
Data Structures to Implement the Sparse Vector in Crout ILU Preconditioner

Sparse Days 2019

11th July 2019

Raju Ram

PhD Student
CC-HPC
Fraunhofer ITWM
Fraunhofer-Platz 1
67663 Kaiserslautern
Germany



Data Structures to Implement the Sparse Vector in Crout ILU Preconditioner

- Iterative Solvers for Sparse Linear Systems
 - GaspILS Linear Solver Library

- Crout Incomplete LU (ILU) factorization of A
 - Serial Crout ILU Method
 - Multilevel Crout ILU Method
 - Parallelization of Crout ILU Method

- Sparse Vector Update in Serial Crout ILU Factorization
 - Data Structures to Implement Sparse Vector
 - Profiler Readings

Sparse Iterative Linear Solvers

- Linear Solvers on Sparse Matrices are the base of Simulations in Science, Engineering.
- Solve for x in $Ax = b$.
- Preconditioning improves the convergence of linear solver since it reduces the condition number of the matrix.
- Typical kernel in Parallel Iterative Solvers:
 - **Preconditioning step (line 4)**
 - Sparse matrix vector multiplication (line 12)
 - Global dot product (line 8, 12)
 - Apxy operation (line 10, 14, 15)
- **Preconditioning Step** is most challenging kernel for scalability in parallel iterative solvers.

Algorithm 1 Preconditioned Conjugate Gradient (PCG) Algorithm

```
1: procedure PCG( $A, b, x^{(0)}, tol, k_{max}, M$ )
2:    $r^{(0)} = b - Ax^{(0)}, k = 1$  ▷ Initialization
3:   while ( $k < k_{max}$  and  $\|r^{(k-1)}\| > tol$ ) do
4:      $z^{(k-1)} = M^{-1}r^{(k-1)}$  ▷ Preconditioning
5:     if  $k = 1$  then
6:        $p^{(1)} = z^{(0)}$ 
7:     else
8:        $\beta_k = \frac{(r^{(k-1)})^T z^{(k-1)}}{(r^{(k-2)})^T z^{(k-2)}}$ 
9:
10:       $p^{(k)} = z^{(k-1)} + \beta_k p^{(k-1)}$  ▷ Search direction
11:    end if
12:     $\alpha_k = \frac{(r^{(k-1)})^T z^{(k-1)}}{(p^{(k)})^T Ap^{(k)}}$ 
13:
14:     $x^{(k)} = x^{(k-1)} + \alpha_k p^{(k)}$  ▷ Iterate update
15:     $r^{(k)} = r^{(k-1)} - \alpha_k Ap^{(k)}$  ▷ Residual update
16:     $k = k + 1$ 
17:  end while
18:  return  $x^{(k-1)}$  ▷ The converged solution
19: end procedure
```

Global Address Space Programming Interface (GASPI)

- Asynchronous, single sided communication based standardized API.
- Developed keeping scalability in mind.
- Applications are developed in machine learning, big data, seismic imaging based on GASPI.
- We are building a scalable linear solver library based on GASPI to solve complex simulations in science and engineering.

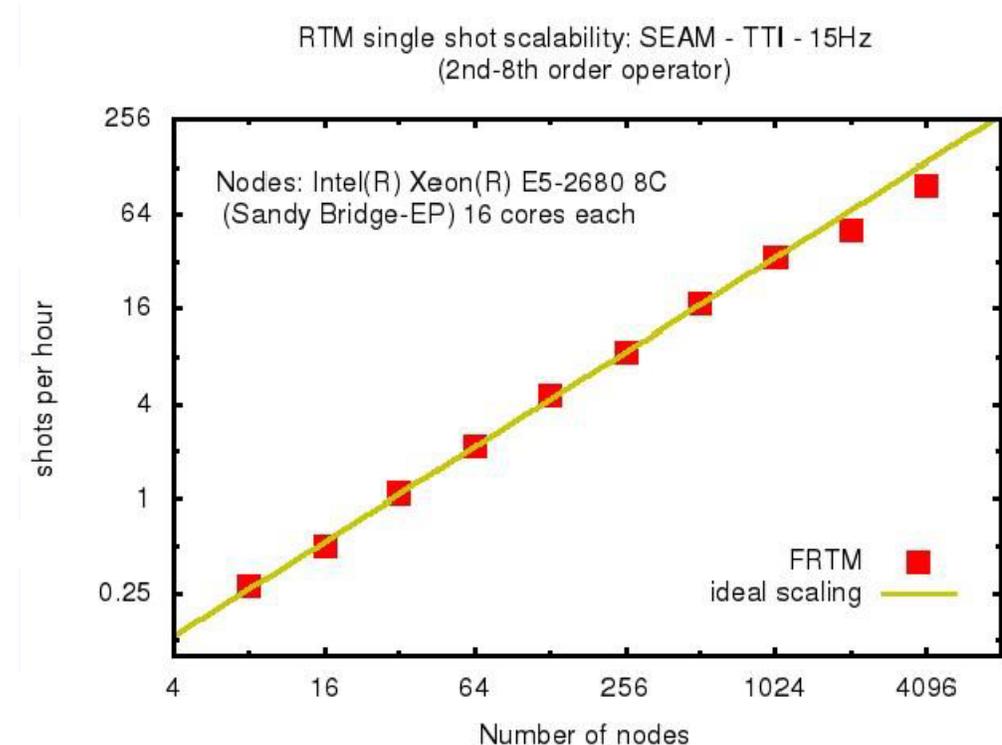


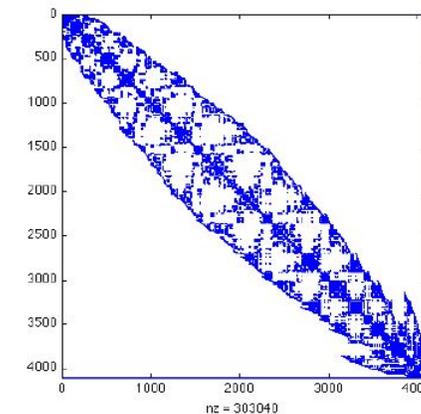
Abbildung: Ideal scalability until 1024 nodes [4]

GaspiLS linear solver library



Scalability, Efficiency, Extendability

- **Gaspi** based C++ Linear Solver Library
- Iterative solvers: (P)CG, BiPCGStab, GMRES
- Preconditioners: Jacobi, **ILU**, ILUM
- MPI interoperable
- Industry proven in CFD and FEM simulations
- OpenSource GPLv3 license library [1]



My research motivation

- Solving for z in $Mz = r$ with Incomplete LU Preconditioner (ILU) consists of two steps:

$$A = \begin{pmatrix} B & F \\ E & C \end{pmatrix} = LDU + E \approx \begin{pmatrix} \triangle & \\ & \diagdown \end{pmatrix} \begin{pmatrix} \diagdown \\ & \end{pmatrix} \begin{pmatrix} \triangle & \\ & \square \end{pmatrix}, \text{ where } L, U \text{ are unit diagonal.}$$

$LDUz = r$, solve for y in $Ly = r$ using forward substitution where $y = DUz$.

$DUz = y$, solve for z in $Uz = D^{-1}y$ using backward substitution.

- LDU Factorization and forward and backward substitution algorithm are serial in nature, thus **difficult to parallelize**.
- We want to decompose the problem into several tasks and run them in parallel as much as possible.

My research motivation

- Solving for z in $Mz = r$ with Incomplete LU Preconditioner (ILU) consists of two steps:

$$A = \begin{pmatrix} B & F \\ E & C \end{pmatrix} = LDU + E \approx \begin{pmatrix} \triangle & \\ & \end{pmatrix} \begin{pmatrix} \diagdown \\ & \end{pmatrix} \begin{pmatrix} \triangle & \\ & \square \end{pmatrix}, \text{ where } L, U \text{ are unit diagonal.}$$

$LDUz = r$, solve for y in $Ly = r$ using forward substitution where $y = DUz$.

$DUz = y$, solve for z in $Uz = D^{-1}y$ using backward substitution.

- LDU Factorization and forward and backward substitution algorithm are serial in nature, thus **difficult to parallelize**.
- We want to decompose the problem into several tasks and run them in parallel as much as possible.

My research motivation

- Solving for z in $Mz = r$ with Incomplete LU Preconditioner (ILU) consists of two steps:

$$A = \begin{pmatrix} B & F \\ E & C \end{pmatrix} = LDU + E \approx \begin{pmatrix} \triangle & \\ & \diagdown \end{pmatrix} \begin{pmatrix} \diagdown \\ & \end{pmatrix} \begin{pmatrix} \triangle & \\ & \square \end{pmatrix}, \text{ where } L, U \text{ are unit diagonal.}$$

$LDUz = r$, solve for y in $Ly = r$ using forward substitution where $y = DUz$.

