Communication-Avoiding Incomplete LU0 (CA-ILU0) Preconditioner

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- Interested in solving $Ax = b$
- CA-Iterative Methods based on **s-step methods**: CA-GMRES, CA-CG
- Few CA-Preconditioners !!

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- Present Communication Avoiding ILU(0) preconditioner (CA-ILU0)

GMRES

- is a Krylov subspace method developed by Saad and Schultz in 1986
- finds the solution of the system $Ax = b$ by minimizing the residual at each iteration

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- builds up an orthonormal basis $q_1, q_2, ..., q_k$ for $\kappa_k(A, r_0) = span\{r_0, Ar_0, A^2r_0, ..., A^{k-1}r_0\}$ using the Arnoldi procedure which is a Modified Gram-Schmidt procedure.
- solves a least square problem using Givens rotations and Backward substitution.

GMRES (x_0, A, b, ϵ, k_{max})

Compute $\boxed{r_0 = b - Ax_0}$, $\rho = ||r_0||_2$, $\beta = \rho$, $q_1 = \frac{r_0}{\rho}$, $P_0 = \beta e_1$, k = 1

While ($\rho \geq \epsilon||b||_2$ and $k < k_{max}$) Do

2. Perform an Arnoldi iteration, generate the $(k+1)^{th}$ vector of the Arnoldi basis Q_{k+1} and the k^{th} column of the Upper Hessenberg matrix H_k

   Compute $\boxed{q_{j+1} = Aq_j}$

   for $j = 1, \ldots, k$

   $h_{j,k} = q_j^t q_{k+1}$ and $q_{k+1} = q_{k+1} - h_{j,k} q_j$

   end

   If $q_{k+1} = 0$ Stop

   Else$h_{k+1,k} = ||q_{k+1}||_2$

   $q_{k+1} = \frac{q_{k+1}}{h_{k+1,k}}$

3. Minimize $||\beta e_1 - H_k y||$ over $\mathbb{R}^k$ to obtain y_k using:

   a. Givens rotations that transform H_k into an upper triangular system

   b. Backward substitution on the system $H_k y = P_k$ where P_k is the transformation of βe_1 under the Givens rotation

4. $\rho = ||P_k - H_k y_k||_2 = |P_k(k+1)|$, $k = k+1$

end

$x = x_0 + Q_{k-1} y_{k-1}$

Preconditioned GMRES (x_0, M, A, b, ϵ, k_{max})

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$s-step$ GMRES

s-step GMRES (x_0, A, b, ϵ, s)

1. Compute $r_0 = b - Ax_0$, $q_1 = r_0/||r_0||_2$
2. Perform an **Arnoldi(s)** iteration
   i. Compute $q_2 = Ar_0, q_3 = A^2r_0, q_4 = A^3r_0, ..., q_{s+1} = A^sr_0$ where $q_i = Aq_{i-1}$
   ii. Orthogonalize $q_1, q_2, ..., q_{s+1}$ using a QR factorization
   iii. Reconstruct the upper Hessenberg matrix H_s
3. Solve the Least Square problem $y_s = min_y||P_s - H_sy||_2$
4. $\rho = ||P_s - H_sy_s||_2$
5. $x_s = x_0 + Q_sy_s$
6. if ($\rho \geq \epsilon||b||_2$)
   Let $x_0 = x_s$ and call s-step GMRES (x_s, A, b, ϵ, s)
   else
   x_s is the approximate solution

CA-GMRES (x_0, A, b, ϵ, s, l)

1. Compute $r_0 = b - Ax_0$, $q_1 = r_0/||r_0||_2$, $\rho = ||r_0||_2$, $i = 0$
2. Perform an **Arnoldi(s,l)** iteration

   While ($\rho \geq \epsilon||b||_2$ and $i < l$)

   i. Compute $q_{si+2}, q_{si+3}, q_{si+4}, ..., q_{si+(s+1)}$ using Matrix Powers Kernel

   ii. Orthogonalize q_{si+j} $(2 \leq j \leq s+1)$ against q_j $(2 \leq j \leq si+1)$ using Block Gram Schmidt

   iii. Orthogonalize $q_{si+1}, q_{si+2}, ..., q_{si+(s+1)}$ using a TSQR factorization

   iv. Reconstruct the upper Hessenberg matrix H_s

   v. Update ρ, $i = i+1$
3. Solve the Least Square problem $y_{si} = min_y||P_s - H_s y||_2$
5. $x_{si} = x_0 + Q_s y_{si}$
6. if ($\rho \geq \epsilon||b||_2$)

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The Parallel $s-step$ Matrix-Vector Multiplication (Matrix Powers Kernel)

The $s-step$ matrix-Vector multiplication consists of performing s matrix vector multiplications at a time Ax till $A^s x$ in parallel by p processors where

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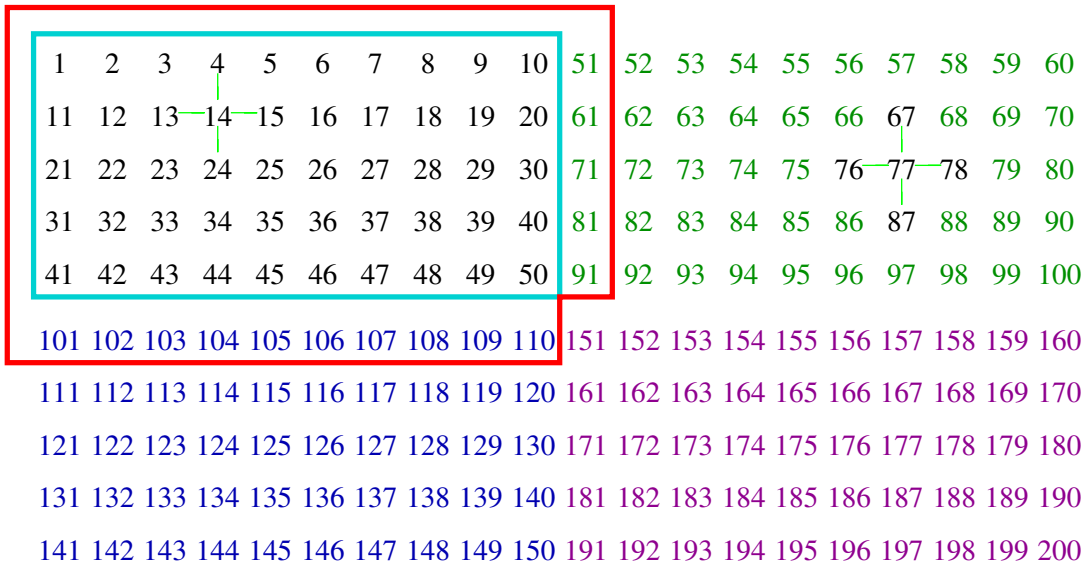
- each processor fetches all the data needed from the beginning
- each processor computes a part of Ax till $A^s x$ without any communication with other processors by performing extra redundanat flops

Domain 1

Domain & ghost zone for one step

Domain & ghost zone for two steps

Domain & ghost zone for three steps



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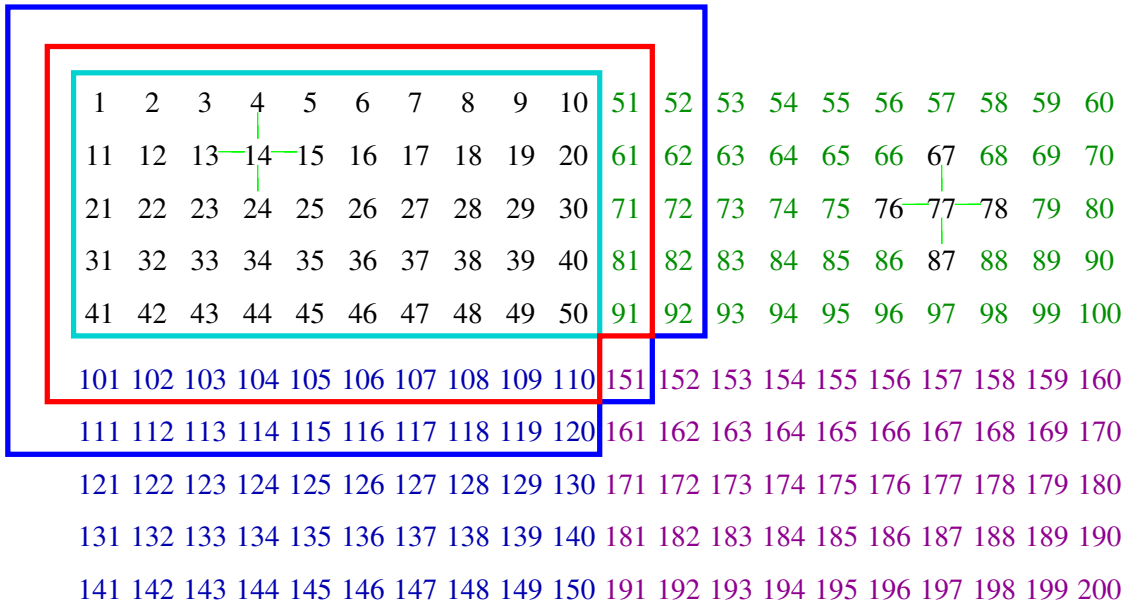

