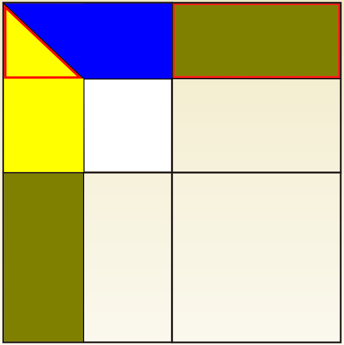
Recursive call

Tile recursive PLUQ algorithm



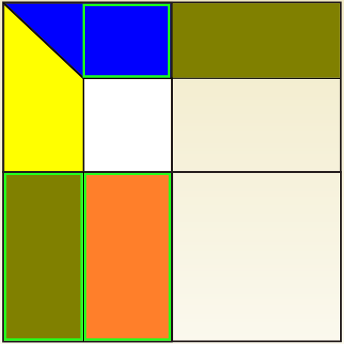
$\texttt{TRSM} : B \leftarrow BU^{-1}$

Tile recursive PLUQ algorithm



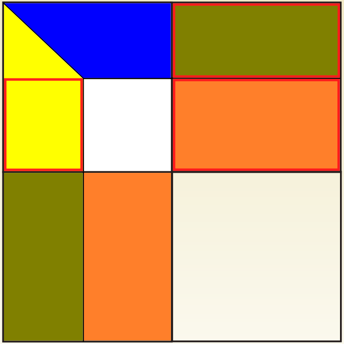
$\texttt{TRSM} : B \leftarrow L^{-1}B$

Tile recursive PLUQ algorithm



$\texttt{fgemm} : C \leftarrow C - A \times B$

Tile recursive PLUQ algorithm



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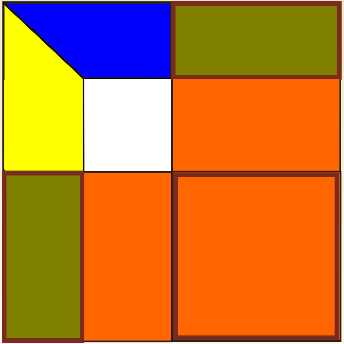

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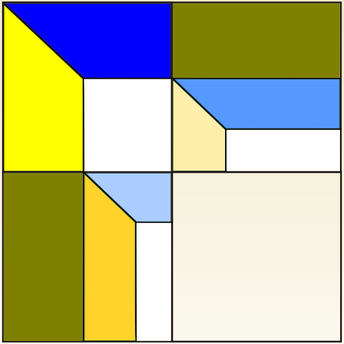
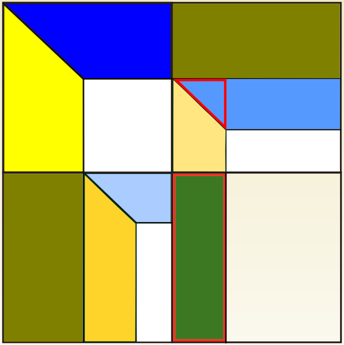


2 independent recursive calls (product order search)

Tile recursive PLUQ algorithm



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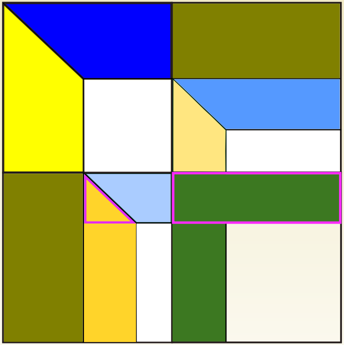

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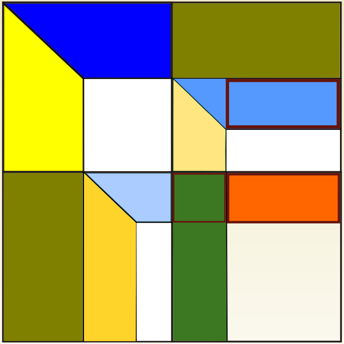

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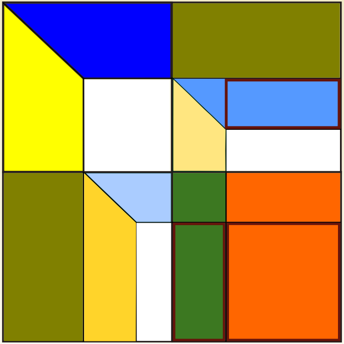

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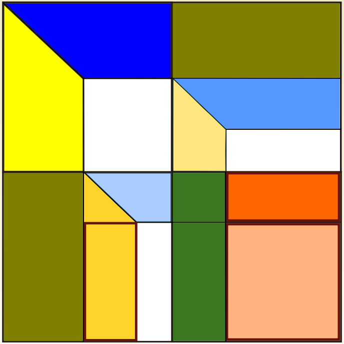