$DUz = y$, solve for z in $Uz = D^{-1}y$ using backward substitution.

- LDU Factorization and forward and backward substitution algorithm are serial in nature, thus **difficult to parallelize**.
- We want to decompose the problem into several tasks and run them in parallel as much as possible.

Data Structures to Implement the Sparse Vector in Crout ILU Preconditioner

- Iterative Solvers for Sparse Linear Systems
- Crout Incomplete LU (ILU) factorization of A
 - Serial Crout ILU Method
 - Multilevel Crout ILU Method
 - Parallelization of Crout ILU Method
- Sparse Vector Update in Serial Crout ILU Factorization

Incomplete LU (ILU) Preconditioner

- The iterative methods frequently incorporate incomplete LU (ILU) preconditioner because of its robustness, accuracy, and usability as a black-box preconditioner.
- The ILU Preconditioner is serial in nature.
- To introduce parallelism, Crout version of ILU is used as a preconditioner.
- Crout ILU may control the growth of error in the preconditioning operation by setting a bound on the inverse of the triangular (L and U) factors.

Incomplete LU (ILU) Preconditioner

- The iterative methods frequently incorporate incomplete LU (ILU) preconditioner because of its robustness, accuracy, and usability as a black-box preconditioner.
- The ILU Preconditioner is serial in nature.
- To introduce parallelism, Crout version of ILU is used as a preconditioner.
- Crout ILU may control the growth of error in the preconditioning operation by setting a bound on the inverse of the triangular (L and U) factors.

Incomplete LU (ILU) Preconditioner

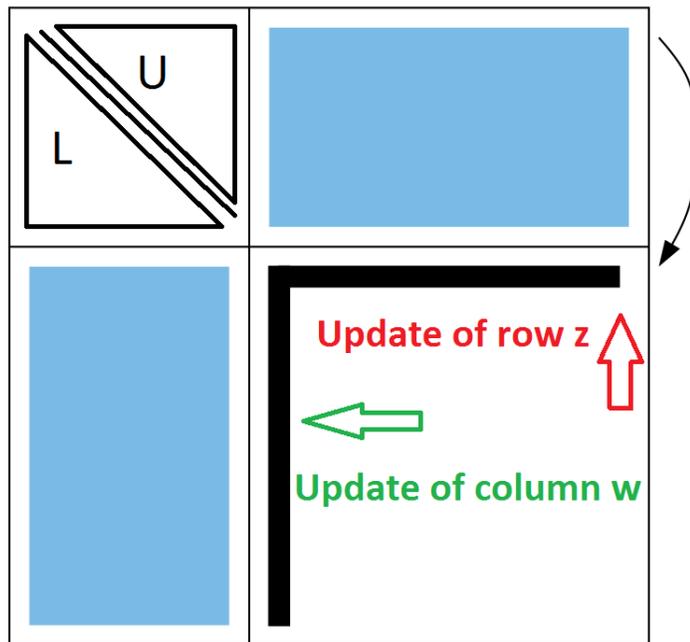
- The iterative methods frequently incorporate incomplete LU (ILU) preconditioner because of its robustness, accuracy, and usability as a black-box preconditioner.
- The ILU Preconditioner is serial in nature.
- To introduce parallelism, Crout version of ILU is used as a preconditioner.
- Crout ILU may control the growth of error in the preconditioning operation by setting a bound on the inverse of the triangular (L and U) factors.

Incomplete LU (ILU) Preconditioner

- The iterative methods frequently incorporate incomplete LU (ILU) preconditioner because of its robustness, accuracy, and usability as a black-box preconditioner.
- The ILU Preconditioner is serial in nature.
- To introduce parallelism, Crout version of ILU is used as a preconditioner.
- Crout ILU may control the growth of error in the preconditioning operation by setting a bound on the inverse of the triangular (L and U) factors.

Crout ILU Algorithm

- Until step $(k - 1)$, LDU factorization of $A(1 : k - 1, 1 : k - 1)$ is computed.
- At k th step, row z ($A(k, k : n)$) and column w ($A(k + 1 : n, k)$) is updated.
- U is stored in CSR and L is stored in CSC format.



Algorithm 2 Crout version of ILU Algorithm: ILUC

```

1: for  $k = 1 : n$  do
2:    $z_{1:k-1} = 0, \quad z_{k:n} = a_{k,k:n}$  ▷ Initialize row z
3:   for  $(1 \leq i \leq k - 1 \text{ and } l_{ki} \neq 0)$  do
4:      $z_{k:n} = z_{k:n} - l_{ki} * u_{i,k:n}$  ▷ Preparation to update  $u_{k,:}$ 
5:   end do
6:    $w_{1:k} = 0, \quad w_{k+1:n} = a_{k+1:n,k}$  ▷ Initialize column z
7:   for  $(1 \leq i \leq k - 1 \text{ and } u_{ik} \neq 0)$  do
8:      $w_{k+1:n} = w_{k+1:n} - u_{ik} * l_{k+1:n,i}$  ▷ Preparation to update  $l_{:,k}$ 
9:   end do
10:  Apply a dropping rule to row z
11:  Apply a dropping rule to column w
12:   $u_{k,:} = z$ 
13:   $l_{:,k} = w / u_{kk}, \quad l_{kk} = 1$ 
14: end do

```

Dropping entries in L and U

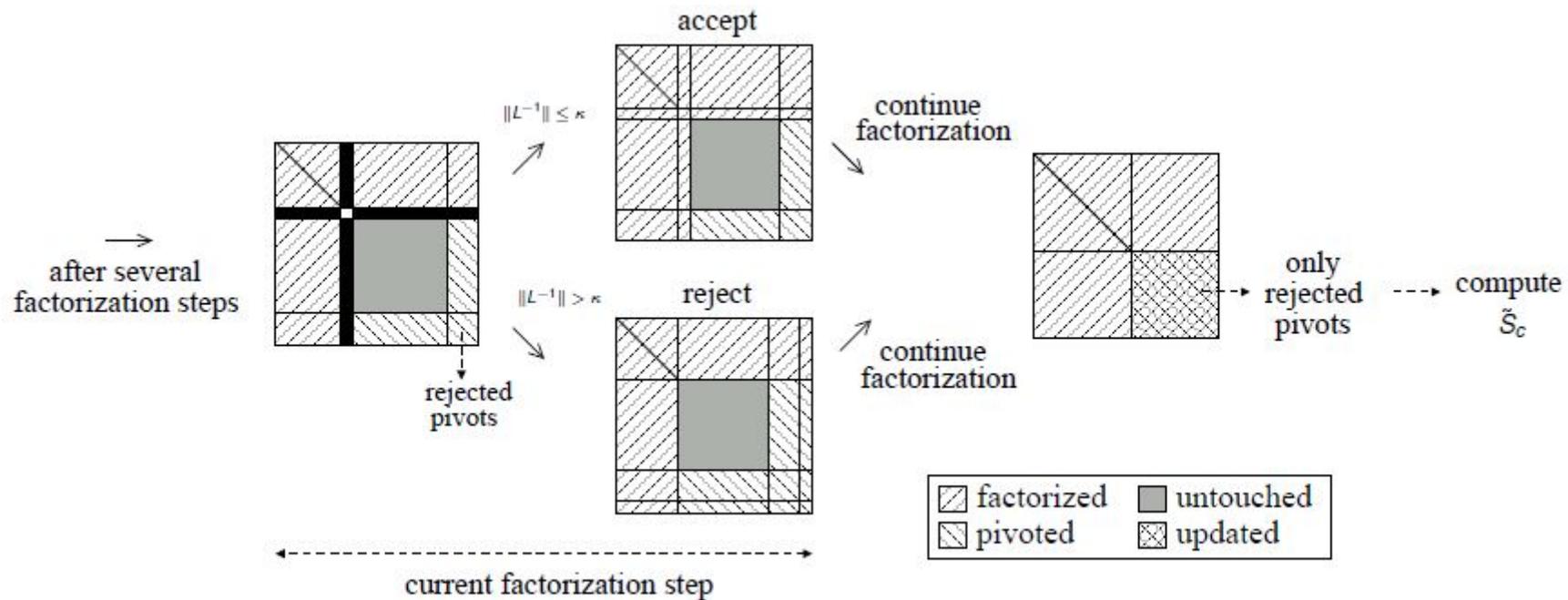
- Why dropping? : The complete LU decomposition of sparse matrix A introduce additional fill-ins in L and U . This leads to computation overhead during solution phase.
- Dropping strategies in $ILU(\tau, \rho)$:
 - τ : Drop an element whose magnitude is less than a tolerance τ .
 - ρ : Only keep ρ largest elements in magnitude in the k -th column of L and k th row of U . Drop all other elements.