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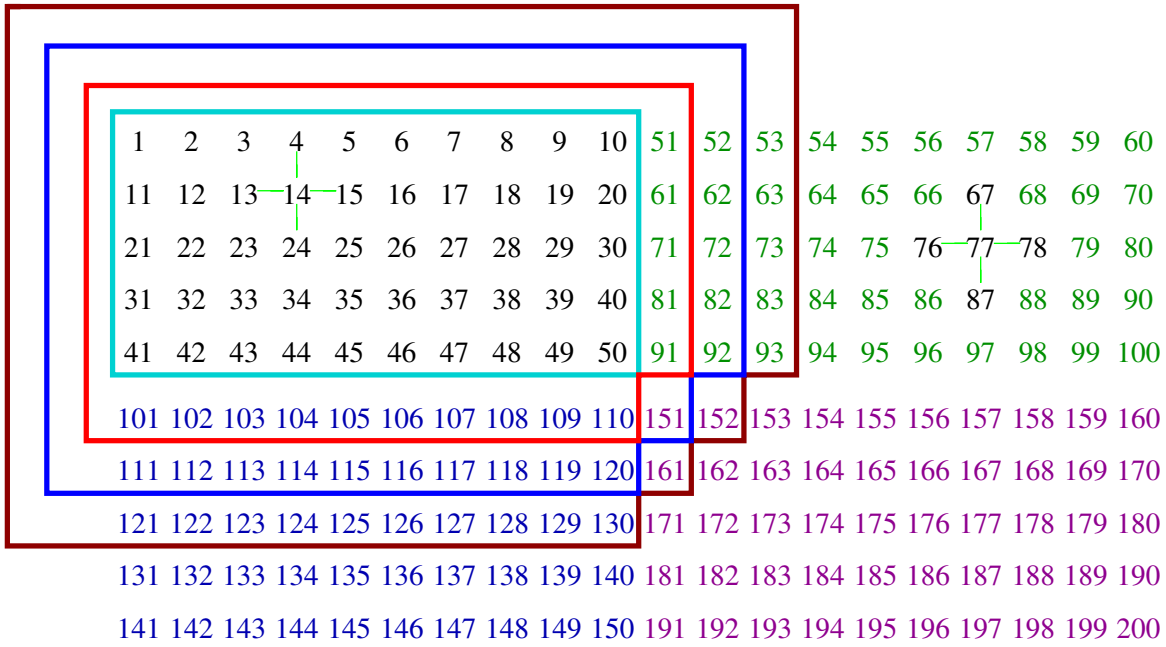

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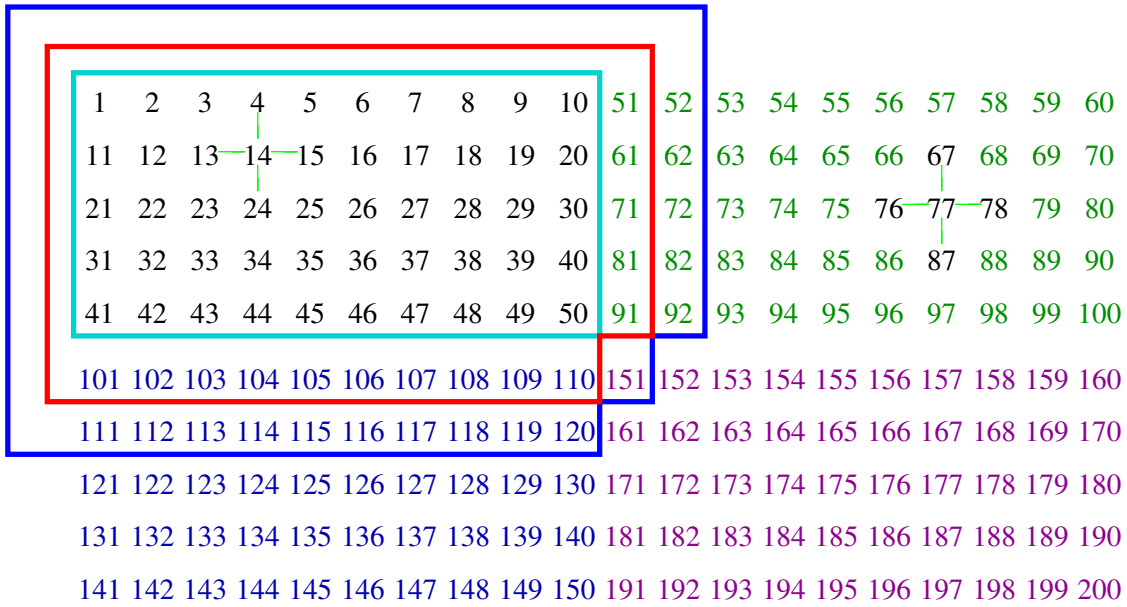

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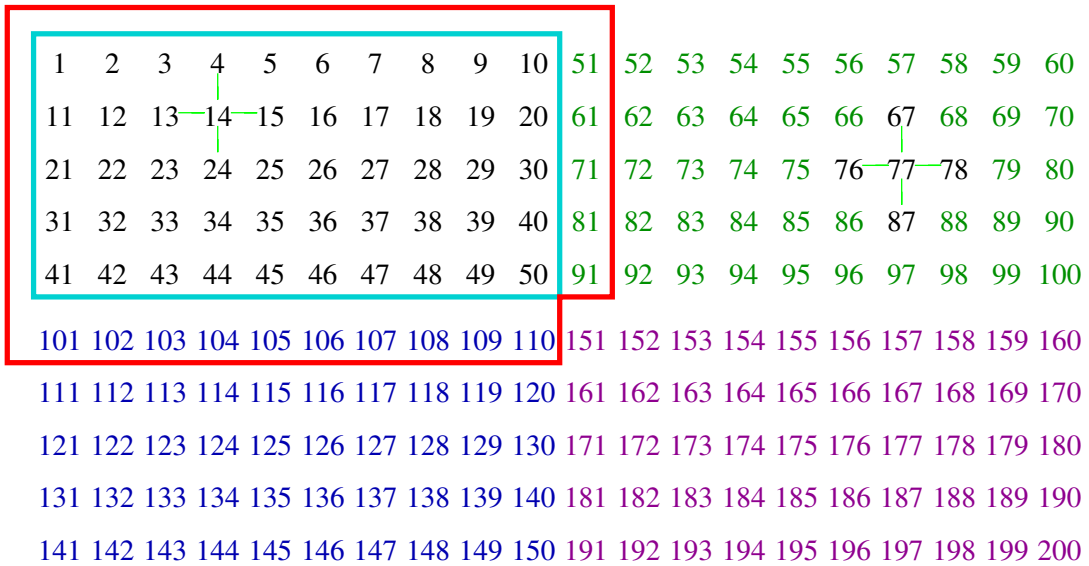

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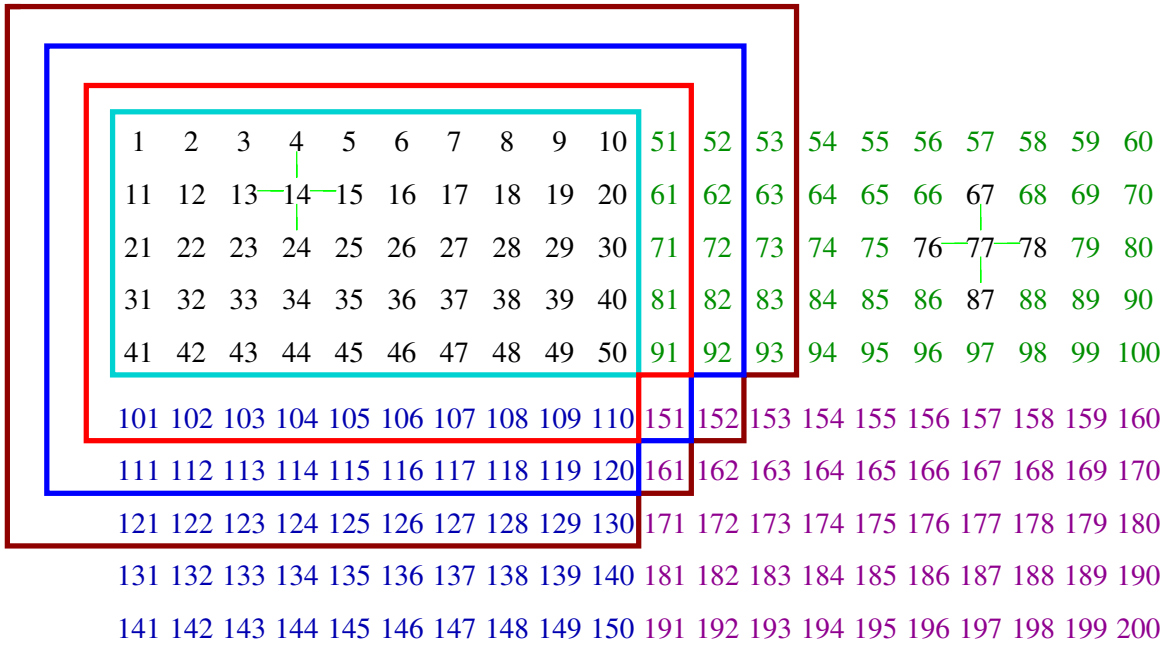