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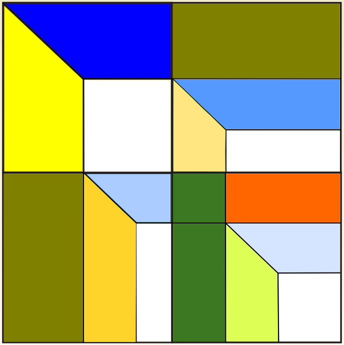
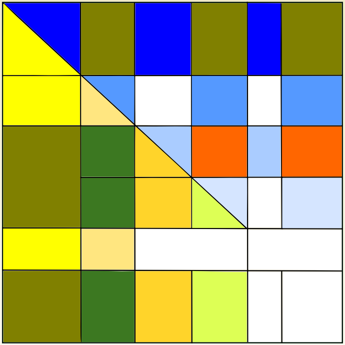


Recursive call

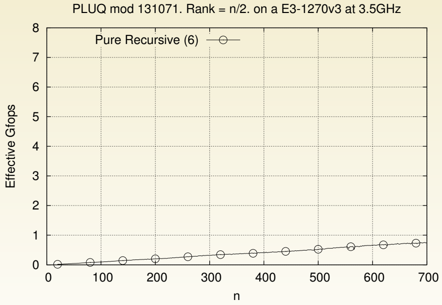
Tile recursive PLUQ algorithm



Puzzle game (block permutations)

New PLUQ algorithm

- New state of the art algo that computes faster PLUQ decomposition
- Computes more information (the rank profile matrix $\mathcal{R}_A$)



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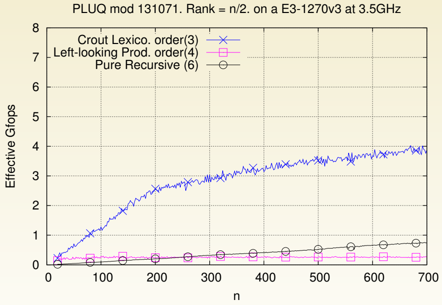

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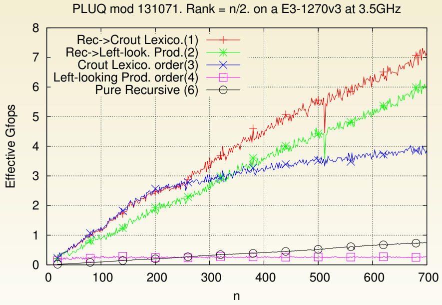

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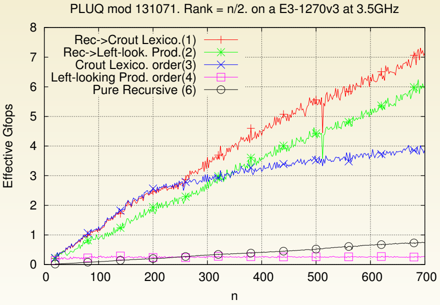

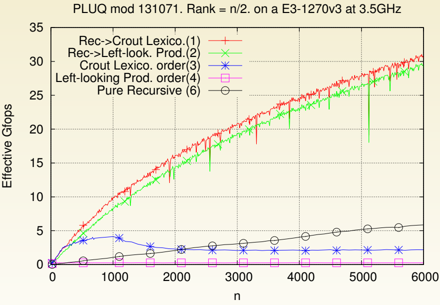

Execution on 1 core (3.5GHz) $\rightarrow$ effective 31 Gfops (AVX2 + sub-cubic complexity)

Outline

FFLAS-FFPACK library

FFLAS-FFPACK features

- High performance implementation of basic linear algebra routines over word size prime fields
- Exact alternative to the numerical BLAS library
- Exact triangularization, Sys. solving, Det, Inv., CharPoly

Parallel FFLAS-FFPACK

Explore :

- several algorithms and variants
- parallel runtimes and languages :
  - unified parallel language harnessing different runtimes (OMP, TBB, xKaapi, ...)
  - Abstraction for the user
- data parallelism vs task parallelism

Parallel computation constraints : exact and numeric

In state of the art numerical libraries :

- Often non singular matrices with fixed static cutting.
  $\rightarrow$ easier to manually map and schedule tasks or threads.
- Use of iterative algorithms $\rightarrow$ often one or two levels of parallelism.

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Our experience in exact linear algebra :

- Sub-cubic complexity : $O(n^\omega)$ [Strassen]
  $\rightarrow$ Coarser grain cutting
  $\rightarrow$ Recursive algorithms.
  $\rightarrow$ Parallel runtime system that implements well recursive tasks.
- Rank deficiencies $\rightarrow$ tasks of unbalanced workloads.
- Recursion and code composition $\rightarrow$ multiple levels of parallelism.

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$\rightarrow$ Need for a high level parallel programming environments

Requirements of high level parallel programming environments

Features required

Portability, Performance and scalability. But more precisely :

- Runtime system with good performance for recursive tasks.
- Handle efficiently unbalanced workloads.
- Efficient range cutting for parallel for.

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Portability, Performance and scalability. But more precisely :

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- Efficient range cutting for parallel for.