Dropping entries in L and U

- Why dropping? : The complete LU decomposition of sparse matrix A introduce additional fill-ins in L and U . This leads to computation overhead during solution phase.
- Dropping strategies in $ILU(\tau, p)$:
 - τ : Drop an element whose magnitude is less than a tolerance τ .
 - p : Only keep p largest elements in magnitude in the k -th column of L and k th row of U . Drop all other elements.

Inverse Based Pivoting in ILU

- Applying Crout ILU on A , we obtain $A = LDU + R$. The matrix R is generated due to dropping.
- Preconditioning matrix: $L^{-1}AU^{-1} = D + L^{-1}RU^{-1}$.
- Error matrix $L^{-1}RU^{-1}$ grows when $\|L^{-1}\|$ and $\|U^{-1}\|$ grows.
- If $\|L^{-1}\| \leq \kappa$ perform factorization, else move the pivot a_{kk} at the end of matrix.



Schur Complement Matrix Computation

- To bound the inverse norm, the matrix is not completely factorized at this stage. Instead, Partial Crout ILU factorization of A such that $B = L_B D_B U_B$.

$$A = \begin{bmatrix} B & E \\ F & C \end{bmatrix} = \begin{bmatrix} L_B & 0 \\ L_E & I \end{bmatrix} \begin{bmatrix} D_B & 0 \\ 0 & S_C \end{bmatrix} \begin{bmatrix} U_B & U_F \\ 0 & I \end{bmatrix} + E$$

- Schur complement matrix S_C is computed that will be factorized at next level.

$$S_C \approx C - L_E D_B U_F.$$

Schur Complement Matrix Computation

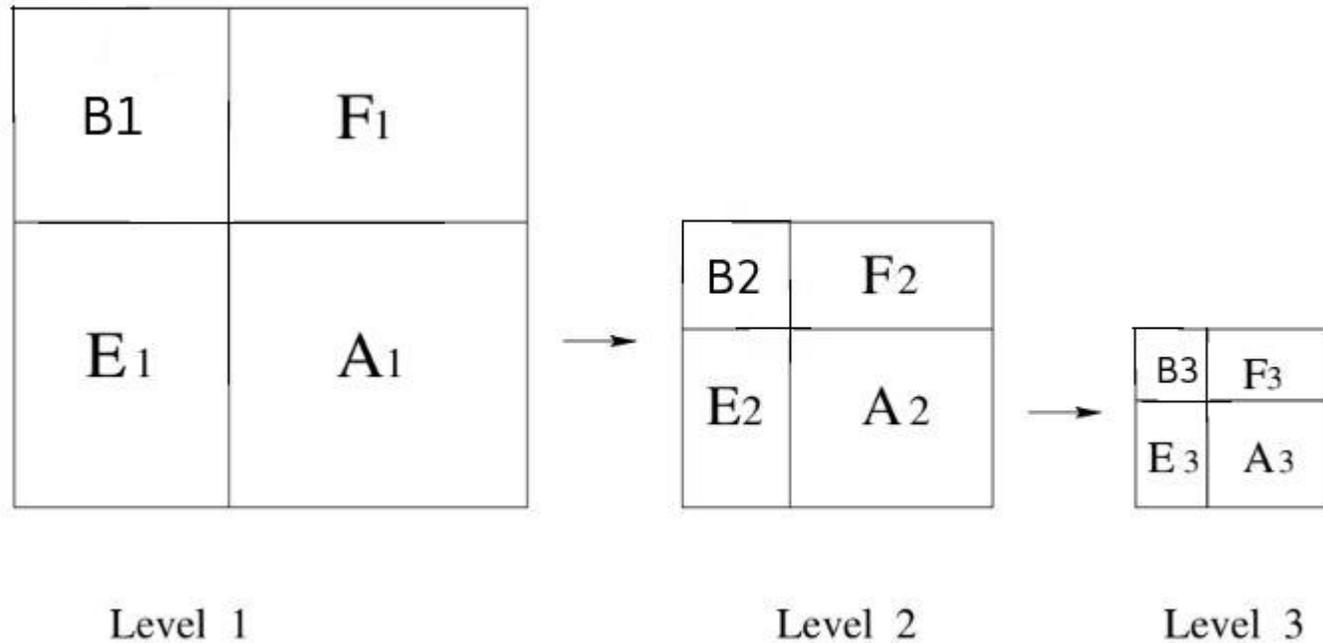
- To bound the inverse norm, the matrix is not completely factorized at this stage. Instead, Partial Crout ILU factorization of A such that $B = L_B D_B U_B$.

$$A = \begin{bmatrix} B & E \\ F & C \end{bmatrix} = \begin{bmatrix} L_B & 0 \\ L_E & I \end{bmatrix} \begin{bmatrix} D_B & 0 \\ 0 & S_C \end{bmatrix} \begin{bmatrix} U_B & U_F \\ 0 & I \end{bmatrix} + E$$

- Schur complement matrix S_C is computed that will be factorized at next level.

$$S_C \approx C - L_E D_B U_F.$$

Multilevel Crout ILU Method



Algorithm 3 Multilevel Crout Algorithm

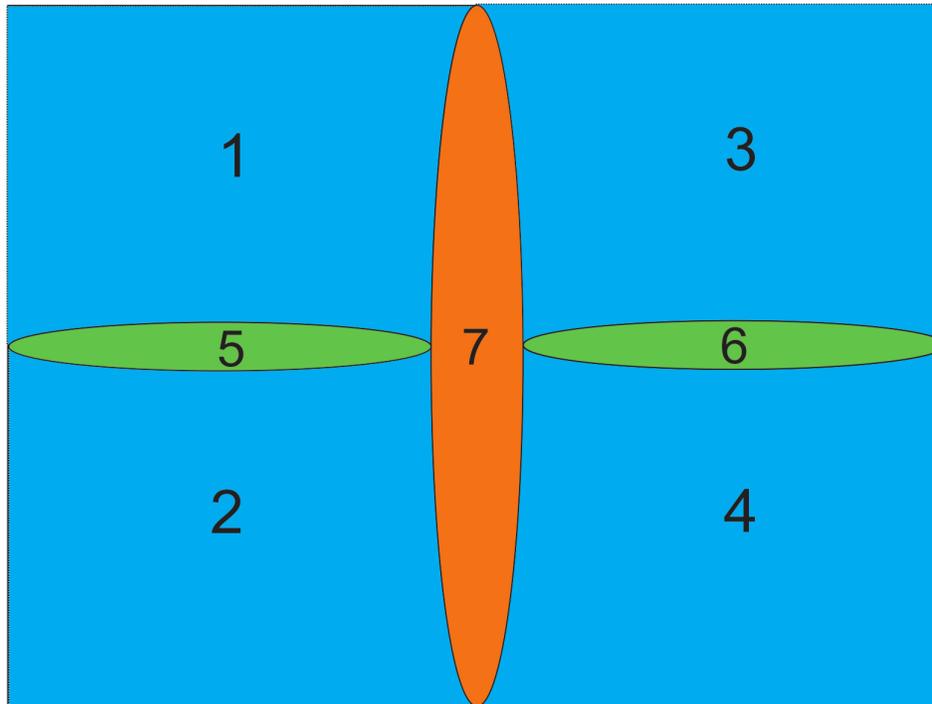
```
1: procedure MULTILEVEL_CROUT_ILU(A)
2:   if (coarsest level) then
3:     Decompose Crout LDU factorization.
4:     return
5:   else
6:     Compute Crout LDU formulation of submatrix  $n_B \times n_B$  of  $A$ 
7:     Compute the Schur complement matrix  $S_C$ 
8:     Call MULTILEVEL_CROUT_ILU ( $S_C$ ).
9:     return
10:  end if
11: end procedure
```