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ILU Preconditioner

- ILU preconditioning techniques based on the incomplete factorization of A

$$A = LU + R$$

$$M = LU$$

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$$A = \begin{pmatrix} \times & \times & 0 & 0 & \times & 0 & \times \\ \times & \times & \times & \times & 0 & 0 & 0 \\ \times & 0 & \times & \times & 0 & 0 & \times \\ 0 & 0 & \times & \times & 0 & \times & \times \\ 0 & \times & 0 & 0 & \times & \times & 0 \\ \times & 0 & \times & 0 & 0 & \times & \times \\ 0 & 0 & \times & 0 & \times & 0 & \times \end{pmatrix}$$

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Processor i has to
Compute part α_0 of

$$\begin{aligned} y_1 &= (LU)^{-1}Ay_0 \\ \\ y_2 &= ((LU)^{-1}A)^2 y_0 \\ &= (LU)^{-1}Ay_1 \\ &\vdots \\ y_s &= ((LU)^{-1}A)^s y_0 \\ &= (LU)^{-1}Ay_{s-1} \end{aligned}$$

without communicating
with other processors

The s-step Data Dependencies

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$$\Longleftrightarrow \begin{cases} f = A y_{i-1} \\ L z = f \\ U y_i = z \end{cases}$$

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s-step Dependencies (A, L, U, s, α_0)

for $j = 1$ *to* s
  Find $\beta_j = R(G(U), \alpha_{j-1})$
  Find $\gamma_j = R(G(L), \beta_j)$
  Find $\delta_j = Adj(G(A), \gamma_j)$
  Set $\alpha_j = \delta_j$
end

ILU Matrix Powers Kernel

ILU Matrix Powers Kernel (A, L, U, s, α_0)

i. Processor i calls the algorithm s-step Dependencies

ii. Processor i fetches the corresponding parts of A, L, U, y_0

iii. for $j = s$ *to* 1

1. Compute $f(\gamma_j) = A(\gamma_j, \delta_j) y_{j-k}(\delta_j)$
2. Solve $L(\gamma_j, \gamma_j) z_{j-k+1}(\gamma_j) = f(\gamma_j)$
3. Solve $U(\beta_j, \beta_j) y_{j-k+1}(\beta_j) = z(\beta_j)$
4. Save $y_{j-k+1}(\alpha_0)$, which is the part that Processor i has to compute
5. Set $y_{j-k} = y_{j-k+1}$

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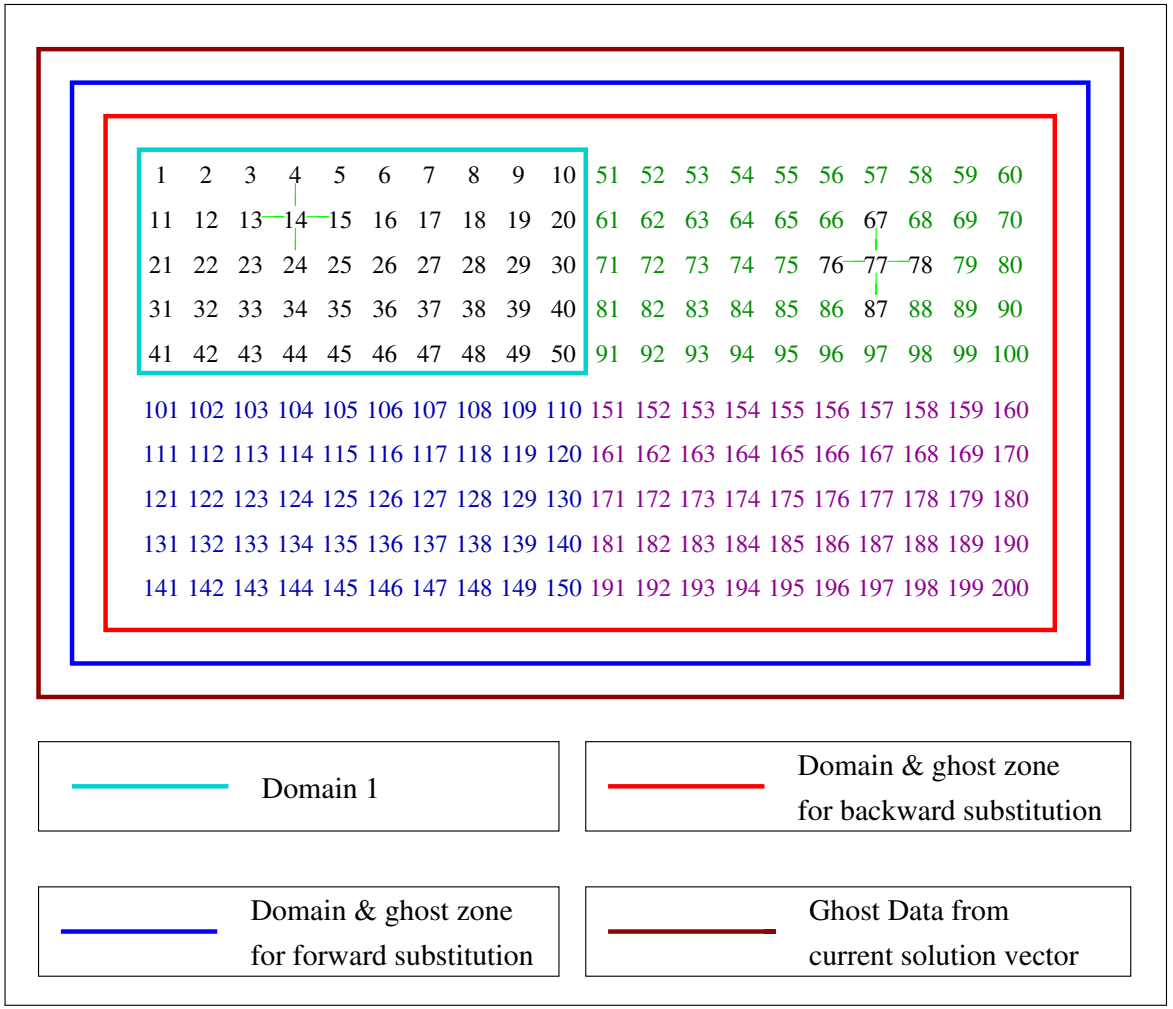
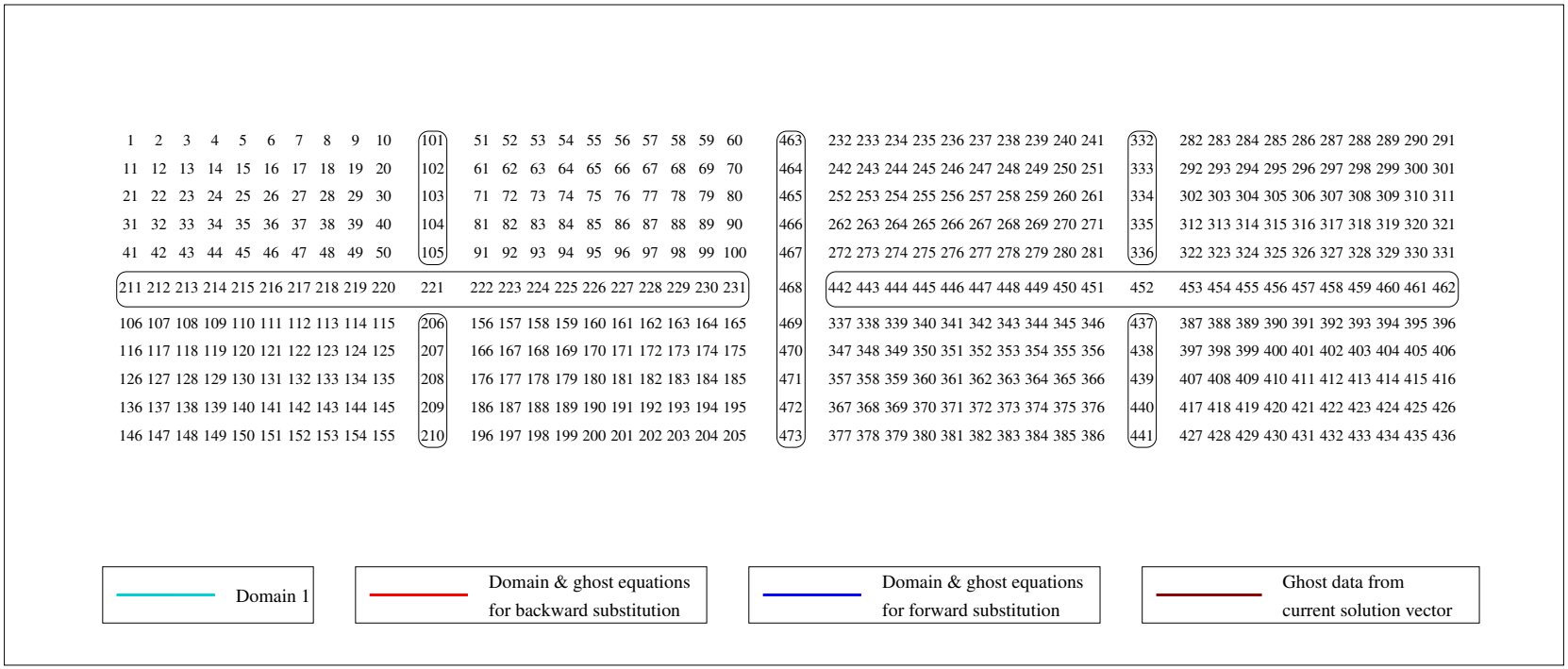
ILU0 Matrix Powers Kernel for $s = 1$