No parallel environment offers all these features
$\rightarrow$ Need to design a code independently from the runtime system
$\rightarrow$ Using runtime systems as a plugin

Runtime systems to be supported

OpenMP3.x and 4.0 supported directives : (using libgomp)

- Data sharing attributes :
  - OMP3 `shared` : data visible and accessible by all threads
  - OMP3 `firstprivate` : local copy of original value
  - OMP4 `depend` : set data dependencies
- Synchronization clauses : `#pragma omp taskwait`

xKaapi : via the libkomp [BDG12] library :

- OpenMP directives → xKaapi tasks.
- Re-implem. of task handling and management.
- Better recursive tasks execution.

TBB : designed for nested and recursive parallelism

- `parallel_for`
- `tbb::task_group, wait(), run()` using C++11 lambda functions

PALADIn

Parallel **A**lgebraic **L**inear **A**lgebra **D**edicated **In**terface

Mainly macro-based keywords

- No function call runtime overhead when using macros.
- No important modifications to be done to original program.
- Macros can be used also for C-based libraries.

Complementary C++ template functions

- Implement the different cutting strategies.
- Store the iterators

PALADIn description : data parallelism

Data parallelism : SPMD programming

- Parallel region : chunks are dispatched on multiple proc.
- Supported : `PARFOR1D`, `PARFOR2D`, `PARFORBLOCK1D`, `PARFORBLOCK2D`.

Example : Loop Summing in C++

```
for(size_t i=0; i<n; ++i){
 T[i] = T1[i] + T2[i];
}
```

Example : Loop Summing in OpenMP

```
#pragma omp parallel for
for(size_t i=0; i<n; ++i){
 T[i] = T1[i] + T2[i];
}
```

Example : Loop Summing in PALADIn

```
PARFOR1D(i, n, SPLITTER(),
         T[i] = T1[i]+T2[i];
        );
```

→ The `SPLITTER` keyword sets the cutting strategy.

Iterative Cutting Strategies 1D

Splitting over one dimension

- `SPLITTER(`p`, THREADS)` : p partitions $= \#tasks$
- `SPLITTER(`p`, GRAIN)` : BlockSize : $BS = p$
- `SPLITTER(`p`, FIXED)` : BlockSize : $BS = 256$
- `SPLITTER(`p`)` : p tasks with default strategy (`THREADS`)
- `SPLITTER()` : default strategy with $p = \#$ available processors

Code example : Matrix add in parallel

```
void pfadd(const Field & F,const Element *A,const Element *B, Element *C, size_t n){
   PARFORBLOCK1D(it , n, SPLITTER(32, THREADS),
            FFLAS::fadd(F, it.end()-it.begin(), n,
                        A+it.begin()*n, n,
                        B+it.begin()*n, n,
                        C+it.begin()*n, n);
            );
 }
```

Iterative cutting strategies 2D

Data parallelism : SPLITTER keyword

- `SPLITTER(`p`, ROW, THREADS)` : p row blocks
- `SPLITTER(`p`, ROW, FIXED)` : row $BS = 256$
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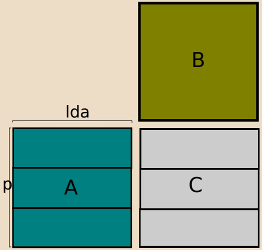

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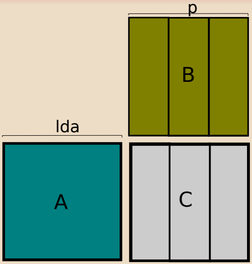

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- `SPLITTER(`p`, BLOCK, THREADS)` : $s \times t$ blocks
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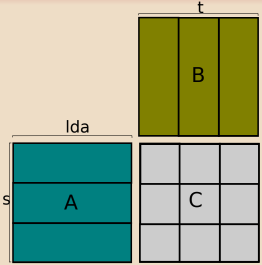

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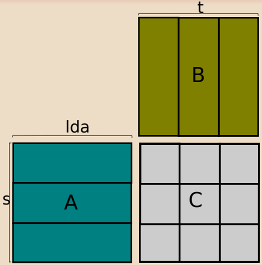
- `NOSPLIT()` : sequential execution



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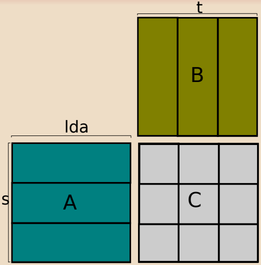


```
PARFORBLOCK2D(iter, m, n, SPLITTER(),
        fgemm( ..., A +iter.ibegin()*lda, lda,
                    B +iter.jbegin(), ldb, beta,
                    C +iter.ibegin()*ldc+iter.jbegin(), ldc);
      );
```

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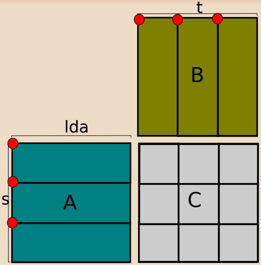