Data Structures to Implement the Sparse Vector in Crout ILU Preconditioner

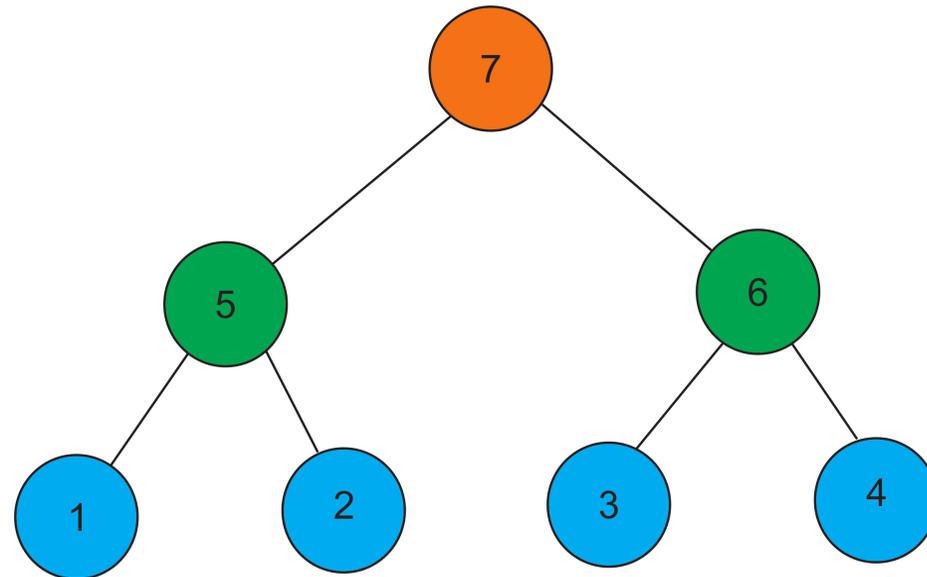
- Iterative Solvers for Sparse Linear Systems
- Crout Incomplete LU (ILU) factorization of A
 - Serial Crout ILU Method
 - Multilevel Crout ILU Method
 - Parallelization of Crout ILU Method
- Sparse Vector Update in Serial Crout ILU Factorization

How to extract Parallelism in Crout LU decomposition

- Sparse matrix A can be represented in an undirected graph G_A .
- Nested Dissection of G_A leads to a binary task tree.



(a) The graph G_A partitioned using 2 level nested dissection



(b) Task dependency tree corresponding to a)

Abbildung: Extracting task level parallelism from ILU algorithm

$$\text{After reordering } A \rightarrow P^T A P = \left[\begin{array}{cccc|cc|c} A_{11} & 0 & 0 & 0 & A_{15} & 0 & A_{17} \\ 0 & A_{22} & 0 & 0 & A_{25} & 0 & A_{27} \\ 0 & 0 & A_{33} & 0 & 0 & A_{36} & A_{37} \\ 0 & 0 & 0 & A_{44} & 0 & A_{46} & A_{47} \\ \hline A_{51} & A_{52} & 0 & 0 & A_{55} & 0 & A_{57} \\ 0 & 0 & A_{63} & A_{64} & 0 & A_{66} & A_{67} \\ \hline A_{71} & A_{72} & A_{73} & A_{74} & A_{75} & A_{76} & A_{77} \end{array} \right] \quad (1)$$

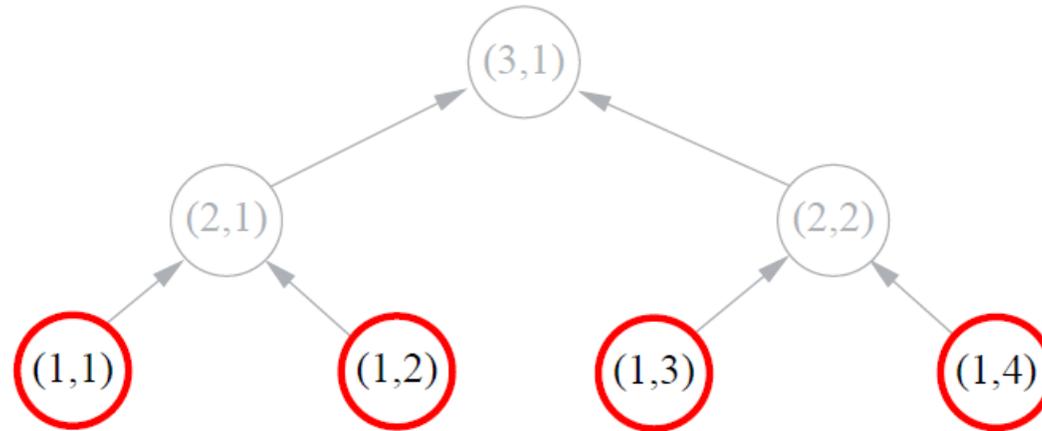
We can disassemble (1) into following independent matrix structures:

$$A_1 = \left[\begin{array}{c|cc} A_{11} & A_{15} & A_{17} \\ \hline A_{51} & A_{55}^1 & A_{57}^1 \\ A_{71} & A_{75}^1 & A_{77}^1 \end{array} \right], \quad A_2 = \left[\begin{array}{c|cc} A_{22} & A_{25} & A_{27} \\ \hline A_{52} & A_{55}^2 & A_{57}^2 \\ A_{72} & A_{75}^2 & A_{77}^2 \end{array} \right] \quad (2)$$

$$A_3 = \left[\begin{array}{c|cc} A_{33} & A_{36} & A_{37} \\ \hline A_{63} & A_{66}^3 & A_{67}^3 \\ A_{73} & A_{76}^3 & A_{77}^3 \end{array} \right], \quad A_4 = \left[\begin{array}{c|cc} A_{44} & A_{46} & A_{47} \\ \hline A_{64} & A_{66}^4 & A_{67}^4 \\ A_{74} & A_{76}^4 & A_{77}^4 \end{array} \right]$$

- These independent sub-matrices can now be processed in parallel.
- Here, we choose $A_{55}^1 = A_{55}^2 = \frac{1}{2}A_{55}$, $A_{57}^1 = A_{57}^2 = \frac{1}{2}A_{57}$, $A_{66}^3 = A_{66}^4 = \frac{1}{2}A_{66}$, $A_{67}^3 = A_{67}^4 = \frac{1}{2}A_{67}$, $A_{77}^1 = A_{77}^2 = A_{77}^3 = A_{77}^4 = \frac{1}{4}A_{77}$.

Parallel Crout ILU factorization at level 1

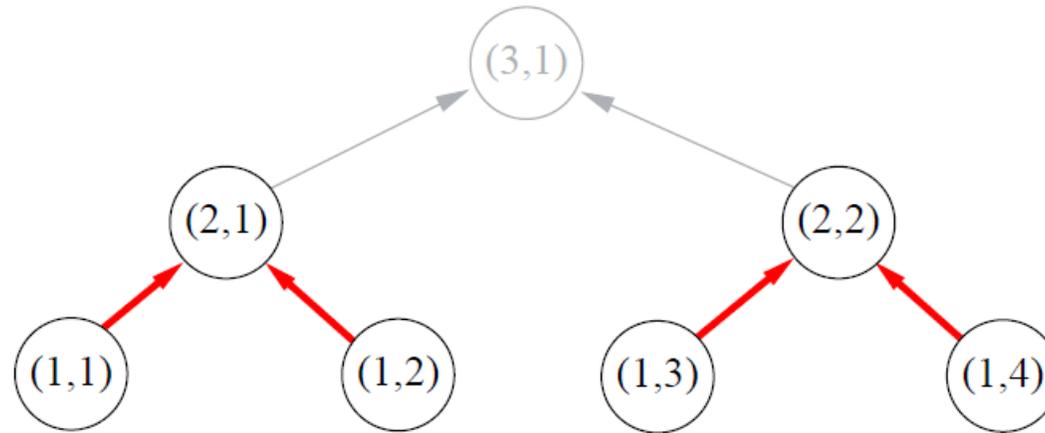


First-level tasks compute in parallel ILUPACK partial ILUs

$$\left(\begin{array}{c|cc} A_{11}^{(1,i)} & A_{12}^{(1,i)} & A_{13}^{(1,i)} \\ \hline A_{21}^{(1,i)} & A_{22}^{(1,i)} & A_{23}^{(1,i)} \\ A_{31}^{(1,i)} & A_{32}^{(1,i)} & A_{33}^{(1,i)} \end{array} \right) \approx \left(\begin{array}{c|cc} L_{11}^{(1,i)} & 0 & 0 \\ \hline L_{21}^{(1,i)} & / & 0 \\ L_{31}^{(1,i)} & 0 & / \end{array} \right) \left(\begin{array}{c|cc} U_{11}^{(1,i)} & U_{12}^{(1,i)} & U_{13}^{(1,i)} \\ \hline 0 & S_{22}^{(1,i)} & S_{23}^{(1,i)} \\ 0 & S_{32}^{(1,i)} & S_{33}^{(1,i)} \end{array} \right)$$