Nested Dissection ILU0 Matrix Powers Kernel for $s = 1$



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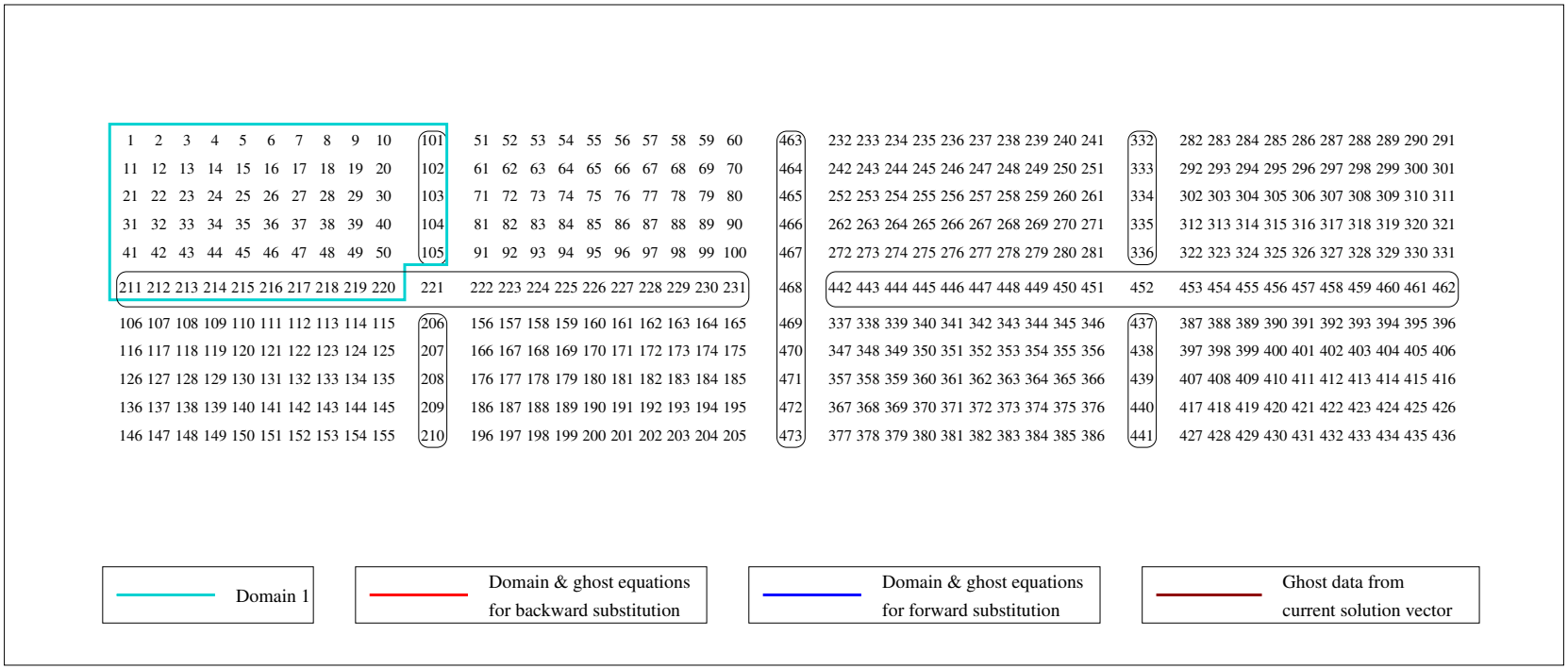

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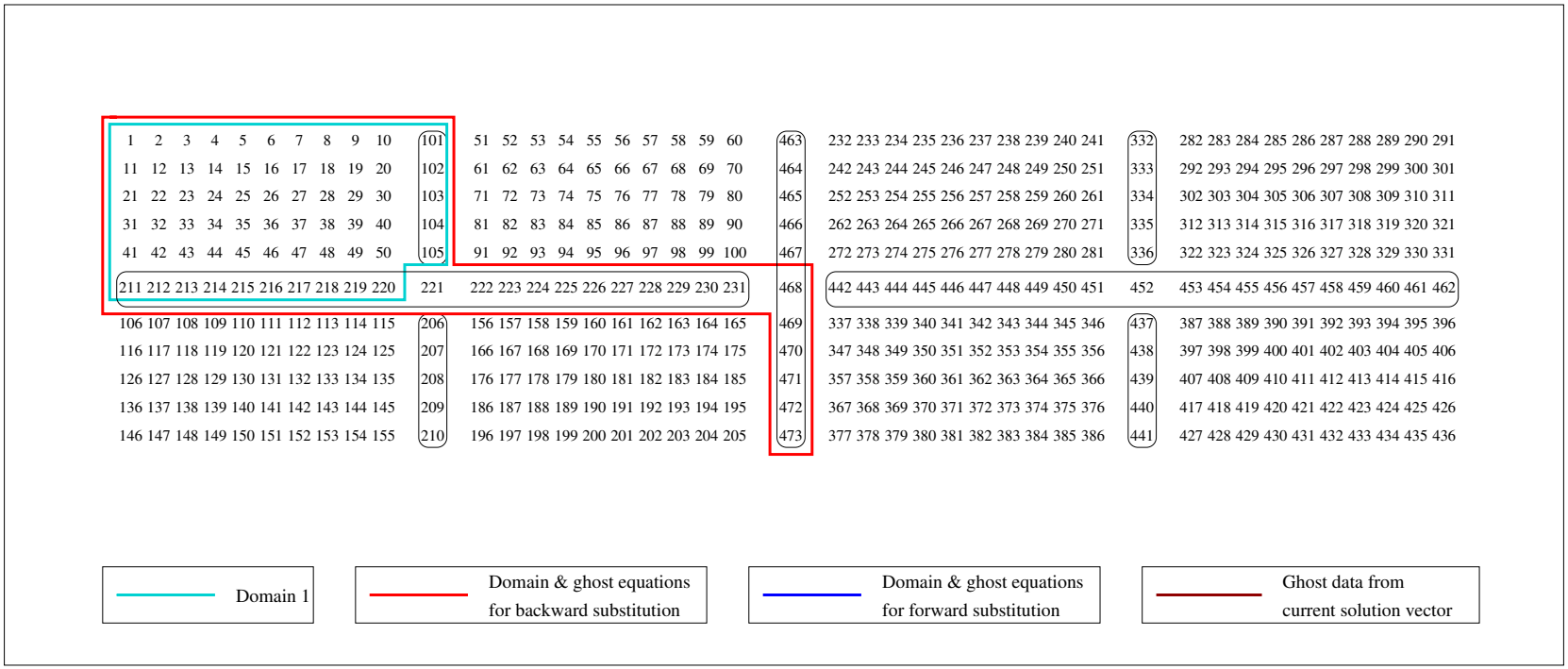