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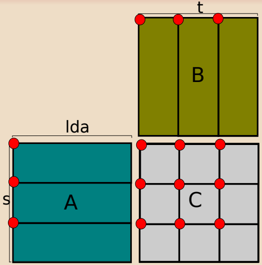


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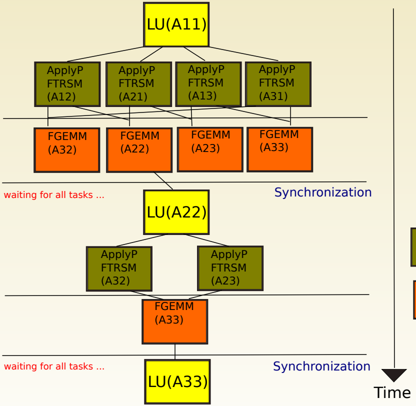
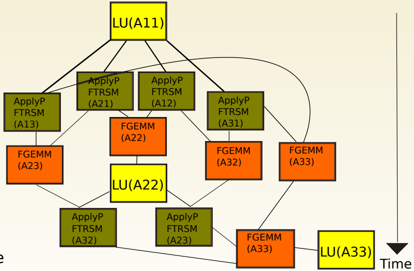
Task parallelism

fork-join model :



data-flow model :



PALADIn description : task parallelism

Task parallelization : fork-join and dataflow models

- `PAR_BLOCK` : opens a parallel region.
- `SYNCH_GROUP` : Group of tasks synchronized upon exit.
- `TASK` : creates a task.
  - `REFERENCE(args...)` : specify variables captured by reference. By default all variables accessed by value.
  - `READ(args...)` : set var. that are read only.
  - `WRITE(args...)` : set var. that are written only.
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Example :

```
void axpy(const Element a, const Element b, Element &y){y += a*x;}
SYNCH_GROUP(
            TASK(MODE(READ(a,x) READWRITE(y)),
                 axpy(a,x,y));
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Now we have a language to test our parallel exact linear algebra algorithms !

Parallel matrix multiplication cascading

Algorithms

- Classical algorithms : $O(n^3)$
- Fast algorithms : $O(n^\omega)$

Problem

What are the best possible cascades ?

Cascading

- Parallel classical variant switches to :
  - sequential fast
  - sequential classical
  - parallel fast
- iterative (BLOCK-THREADS)
- recursive (1D, 2D, 3D splitting)

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- recursive (1D, 2D, 3D splitting)
- Parallel fast variant switches to :
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  - sequential classical
  - parallel classical
- recursive (Strassen-Winograd)

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- recursive (Strassen-Winograd)

Performance of pfgemm

pfgemm : Parallel classical variant → Sequential fast

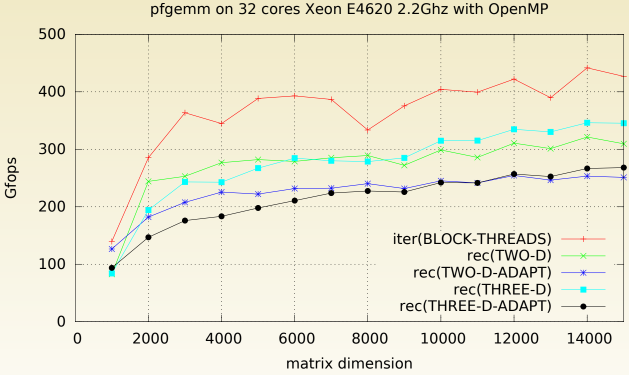


FIGURE : Speed of different matrix multiplication cutting strategies using OpenMP tasks

Performance of pfgemm

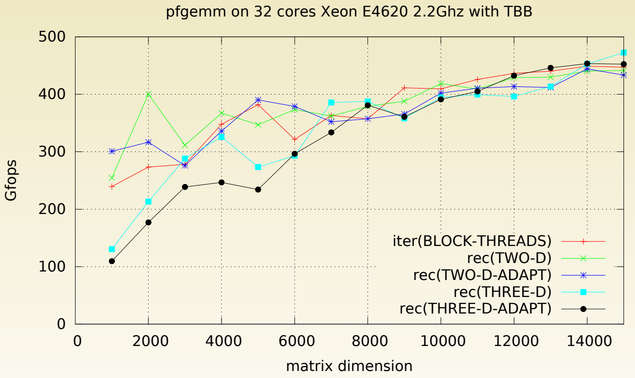


FIGURE : Speed of different matrix multiplication cutting strategies using TBB tasks

Performance of pfgemm

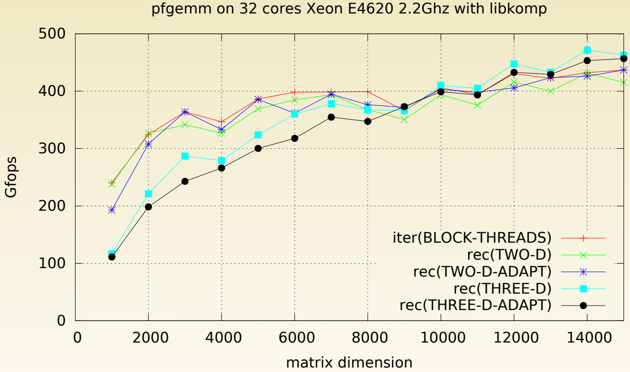