where $i = 1, \dots, 4$

Parallel Assembly of Schur Complement Matrices at level 2



Second-level tasks “merge” the Schur complements of its children

$$\begin{pmatrix} A_{22}^{(2,i)} & A_{23}^{(2,i)} \\ A_{32}^{(2,i)} & A_{33}^{(2,i)} \end{pmatrix} = \begin{pmatrix} S_{22}^{(1,2i-1)} & S_{23}^{(1,2i-1)} \\ S_{32}^{(1,2i-1)} & S_{33}^{(1,2i-1)} \end{pmatrix} + \begin{pmatrix} S_{22}^{(1,2i)} & S_{23}^{(1,2i)} \\ S_{32}^{(1,2i)} & S_{33}^{(1,2i)} \end{pmatrix},$$

where $i = 1, 2$

Parallel Crout ILU factorization at level 2

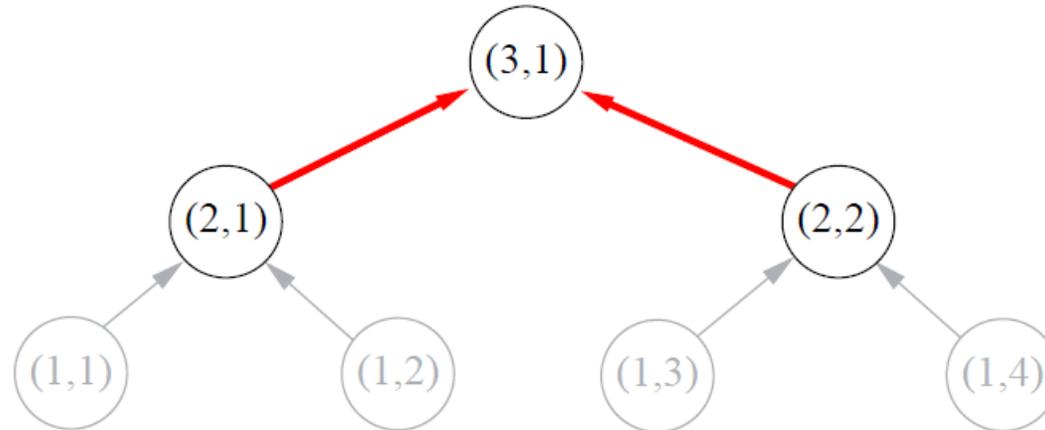


Second-level tasks compute in parallel ILUPACK partial ILUs,

$$\left(\begin{array}{c|c} A_{22}^{(2,i)} & A_{23}^{(2,i)} \\ \hline A_{32}^{(2,i)} & A_{33}^{(2,i)} \end{array} \right) \approx \left(\begin{array}{c|c} L_{22}^{(2,i)} & 0 \\ \hline L_{32}^{(2,i)} & I \end{array} \right) \left(\begin{array}{c|c} U_{22}^{(2,i)} & U_{23}^{(2,i)} \\ \hline 0 & S_{33}^{(2,i)} \end{array} \right),$$

where now $i = 1, 2$

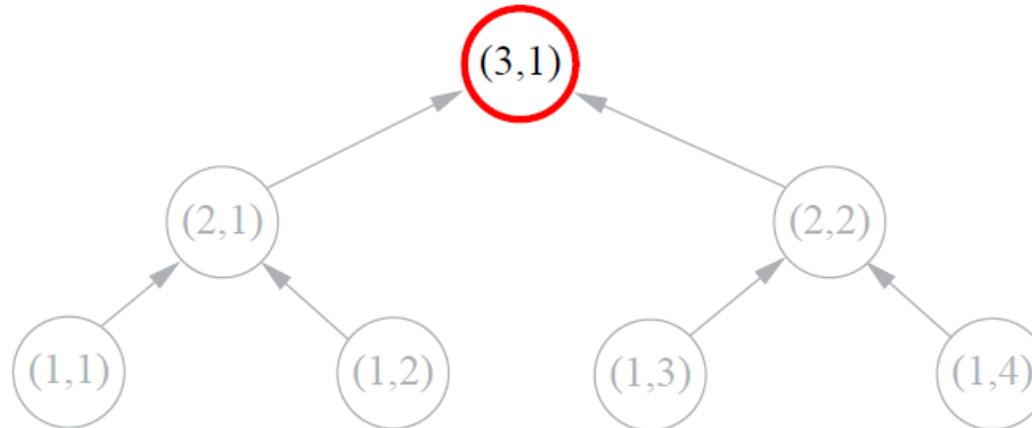
Assembly of Schur Complement Matrices at level 3



The root task “merges” the Schur complements of its children

$$A_{33}^{(3,1)} = S_{33}^{(2,1)} + S_{33}^{(2,2)}$$

Crout complete ILU factorization at level 3



Finally, the root task completes the parallel ILU

$$A_{33}^{(3,1)} \approx L_{33}^{(3,1)} U_{33}^{(3,1)}$$

Why Sparse Vector Update matters to us?

- Serial Crout ILU factorization takes place at every node in the task tree. Therefore its efficient implementation is crucial for the parallel factorization.
- Sparse vector z and w update is most time consuming kernel in serial factorization. Hence its implementation should be properly investigated.

Algorithm 4 Crout version of ILU Algorithm: ILUC

```
1: for  $k = 1 : n$  do
2:    $z_{1:k-1} = 0, \quad z_{k:n} = a_{k,k:n}$  ▷ Initialize row z
3:   for  $(1 \leq i \leq k-1 \text{ and } l_{ki} \neq 0)$  do
4:      $z_{k:n} = z_{k:n} - l_{ki} * u_{i,k:n}$  ▷ Preparation to update  $u_{k,:}$ 
5:   end do
6:    $w_{1:k} = 0, \quad w_{k+1:n} = a_{k+1:n,k}$  ▷ Initialize column z
7:   for  $(1 \leq i \leq k-1 \text{ and } u_{ik} \neq 0)$  do
8:      $w_{k+1:n} = w_{k+1:n} - u_{ik} * l_{k+1:n,i}$  ▷ Preparation to update  $l_{:,k}$ 
9:   end do
10:  Apply a dropping rule to row  $z$ 
11:  Apply a dropping rule to column  $w$ 
12:   $u_{k,:} = z$ 
13:   $l_{:,k} = w / u_{kk}, \quad l_{kk} = 1$ 
14: end do
```

Handling Sparsity at the Step k

- Row vector z is updated using the linear combination of preceding rows of U .

Algorithm 5 Update in sparse vector z

```
1: for ( $1 \leq i \leq k - 1$  and  $l_{ki} \neq 0$ ) do  
2:    $z_{k:n} = z_{k:n} - l_{ki} * u_{i,k:n}$   
3: end do
```

- We only store the non-zero entries in the sparse vector z .
- Features required in sparse Vector z :
 - Column Index j lookup: Should be $O(1)$ for faster lookups,
 - Insertion of entry $z[j]$: Should be $O(1)$,
 - Erasing entry $z[j]$: Should be $O(1)$,
 - Sorting z based on the column index j : Avg case $O(n \log(n))$.

Handling Sparsity at the Step k

- Row vector z is updated using the linear combination of preceding rows of U .

Algorithm 6 Update in sparse vector z

```
1: for ( $1 \leq i \leq k - 1$  and  $l_{ki} \neq 0$ ) do  
2:    $z_{k:n} = z_{k:n} - l_{ki} * u_{i,k:n}$   
3: end do
```

- We only store the non-zero entries in the sparse vector z .
- Features required in sparse Vector z :
 - Column Index j lookup: Should be $O(1)$ for faster lookups,
 - Insertion of entry $z[j]$: Should be $O(1)$,
 - Erasing entry $z[j]$: Should be $O(1)$,
 - Sorting z based on the column index j : Avg case $O(n \log(n))$.

Handling Sparsity at the Step k

- Row vector z is updated using the linear combination of preceding rows of U .

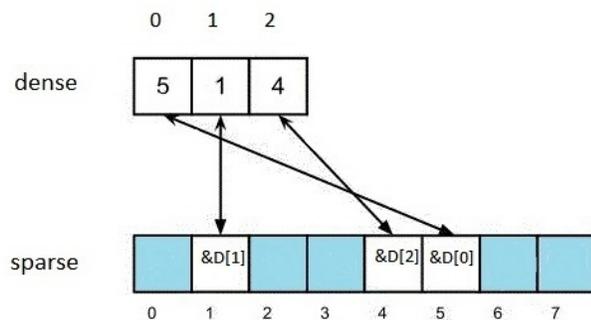
Algorithm 7 Update in sparse vector z

```
1: for ( $1 \leq i \leq k - 1$  and  $l_{ki} \neq 0$ ) do
2:    $z_{k:n} = z_{k:n} - l_{ki} * u_{i,k:n}$ 
3: end do
```

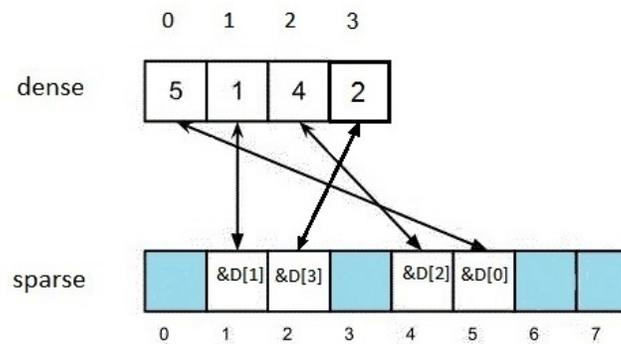
- We only store the non-zero entries in the sparse vector z .
- Features required in sparse Vector z :
 - Column Index j lookup: Should be $O(1)$ for faster lookups,
 - Insertion of entry $z[j]$: Should be $O(1)$,
 - Erasing entry $z[j]$: Should be $O(1)$,
 - Sorting z based on the column index j : Avg case $O(n \log(n))$.