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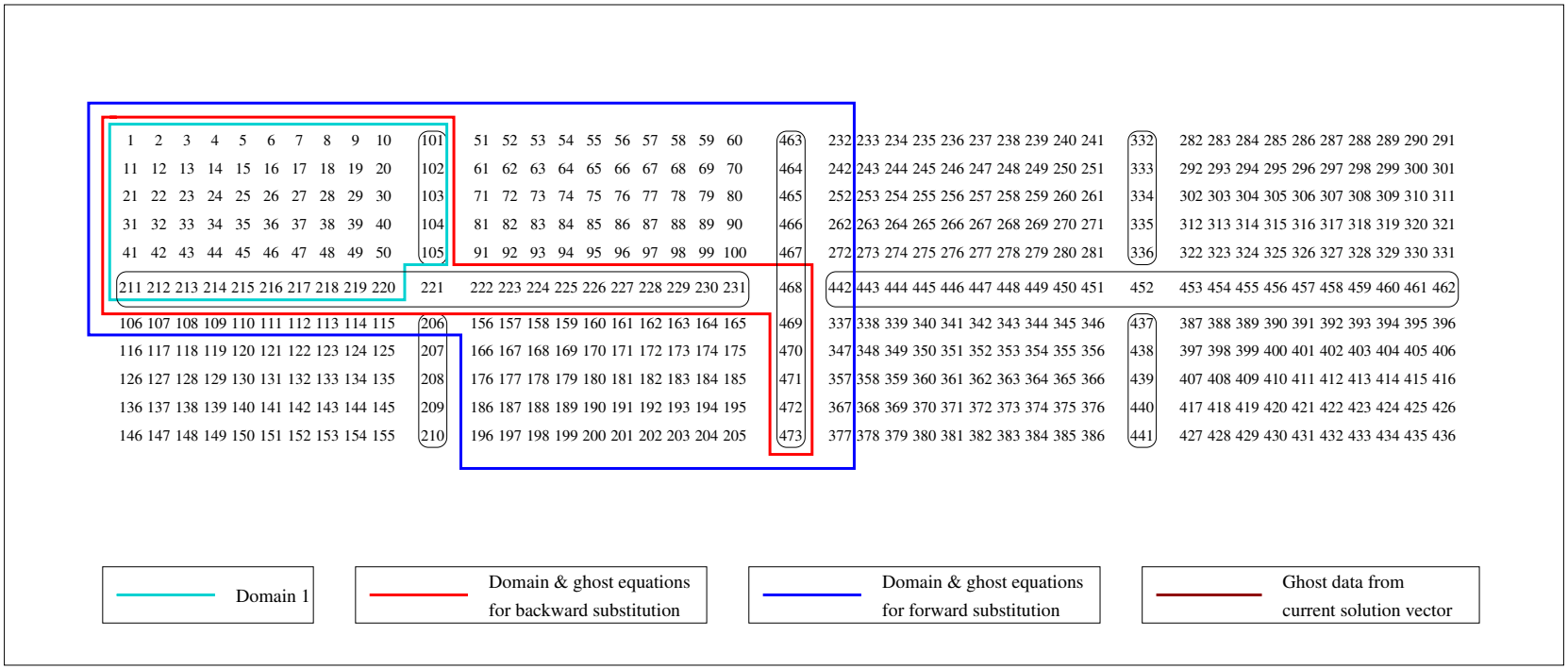

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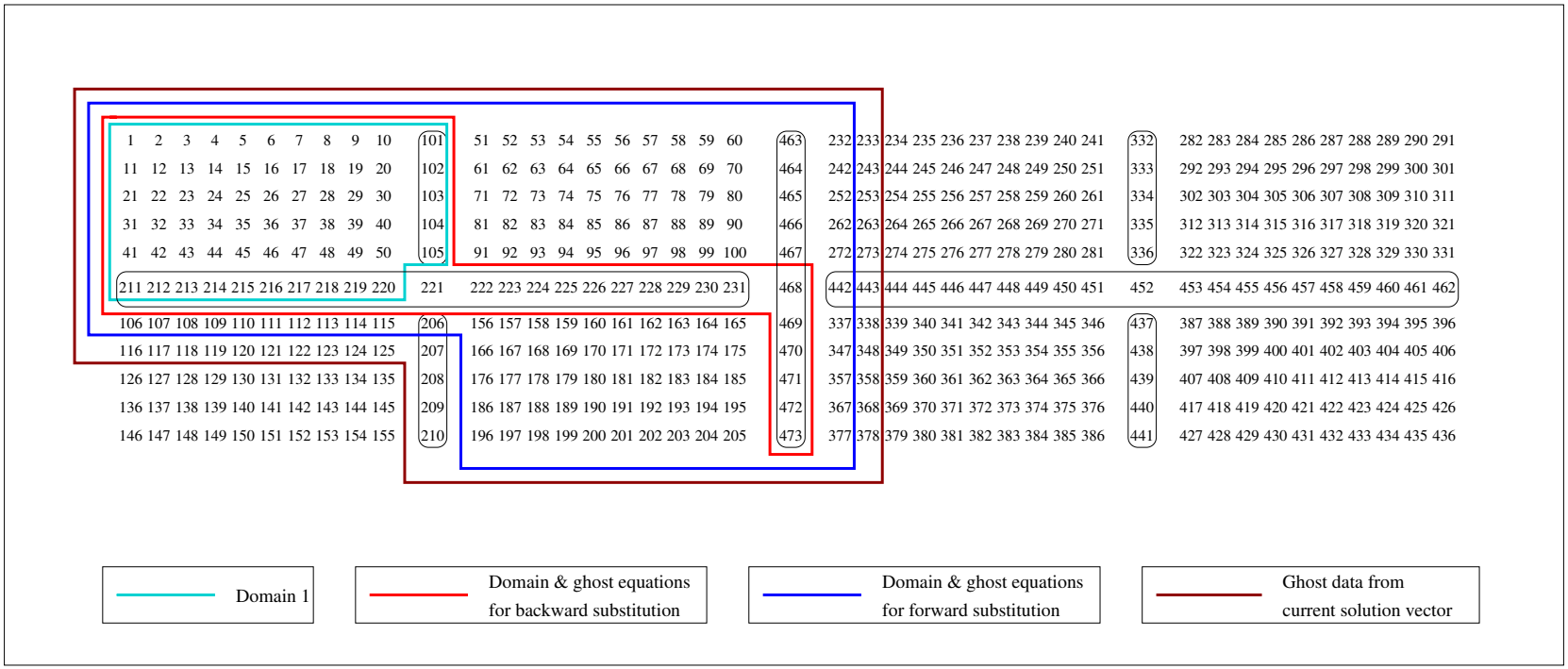