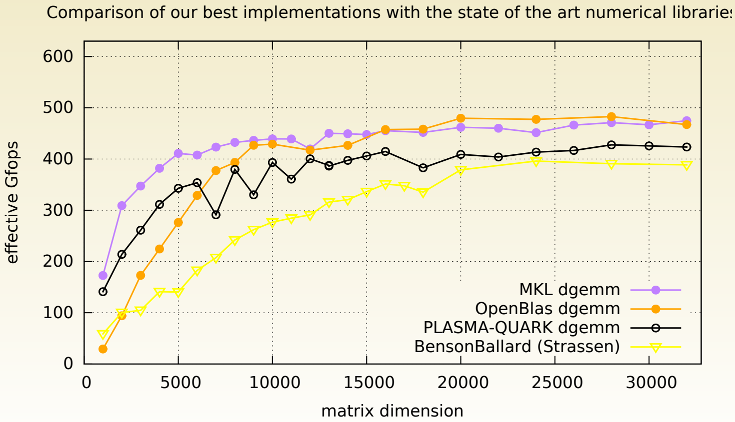


FIGURE : Speed of different matrix multiplication cutting strategies using xKaapi tasks

Parallel Matrix Multiplication : State of the art

HPAC server : 32 cores Xeon E4620 2.2Ghz (4 NUMA sockets)



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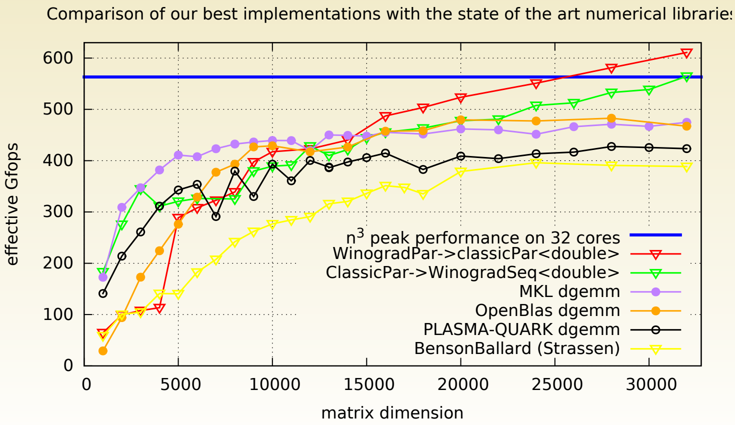
Effective Gfops = $\dfrac{\text{\# of field ops using classic matrix product}}{\text{time}}$.



Outline

Gaussian elimination design

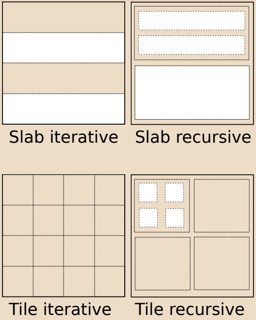
Reducing to MatMul : block versions

$\rightarrow$ Asymptotically faster ($O(n^\omega)$)
$\rightarrow$ Better cache efficiency

Variants of block versions

Split on one dimension :
$\rightarrow$ Row or Column slab cutting

Split on 2 dimensions :
$\rightarrow$ Tile cutting



Gaussian elimination design

Reducing to MatMul : block versions

$\rightarrow$ Asymptotically faster ($O(n^\omega)$)
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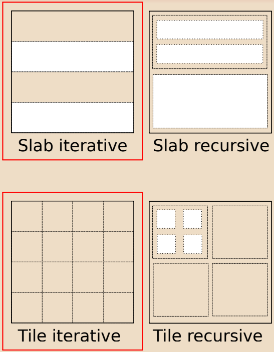
Variants of block versions

Iterative :

- Static $\rightarrow$ better data mapping control
- Dataflow parallel model $\rightarrow$ less sync

Recursive :

- Adaptive
- sub-cubic complexity
- No Dataflow $\rightarrow$ more sync



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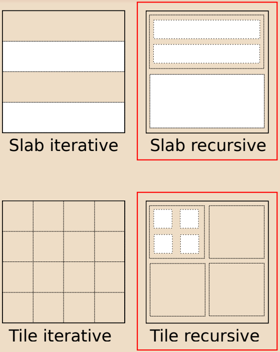
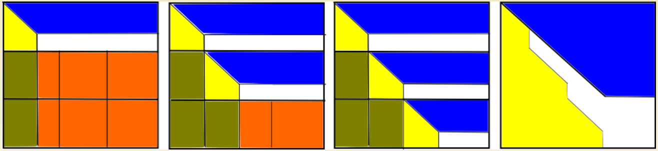


Slab iterative



Slab iterative

Expensive costly tasks in the critical path

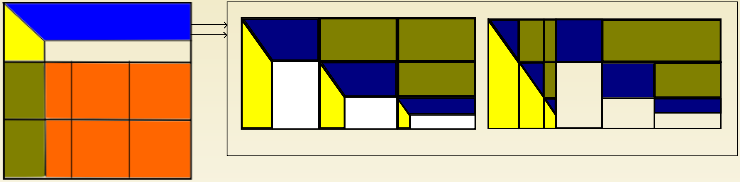
- Panel factorization in sequential

Rank dynamically revealed :

- Varying workload of each block op.

Tiled iterative PLUQ decomposition

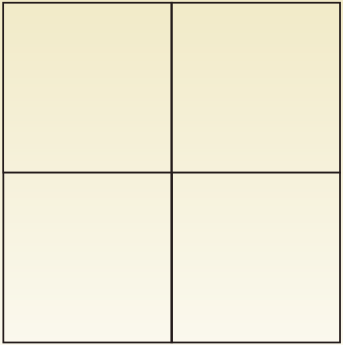
$\rightarrow$ Panel PLUQ decomposition on each slab



Slab iterative CUP to tile iterative PLUQ

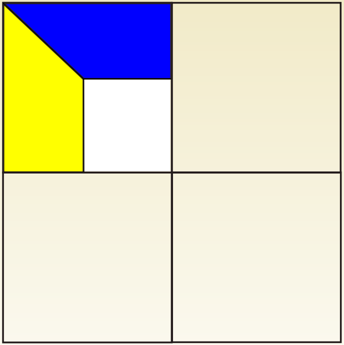
- Cutting according to columns
- Creating "more parallelism" : update tasks are concurrent
- Recovering rank profiles thanks to our pivoting strategies

Parallel tile recursive PLUQ algorithm



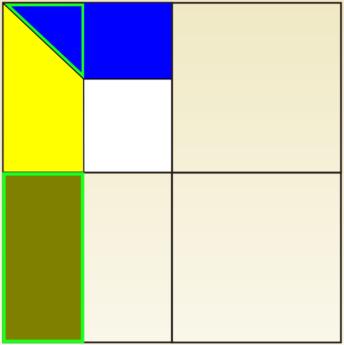
2×2 block splitting

Parallel tile recursive PLUQ algorithm



Recursive call

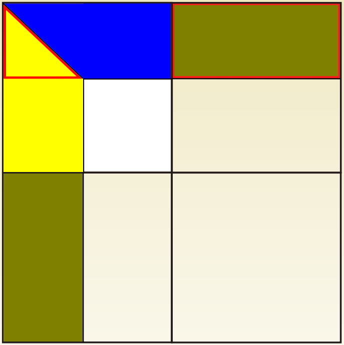
Parallel tile recursive PLUQ algorithm



$\mathrm{pTRSM} : B \leftarrow BU^{-1}$