Different data structures that implements the sparse vector z

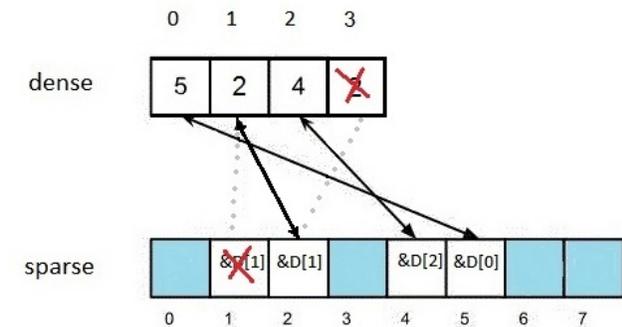
- We have used `std::map`, `std::unordered_map` and a custom implementation to implement sparse vector z .
- Custom Implementation:



(a) Dense (length n) and sparse vector (length N)



(b) Insertion at index 2



(c) Deletion at index 1

[2] Fast Implementations of Sparse Sets in C++

<https://www.codeproject.com/Articles/859324/Fast-Implementations-of-Sparse-Sets-in-Cplusplus>

Complexity of different data structures

	<code>std::map</code>	<code>std::unordered_map</code>	Custom Implementation
Lookup (find)	$O(\log(n))$	$O(n)$ worst case, $O(1)$ avg case	$O(1)$
Insertion	$O(\log(n))$	$O(n)$ worst case, $O(1)$ avg case	$O(1)$
Deletion (erase)	$O(\log(n))$	$O(n)$ worst case, $O(1)$ avg case	$O(1)$
Sort	Already Sorted	$O(n \log n)$	$O(n \log n)$

Tabelle: Time complexity

	<code>std::map</code>	<code>std::unordered_map</code>	Custom Implementation
Space Complexity	$O(n)$	$O(n)$	$O(N) + O(n)$

Tabelle: Space complexity

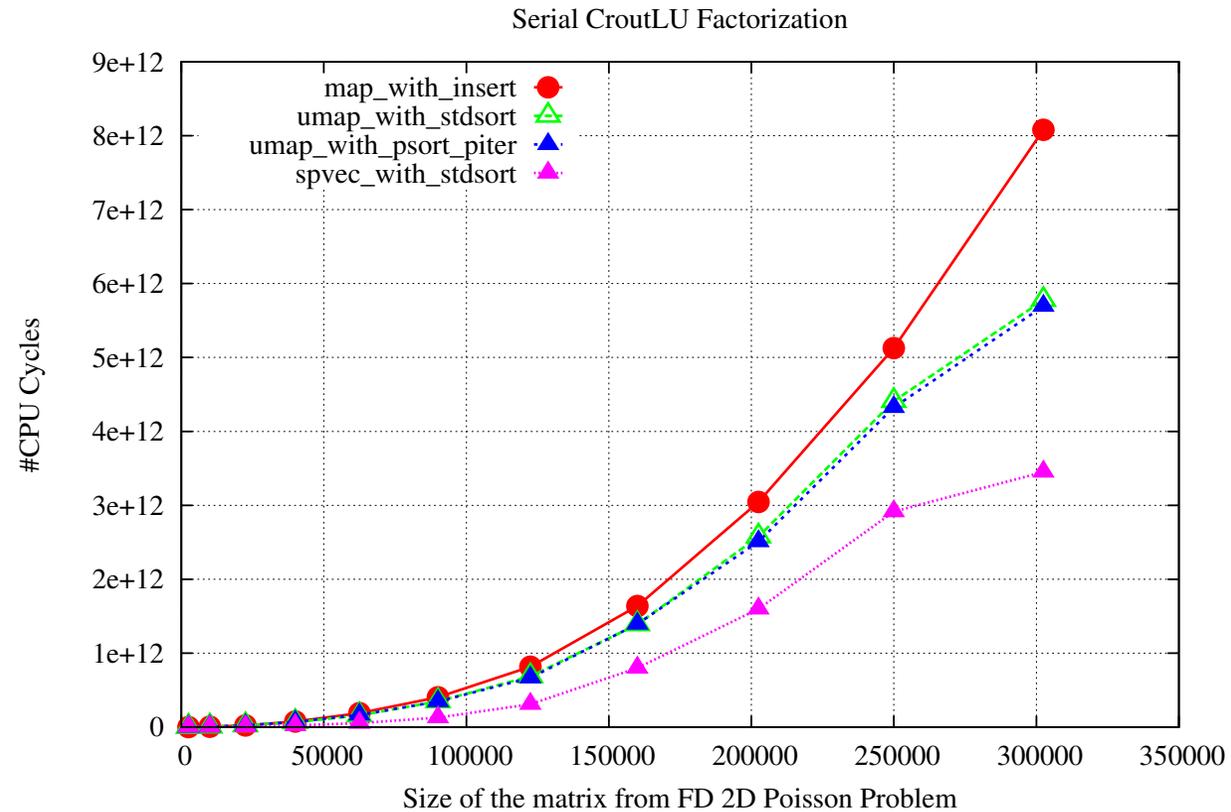
- n : length of the dense vector,
- N : length of the sparse vector ($n \ll N$).

Computational cost to generate the sparse vector z

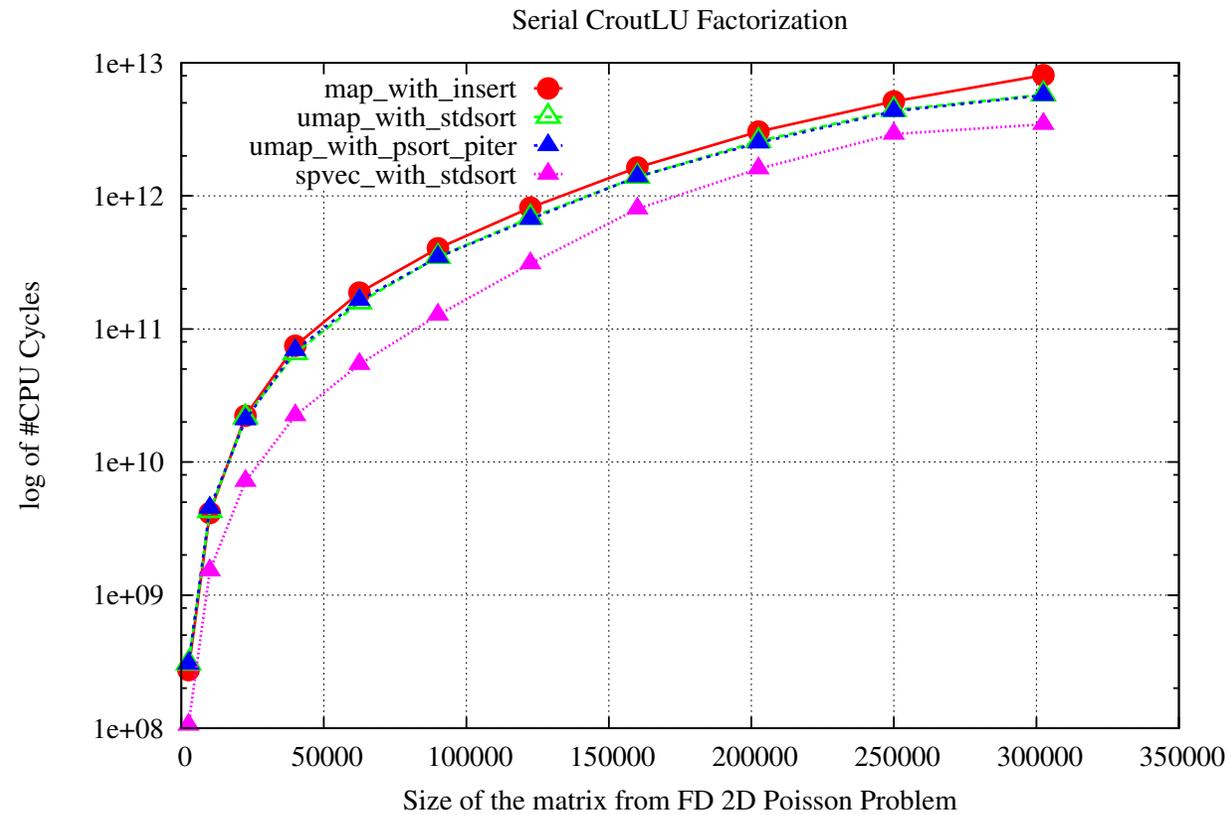
	<code>std::map</code>	<code>std::unordered_map</code>	Custom Implementation
Fill sparse vector z with $A(k,k:n)$	$O(C_0)$	$O(C_0)$	$O(C_0)$
Lookup and insert	$n \log(n) + O(n)$	$O(n^2)$ in worst case, $O(n)$ in avg case	$O(n)$
Dropping ($\tau + p$)	$2 * O(n) + n * \log(p)$	$2 * O(n) + n * \log(p)$	$2 * O(n) + n * \log(p)$
Sort based on index	Already sorted	$O(p \log(p))$	$O(p \log(p))$
Total Computation Cost	$n \log(n) + \log(p) * n + O(n)$	Worst Case: $O(n^2) + \log(p) * n + O(n)$ Avg Case: $O(\log(p) * n) + O(n)$	$\log(p) * n + O(n)$