CR-ILU0 reordering

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CA-ILU0(s) reordering

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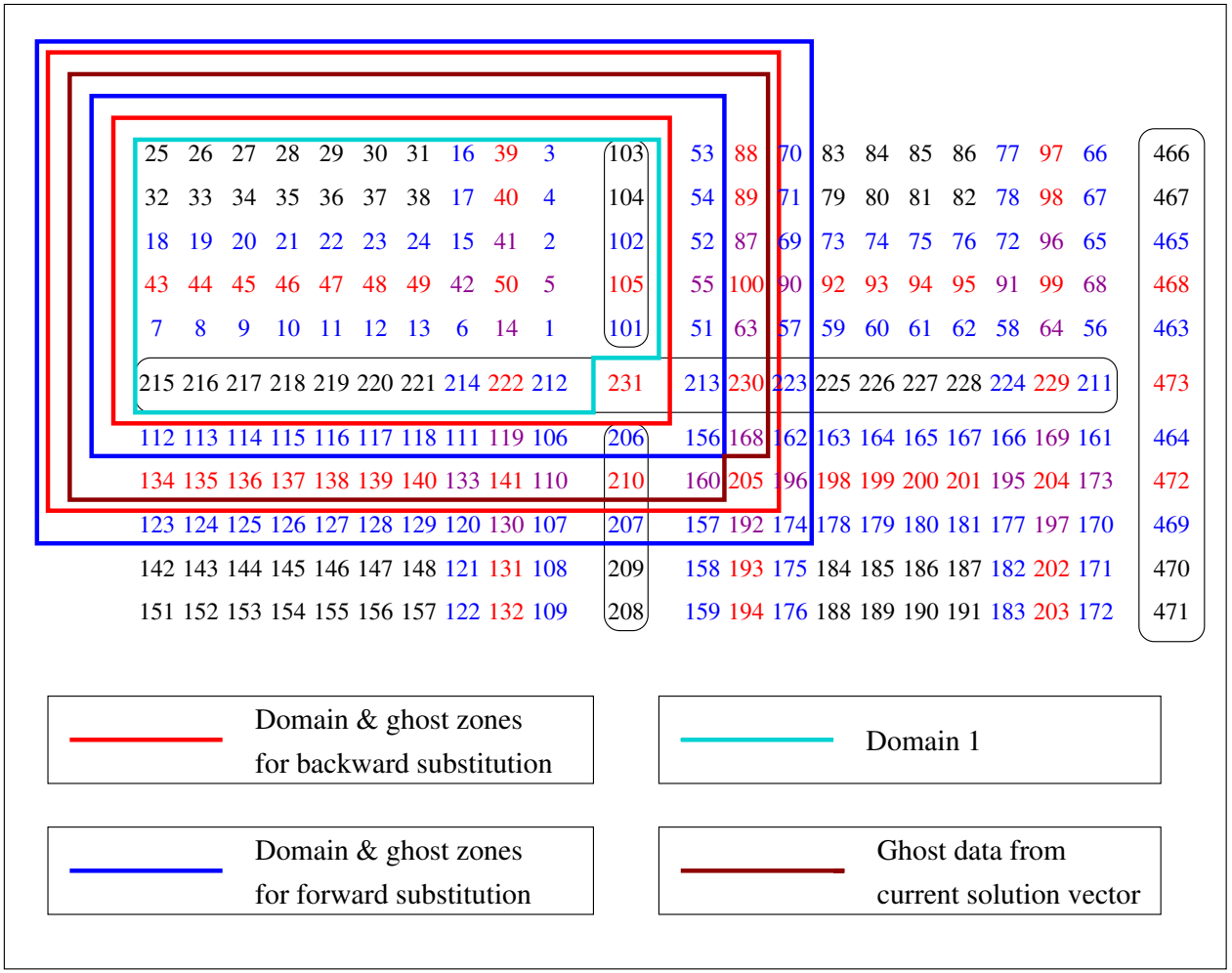
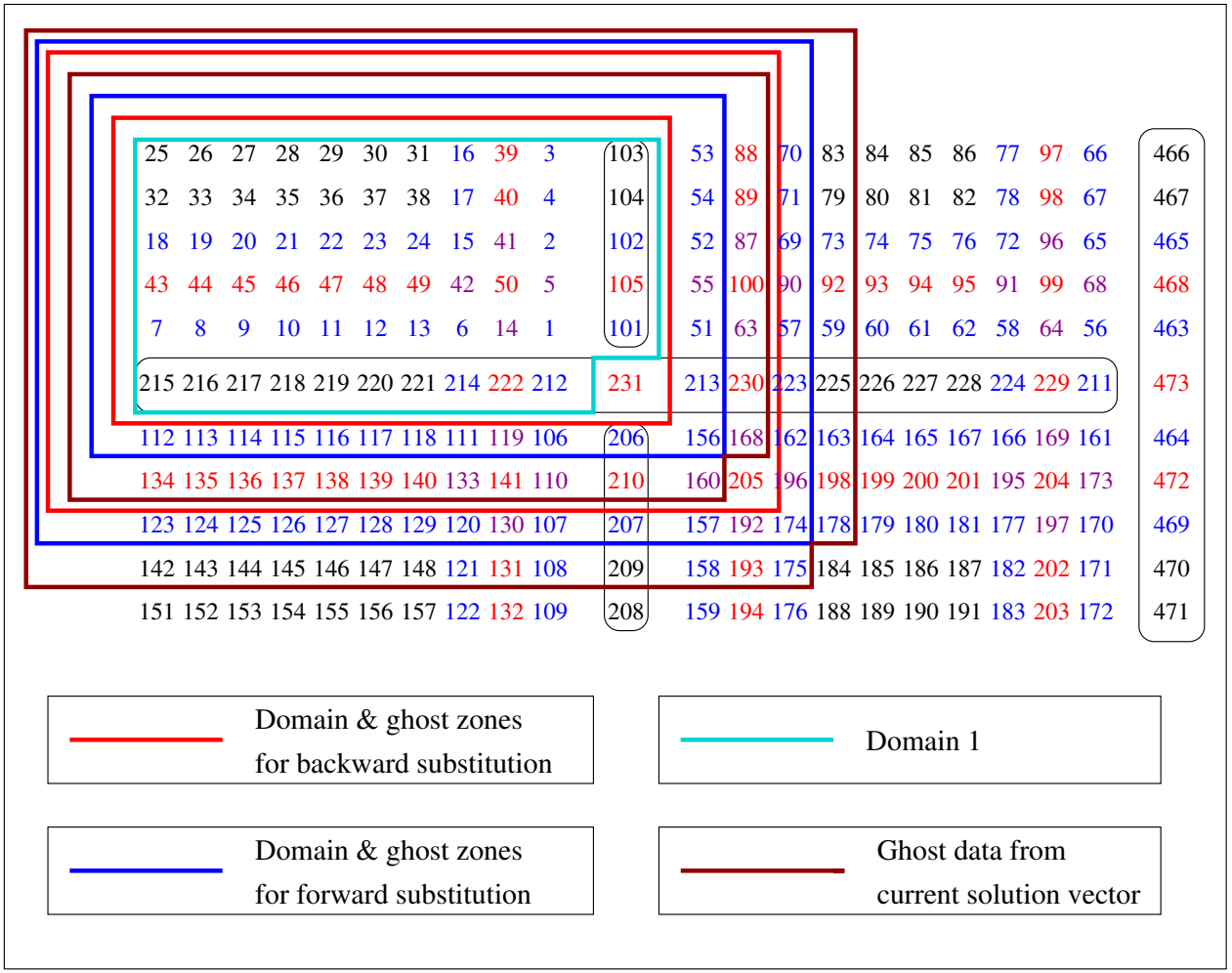


CA-ILU0(s) reordering



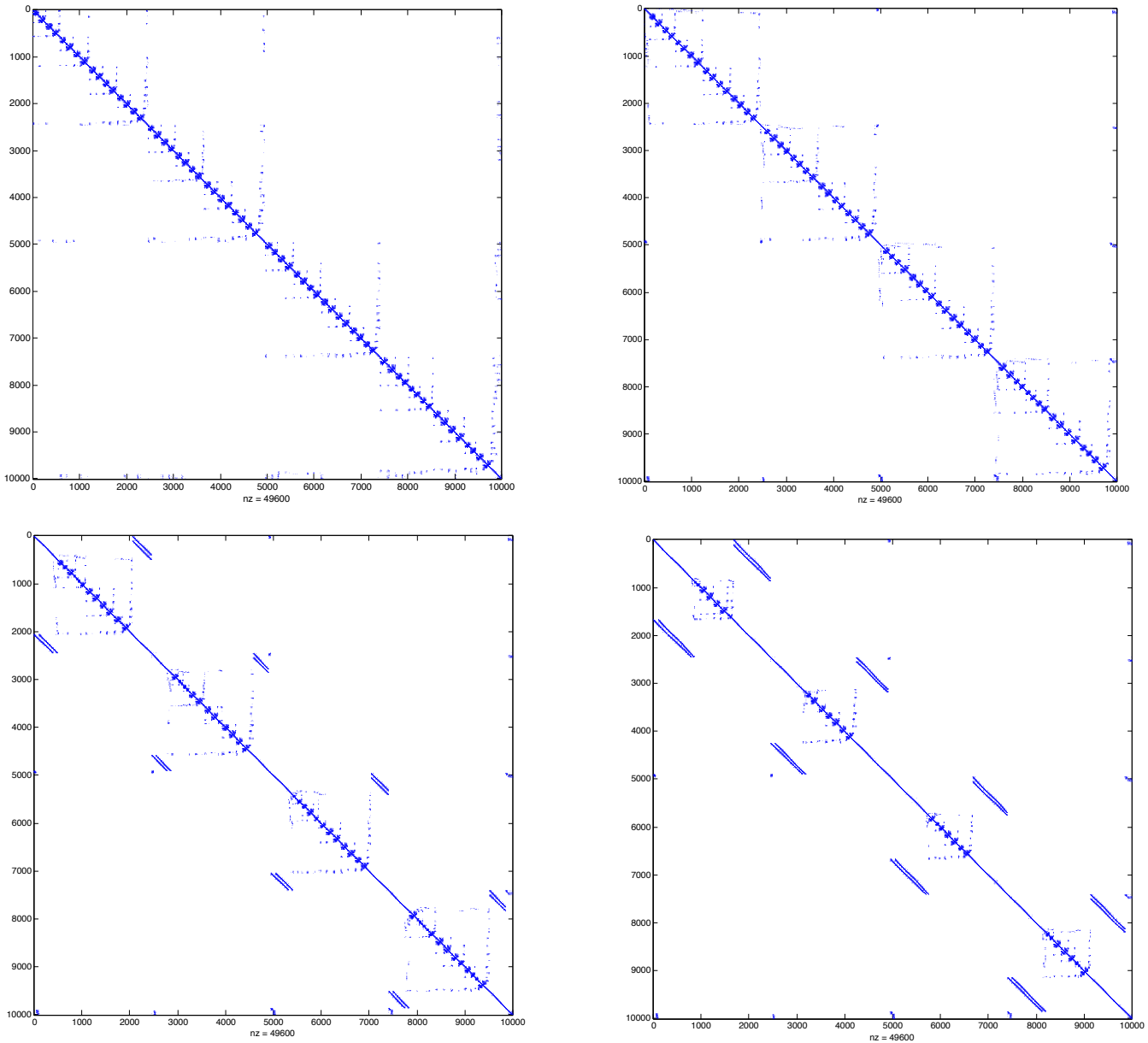


Figure:
Comparison of the sparsity patterns of the ND, CR-ILU0, CA-ILU0(5) and CA-ILU0(10) reordering matrix matvf2DNH100100 of size $10^4 \times 10^4$ with P=4

The complexity of the CA-ILU0(s) reordering

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$$2|D_t(l_{max})| + (3log(P) - 2)|S_{max}(m_{max})|$$

where $D_t(l_{max})$ is the largest subdomain and $S_{max}(m_{max})$ is the largest separator.