```
TASK(MODE(READ(A) READWRITE(B)),
      pftrsm(..., A, lda, B, ldb));
```

Parallel tile recursive PLUQ algorithm



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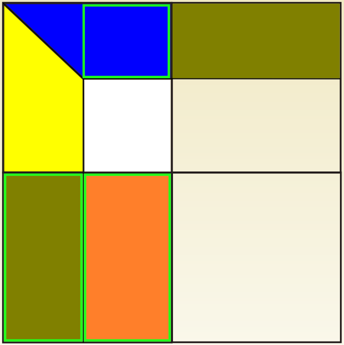
Parallel tile recursive PLUQ algorithm



$\texttt{pfgemm} : C \leftarrow C - A \times B$

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TASK(MODE(READ(A,B) READWRITE(C)),
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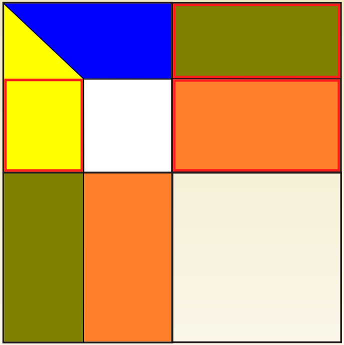
Parallel tile recursive PLUQ algorithm



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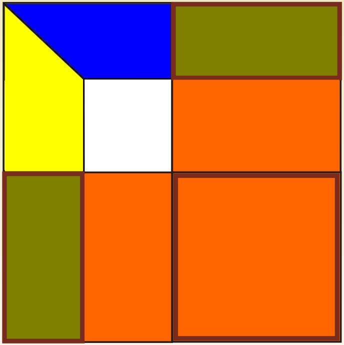

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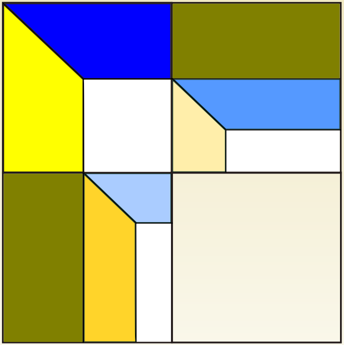
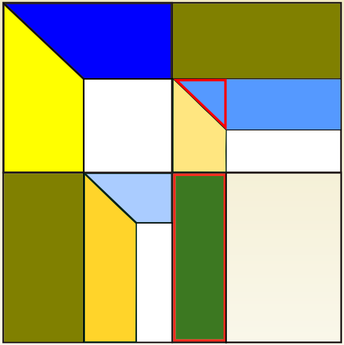


2 independent recursive calls (concurrent → tasks)