- $p = \text{constant}$ in general, $p = n$ in case of full fill-in in z .

Computational Time vs Matrix Size



Log of Computational Time vs Matrix Size



Profiler reading: using std::map to store the sparse vector

insert in std::map takes up 65.6 % time of the Crout LU factorization.

Function	0.0%	100.0%	0
Total	0.0%	100.0%	0
_start	0.0%	100.0%	0
__libc_start_main	0.0%	100.0%	0
main	0.0%	100.0%	0
GaspiLS::CroutLUSolver<GaspiLS::implementation::CSRChunk<int, double>, GaspiLS::implementation::CSCChunk<int, double>, std::vector<double, std::allocator<double>>>::factorizeAintoLU	0.0%	99.4%	0
std::map<unsigned long, double, std::less<unsigned long>, std::allocator<std::pair<unsigned long const, double>>>::insert<std::pair<unsigned long, double>, void>	0.0%	35.0%	0
std::_Rb_tree<unsigned long, std::pair<unsigned long const, double>, std::_Select1st<std::pair<unsigned long const, double>>, std::less<unsigned long>, std::allocator<std::pair<unsigned long const, double>>>::_M_insert_unique<std::pair<unsigned long const, double>>	0.0%	35.0%	0
std::_Rb_tree<unsigned long, std::pair<unsigned long const, double>, std::_Select1st<std::pair<unsigned long const, double>>, std::less<unsigned long>, std::allocator<std::pair<unsigned long const, double>>>::_M_get_insert_unique_ptr	0.0%	32.5%	0
std::_Rb_tree<unsigned long, std::pair<unsigned long const, double>, std::_Select1st<std::pair<unsigned long const, double>>, std::less<unsigned long>, std::allocator<std::pair<unsigned long const, double>>>::_S_right	0.0%	10.0%	0
std::_Rb_tree<unsigned long, std::pair<unsigned long const, double>, std::_Select1st<std::pair<unsigned long const, double>>, std::less<unsigned long>, std::allocator<std::pair<unsigned long const, double>>>::_S_left	0.0%	6.9%	0
std::_Rb_tree_iterator<std::pair<unsigned long const, double>>::operator--	0.0%	6.9%	0
std::_Rb_tree<unsigned long, std::pair<unsigned long const, double>, std::_Select1st<std::pair<unsigned long const, double>>, std::less<unsigned long>, std::allocator<std::pair<unsigned long const, double>>>::_M_begin	0.0%	5.0%	0
std::_Rb_tree_iterator<std::pair<unsigned long const, double>>::_Rb_tree_iterator	0.0%	1.3%	0
std::less<unsigned long>::operator()	0.0%	1.2%	0
std::_Rb_tree<unsigned long, std::pair<unsigned long const, double>, std::_Select1st<std::pair<unsigned long const, double>>, std::less<unsigned long>, std::allocator<std::pair<unsigned long const, double>>>::_M_insert<std::pair<unsigned long const, double>>	0.0%	2.5%	0
std::map<unsigned long, double, std::less<unsigned long>, std::allocator<std::pair<unsigned long const, double>>>::insert<std::pair<unsigned long, double>, void>	0.0%	30.6%	0
std::_Rb_tree<unsigned long, std::pair<unsigned long const, double>, std::_Select1st<std::pair<unsigned long const, double>>, std::less<unsigned long>, std::allocator<std::pair<unsigned long const, double>>>::_M_insert_unique<std::pair<unsigned long const, double>>	0.0%	30.6%	0
std::_Rb_tree<unsigned long, std::pair<unsigned long const, double>, std::_Select1st<std::pair<unsigned long const, double>>, std::less<unsigned long>, std::allocator<std::pair<unsigned long const, double>>>::_M_get_insert_unique_ptr	0.0%	30.0%	0
std::_Rb_tree<unsigned long, std::pair<unsigned long const, double>, std::_Select1st<std::pair<unsigned long const, double>>, std::less<unsigned long>, std::allocator<std::pair<unsigned long const, double>>>::_S_right	0.0%	12.5%	0
std::_Rb_tree_iterator<std::pair<unsigned long const, double>>::operator--	0.0%	7.5%	0
std::_Rb_tree<unsigned long, std::pair<unsigned long const, double>, std::_Select1st<std::pair<unsigned long const, double>>, std::less<unsigned long>, std::allocator<std::pair<unsigned long const, double>>>::_S_left	0.0%	5.0%	0
std::_Rb_tree<unsigned long, std::pair<unsigned long const, double>, std::_Select1st<std::pair<unsigned long const, double>>, std::less<unsigned long>, std::allocator<std::pair<unsigned long const, double>>>::_M_begin	0.0%	3.1%	0
std::_Rb_tree<unsigned long, std::pair<unsigned long const, double>, std::_Select1st<std::pair<unsigned long const, double>>, std::less<unsigned long>, std::allocator<std::pair<unsigned long const, double>>>::_M_insert<std::pair<unsigned long const, double>>	0.0%	0.6%	0
GaspiLS::CroutLUSolver<GaspiLS::implementation::CSRChunk<int, double>, GaspiLS::implementation::CSCChunk<int, double>, std::vector<double, std::allocator<double>>>::update_IFirst_uList	0.0%	10.0%	0
GaspiLS::CroutLUSolver<GaspiLS::implementation::CSRChunk<int, double>, GaspiLS::implementation::CSCChunk<int, double>, std::vector<double, std::allocator<double>>>::update_uFirst_lList	0.0%	7.5%	0
GaspiLS::CroutLUSolver<GaspiLS::implementation::CSRChunk<int, double>, GaspiLS::implementation::CSCChunk<int, double>, std::vector<double, std::allocator<double>>>::addColinL	0.0%	2.5%	0
GaspiLS::CroutLUSolver<GaspiLS::implementation::CSRChunk<int, double>, GaspiLS::implementation::CSCChunk<int, double>, std::vector<double, std::allocator<double>>>::fillVectorZ	0.0%	1.9%	0
GaspiLS::CroutLUSolver<GaspiLS::implementation::CSRChunk<int, double>, GaspiLS::implementation::CSCChunk<int, double>, std::vector<double, std::allocator<double>>>::addRowinU	0.0%	1.3%	0
GaspiLS::CroutLUSolver<GaspiLS::implementation::CSRChunk<int, double>, GaspiLS::implementation::CSCChunk<int, double>, std::vector<double, std::allocator<double>>>::fillVectorW	0.0%	1.2%	0
std::vector<double, std::allocator<double>>::operator[]	0.0%	0.6%	0
std::vector<double, std::allocator<double>>::operator[]	0.0%	0.6%	0
std::ostream::_M_insert<double>	0.0%	0.6%	0

Profiler reading: using `std::unordered_map` to store the sparse vector

`find` in `std::unordered_map` takes up **35.6 %** time of the Crout LU factorization.