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- Thus, our algorithm is of linear complexity.

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4. Each processor i fetches its corresponding $A(\gamma_s, :)$ and $y_0(\delta_s)$
5. Each processor i performs the CA-ILU(0) factorization of $A(\gamma_s, :)$ to obtain the corresponding $L(\gamma_s, :)$ and $U(\gamma_s, :)$ matrices

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5. Each processor i performs the CA-ILU(0) factorization of $A(\gamma_s, :)$ to obtain the corresponding $L(\gamma_s, :)$ and $U(\gamma_s, :)$ matrices
6. Each processor i performs the s multiplications of the form $y_{i+1} = [L(\gamma_{s-i}, \gamma_{s-i})U(\beta_{s-i}, \beta_{s-i})]^{-1} A(\gamma_{s-i}, \delta_{s-i}) y_i(\delta_{s-i})$ using the ILU Matrix Powers Kernel

CA-ILU0 Preconditioner

1. Partitioning the graph of A to obtain P subdomains
2. Each processor is assigned a subdomain and reorders its subdomains in parallel, using the CA-ILU0(s) reordering
3. Then finds the redundant/ghost data that it needs
4. Each processor i fetches its corresponding $A(\gamma_s, :)$ and $y_0(\delta_s)$
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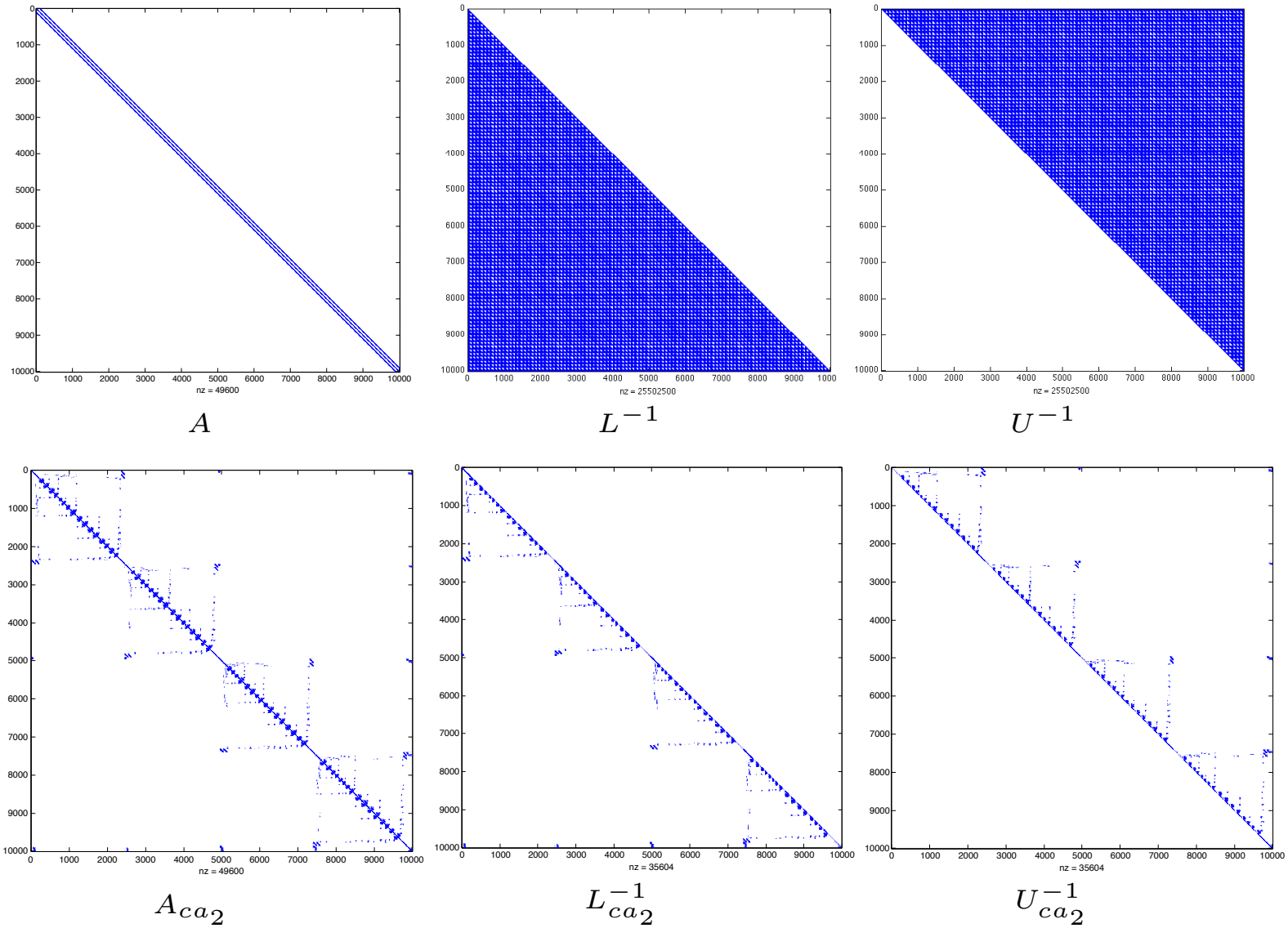
7. The processors communicate to fetch the needed data to proceed with the CA-GMRES algorithm
8. If the method hasn't converged, then each processor fetches $y_s(\delta_s)$ and performs step 6 and on.