```
TASK(MODE(READWRITE(A)),
     pluq(..., A, lda));
```

Parallel tile recursive PLUQ algorithm



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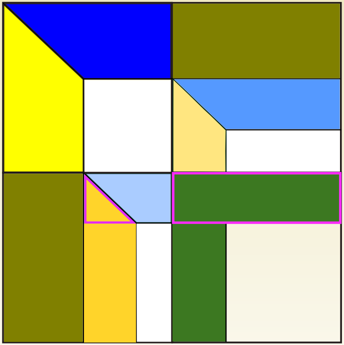

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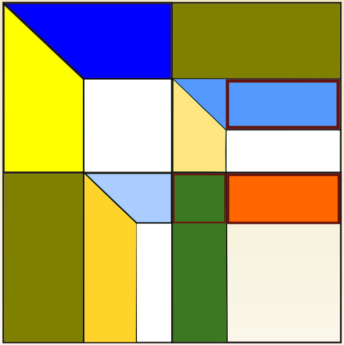

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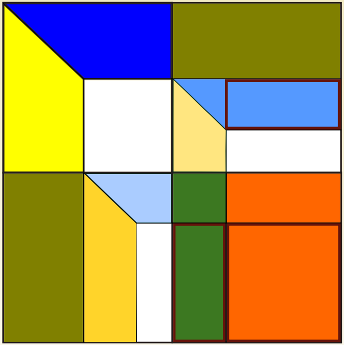

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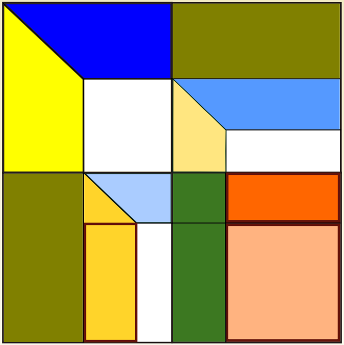

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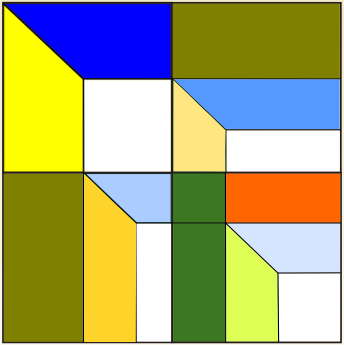

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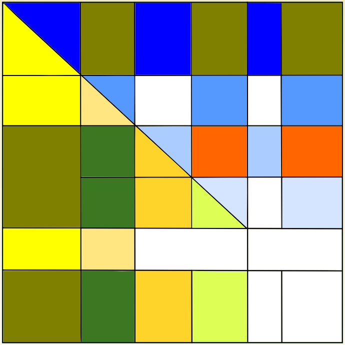
Parallel tile recursive PLUQ algorithm

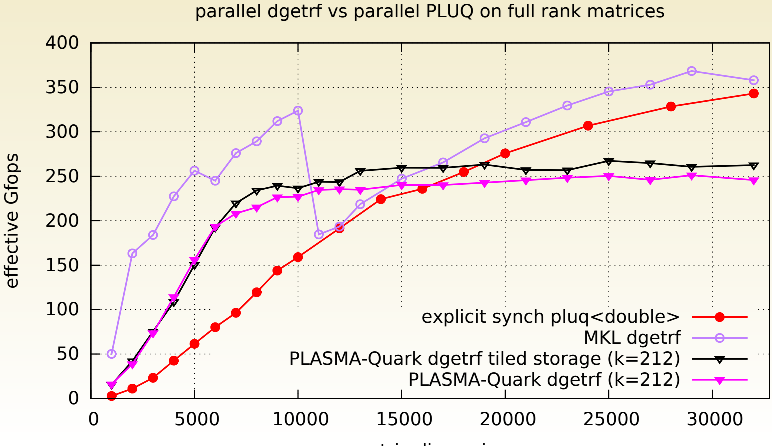


Puzzle game (block permutations)
Tile rec : better data locality and more square blocks for M.M.

State of the art : exact vs numerical linear algebra

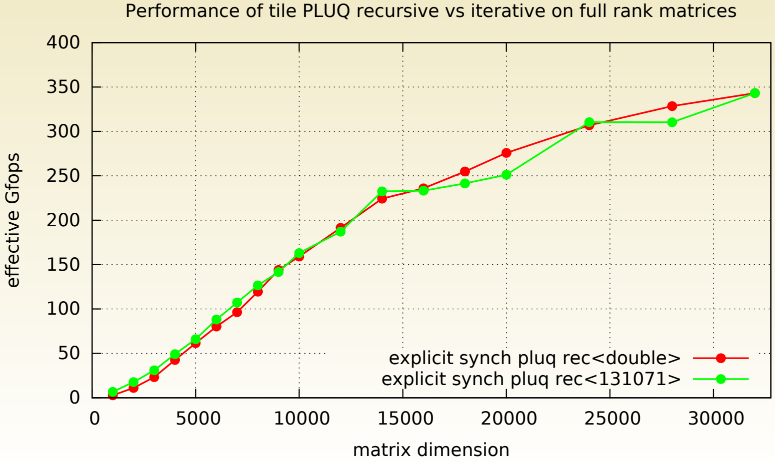
State of the art comparison :

- Exact PLUQ using PALADIn language : best performance with xKaapi
- Numerical LU (dgetrf) of PLASMA-Quark and MKL dgetrf



Performance of parallel PLUQ decomposition

Low impact of modular reductions in parallel
$\rightarrow$ Efficient SIMD implementation

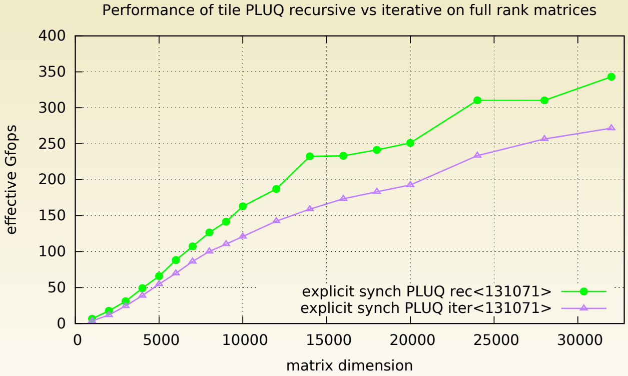


Modular reductions

Iterative Right looking	$\mathbf{\frac{1}{3}n^3} - \frac{1}{3}n$