Function	Time	Percentage	Count
Total	0.0%	100.0%	0.0%
_start	0.0%	100.0%	0.0%
__libc_start_main	0.0%	100.0%	0.0%
main	0.0%	100.0%	0.0%
GaspiLS::CroutLUSolver<GaspiLS::implementation::CSRChunk<int, double>, GaspiLS::implementation::CSCChunk<int, double>, std::vector<double, std::allocator<double>>>::factorizeAintoLU	0.0%	100.0%	0.0%
std::unordered_map<unsigned long, double, std::hash<unsigned long>, std::equal_to<unsigned long>, std::allocator<std::pair<unsigned long const, double>>>::find	0.0%	23.7%	0.0%
std::_Hashtable<unsigned long, std::pair<unsigned long const, double>, std::allocator<std::pair<unsigned long const, double>>, std::_detail::_Select1st, std::equal_to<unsigned long>, std::hash<unsigned long>, std::allocator<std::pair<unsigned long const, double>>>::find	0.0%	23.7%	0.0%
std::_Hashtable<unsigned long, std::pair<unsigned long const, double>, std::allocator<std::pair<unsigned long const, double>>, std::_detail::_Select1st, std::equal_to<unsigned long>, std::hash<unsigned long>, std::allocator<std::pair<unsigned long const, double>>>::find	0.0%	14.1%	0.0%
std::_Hashtable<unsigned long, std::pair<unsigned long const, double>, std::allocator<std::pair<unsigned long const, double>>, std::_detail::_Select1st, std::equal_to<unsigned long>, std::hash<unsigned long>, std::allocator<std::pair<unsigned long const, double>>>::find	0.0%	8.5%	0.0%
GaspiLS::CroutLUSolver<GaspiLS::implementation::CSRChunk<int, double>, GaspiLS::implementation::CSCChunk<int, double>, std::vector<double, std::allocator<double>>>::update_lFirst_uList	0.0%	13.6%	0.0%
std::unordered_map<unsigned long, double, std::hash<unsigned long>, std::equal_to<unsigned long>, std::allocator<std::pair<unsigned long const, double>>>::find	0.0%	11.9%	0.0%
std::_Hashtable<unsigned long, std::pair<unsigned long const, double>, std::allocator<std::pair<unsigned long const, double>>, std::_detail::_Select1st, std::equal_to<unsigned long>, std::hash<unsigned long>, std::allocator<std::pair<unsigned long const, double>>>::find	0.0%	11.9%	0.0%
std::_Hashtable<unsigned long, std::pair<unsigned long const, double>, std::allocator<std::pair<unsigned long const, double>>, std::_detail::_Select1st, std::equal_to<unsigned long>, std::hash<unsigned long>, std::allocator<std::pair<unsigned long const, double>>>::find	0.0%	10.7%	0.0%
std::_Hashtable<unsigned long, std::pair<unsigned long const, double>, std::allocator<std::pair<unsigned long const, double>>, std::_detail::_Select1st, std::equal_to<unsigned long>, std::hash<unsigned long>, std::_detail::_Mod_range_hashing, std::allocator<std::pair<unsigned long const, double>>>::find	0.0%	10.7%	0.0%
std::_detail::_Hashtable_base<unsigned long, std::pair<unsigned long const, double>, std::_detail::_Select1st, std::equal_to<unsigned long>, std::hash<unsigned long>, std::_detail::_Mod_range_hashing, std::allocator<std::pair<unsigned long const, double>>>::find	0.0%	4.5%	0.0%
GaspiLS::CroutLUSolver<GaspiLS::implementation::CSRChunk<int, double>, GaspiLS::implementation::CSCChunk<int, double>, std::vector<double, std::allocator<double>>>::update_uFirst_lList	0.0%	7.9%	0.0%
std::unordered_map<unsigned long, double, std::hash<unsigned long>, std::equal_to<unsigned long>, std::allocator<std::pair<unsigned long const, double>>>::operator[]	0.0%	4.5%	0.0%
GaspiLS::CroutLUSolver<GaspiLS::implementation::CSRChunk<int, double>, GaspiLS::implementation::CSCChunk<int, double>, std::vector<double, std::allocator<double>>>::addColinL_UnorderedMapCase	0.0%	3.4%	0.0%
GaspiLS::CroutLUSolver<GaspiLS::implementation::CSRChunk<int, double>, GaspiLS::implementation::CSCChunk<int, double>, std::vector<double, std::allocator<double>>>::addRowinU_UnorderedMapCase	0.0%	2.3%	0.0%
std::unordered_map<unsigned long, double, std::hash<unsigned long>, std::equal_to<unsigned long>, std::allocator<std::pair<unsigned long const, double>>>::operator[]	0.0%	2.3%	0.0%
std::vector<double, std::allocator<double>>::operator[]	0.0%	1.1%	0.0%
std::vector<unsigned long, std::allocator<unsigned long>>::operator[]	0.0%	1.1%	0.0%
std::unordered_map<unsigned long, double, std::hash<unsigned long>, std::equal_to<unsigned long>, std::allocator<std::pair<unsigned long const, double>>>::operator[]	0.0%	0.6%	0.0%
Selected 2 rows:	0.0%	35.6%	0.0%

Profiler reading: Custom implementation for the sparse vector

insert in the custom implementation takes up only **18.4 %** time of the Crout LU factorization.

	Idle	Poor	Ok	
▼ Total	0.0%	100.0%	0.0%	0.0%
▼ _start	0.0%	100.0%	0.0%	0.0%
▼ __libc_start_main	0.0%	100.0%	0.0%	0.0%
▼ main	0.0%	98.7%	0.0%	0.0%
▼ GaspiLS::CroutLUSolver<GaspiLS::implementation::CSRChunk<int, double>, GaspiLS::implementation::CSCChunk<int, double>, std::vector<double, std::allocator<double>>>::factorizeAintoLU	0.0%	98.7%	0.0%	0.0%
▶ GaspiLS::CroutLUSolver<GaspiLS::implementation::CSRChunk<int, double>, GaspiLS::implementation::CSCChunk<int, double>, std::vector<double, std::allocator<double>>>::update_uFirst_IList	0.0%	29.0%	0.0%	0.0%
▶ GaspiLS::CroutLUSolver<GaspiLS::implementation::CSRChunk<int, double>, GaspiLS::implementation::CSCChunk<int, double>, std::vector<double, std::allocator<double>>>::update_lFirst_uList	0.0%	19.7%	0.0%	0.0%
▶ GaspiLS::SparseVector<unsigned long, double>::insert	0.0%	10.5%	0.0%	0.0%
▶ GaspiLS::SparseVector<unsigned long, double>::insert	0.0%	7.9%	0.0%	0.0%
▶ GaspiLS::CroutLUSolver<GaspiLS::implementation::CSRChunk<int, double>, GaspiLS::implementation::CSCChunk<int, double>, std::vector<double, std::allocator<double>>>::addColinL_SpVector	0.0%	5.3%	0.0%	0.0%
▶ GaspiLS::CroutLUSolver<GaspiLS::implementation::CSRChunk<int, double>, GaspiLS::implementation::CSCChunk<int, double>, std::vector<double, std::allocator<double>>>::addRowinU_SpVector	0.0%	3.9%	0.0%	0.0%
▶ GaspiLS::CroutLUSolver<GaspiLS::implementation::CSRChunk<int, double>, GaspiLS::implementation::CSCChunk<int, double>, std::vector<double, std::allocator<double>>>::fillVectorW	0.0%	1.3%	0.0%	0.0%
▶ std::vector<double, std::allocator<double>>::operator[]	0.0%	1.3%	0.0%	0.0%
▶ [Unknown stack frame(s)]	0.0%	1.3%	0.0%	0.0%

Summary and future outlook

- Understood Multilevel Parallel Crout ILU factorization algorithm of matrix A .
- Insert in Sparse vector is the bottleneck in Serial implementation.
- Optimized using custom implementation of Sparse vector.
- Since the serial implementation looks good (reasonably optimal), we will start parallel implementation.

Questions/Discussion?

References

-  <http://www.gaspils.de/>.
-  <https://www.codeproject.com/Articles/859324/Fast-Implementations-of-Sparse-Sets-in-Cplusplus>.
-  José Ignacio Aliaga, Rosa M. Badia, Maria Barreda, Matthias Bollhöfer, Ernesto Dufrechou, Pablo Ezzatti, and Enrique S. Quintana-Ortí.
Exploiting task and data parallelism in ilupack's preconditioned CG solver on NUMA architectures and many-core accelerators.
Parallel Computing, 54:97–107, 2016.
-  Daniel Gruenewald Christian Simmendinger Mirko Rahn.
Gaspi tutorial.
-  Alberto F. Martin Enrique S. Quintana-Orti Jose I. Aliaga, Matthias Bollheofer.
Scheduling strategies for parallel sparse backward/forward substitution.