Iterative Left Looking	$\mathbf{\frac{3}{2}n^2} - \frac{5}{2}n + 1$
Iterative Crout	$\mathbf{\frac{3}{2}n^2} - \frac{5}{2}n + 1$
Tile Recursive	$\mathbf{2n^2} - n\log_2 n - 2n$
Slab Recursive	$(\mathbf{1} + \mathbf{\frac{1}{4}\log_2 n})\mathbf{n^2} - \frac{1}{2}n\log_2 n - n$

TABLE : Counting modular reductions in full rank LU factorization of an $n \times n$ matrix modulo p when $n(p-1)^2 < 2^{\text{mantissa}}$.

Performance of task parallelism : dataflow model



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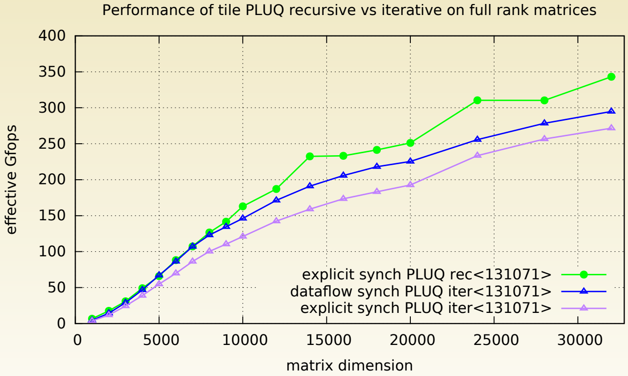

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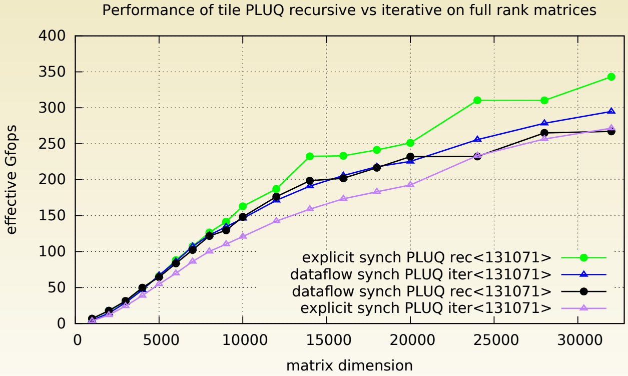

Possible improvement : implementation of the delegation of recursive tasks dependencies (Postpone access mode in the parallel programming environments)

Conclusion & Perspectives

HPAC DLP challenge : ~8 years → today feasible in ~3 months on 32 cores.

Defended theses

Sub-cubic : scale up in parallel in practice.

PALADIn : parallel programming environments as a plugin

The rank profile matrix : global information - efficient algorithms
Requires deep and precise understanding of pivoting

Perspectives

- Study the scaling of sub-cubic exact linear algebra algorithms on distributed machines.
- PALADIn on GPUs and distributed memory machines
- Adapt Communication avoiding algorithms to compute the rank profile information