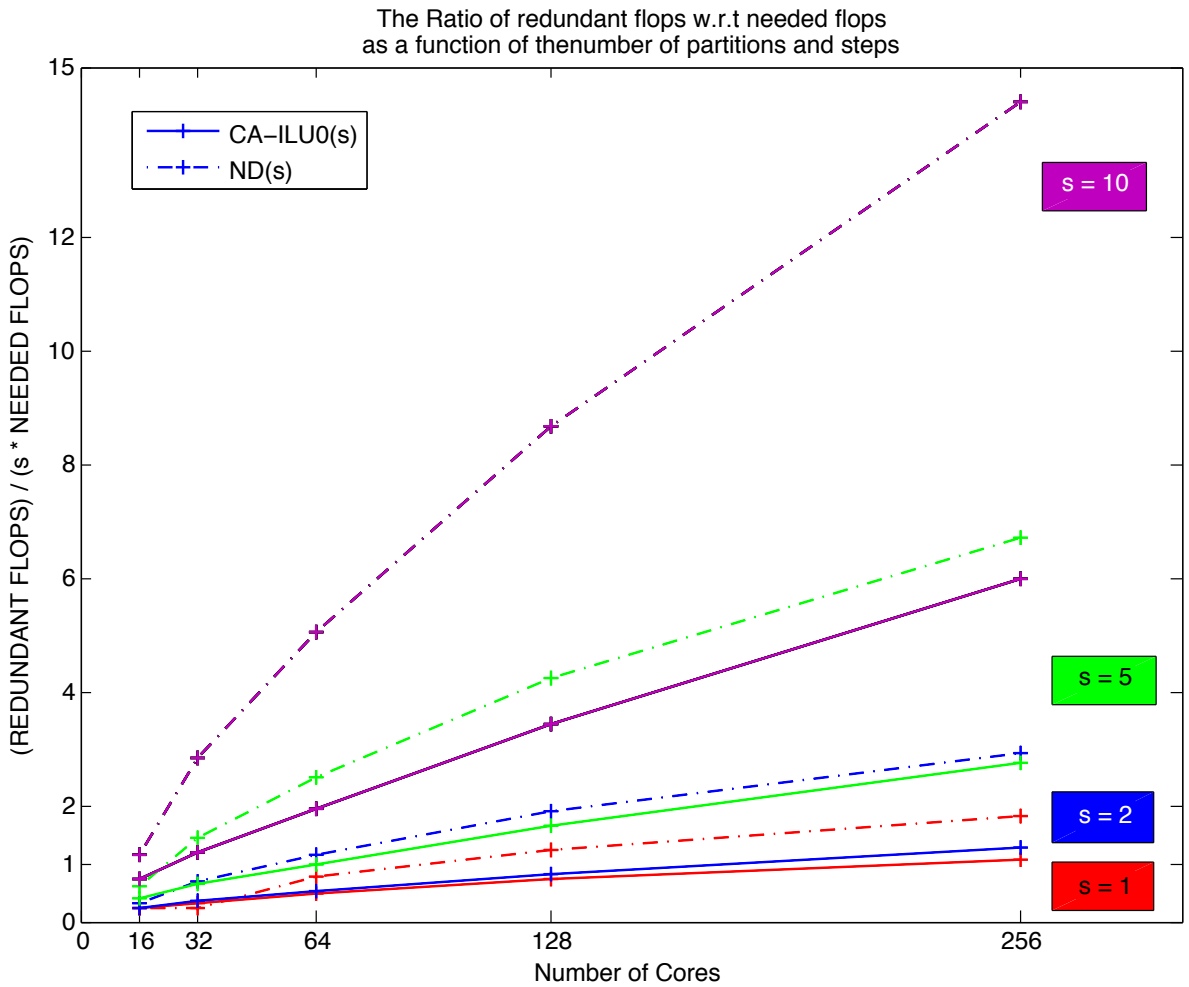


A L^{-1} U^{-1}

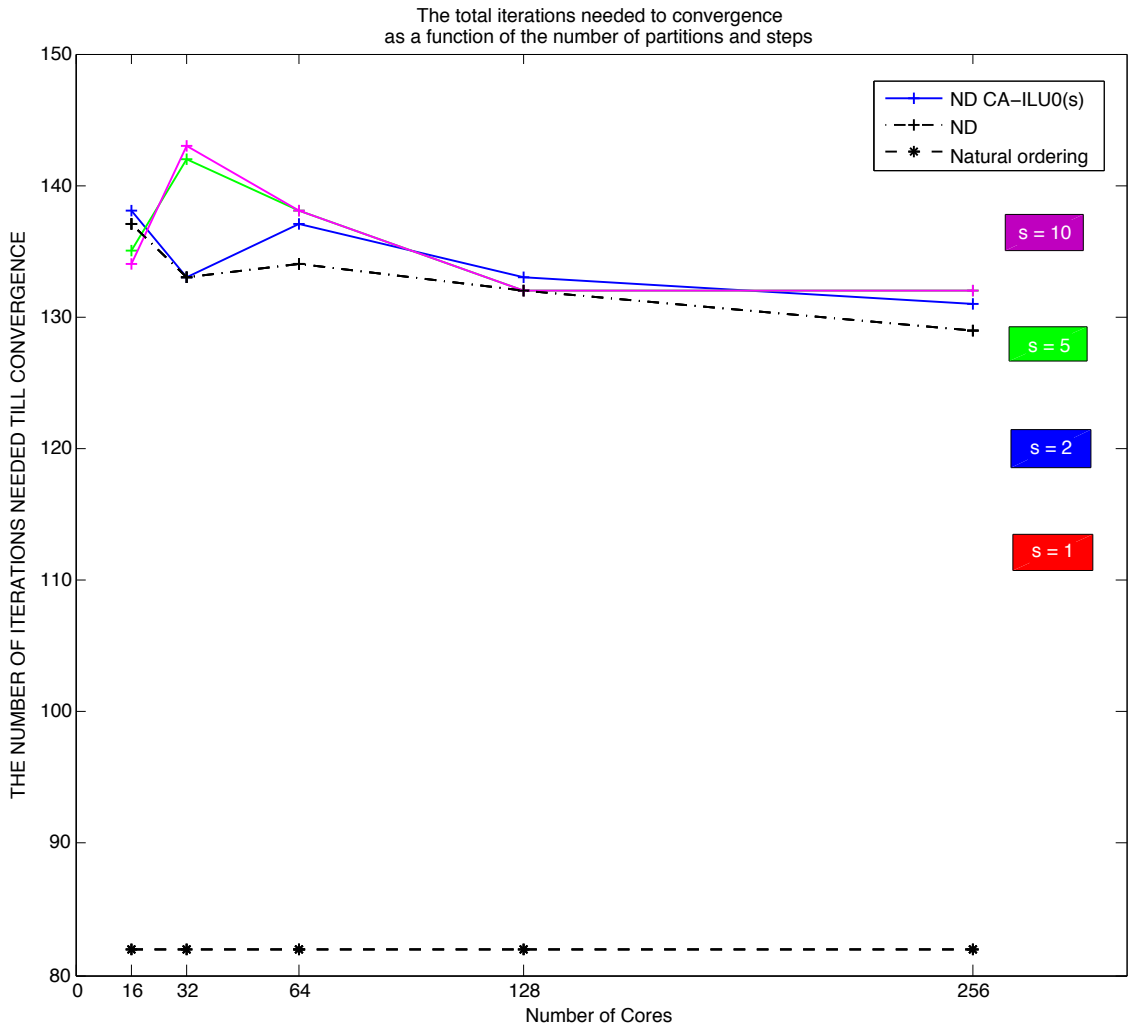
A_{ca_2} $L^{-1}_{ca_2}$ $U^{-1}_{ca_2}$

Figure: The fill-ins in the ILU(0) factorization of a 2D matrix A and its CA-ILU0(2) reordered version A_{ca}

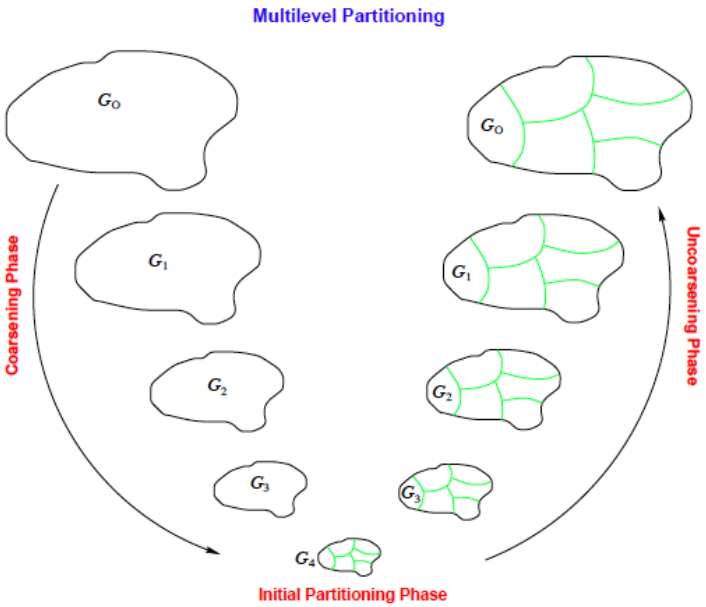
Redundant Flops in ILU-Matrix Powers Kernel



The effect of reordering A on GMRES's Convergence



k-way Partitioning

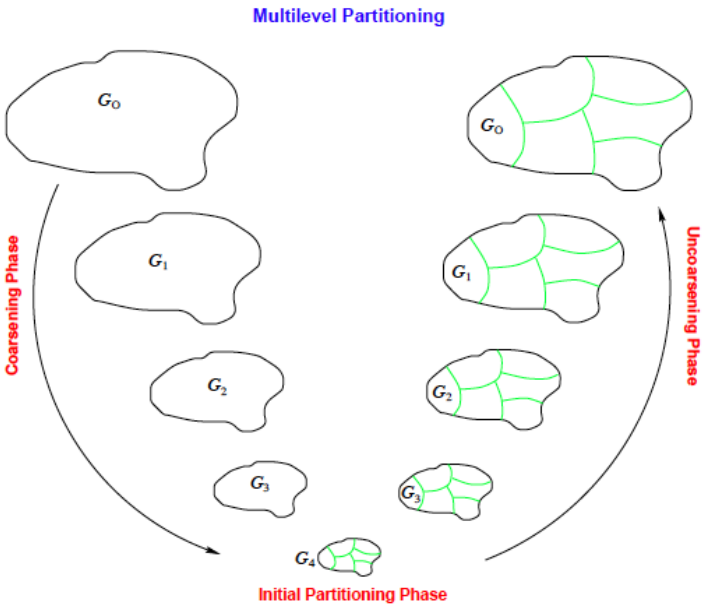


Source: METIS 5.0 Manual

The three phases of multilevel k-way graph partitioning:

- The coarsening phase: the size of the graph is successively decreased

k-way Partitioning



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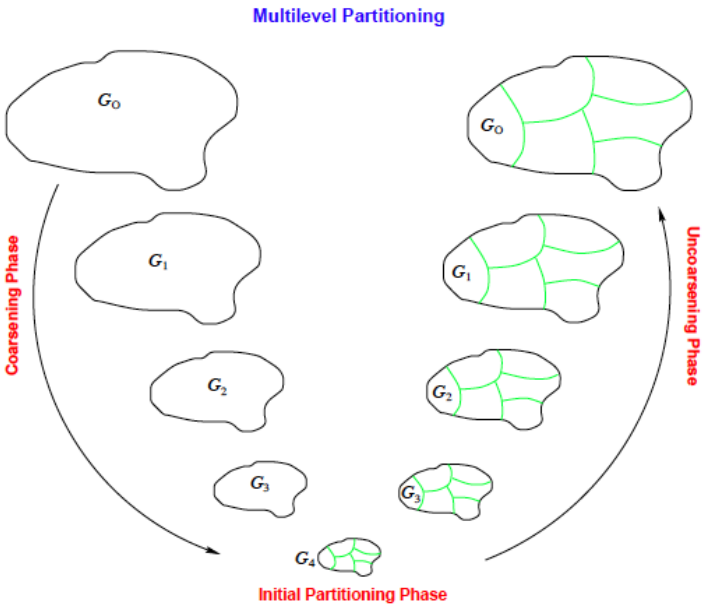

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CR-ILU0 reordering

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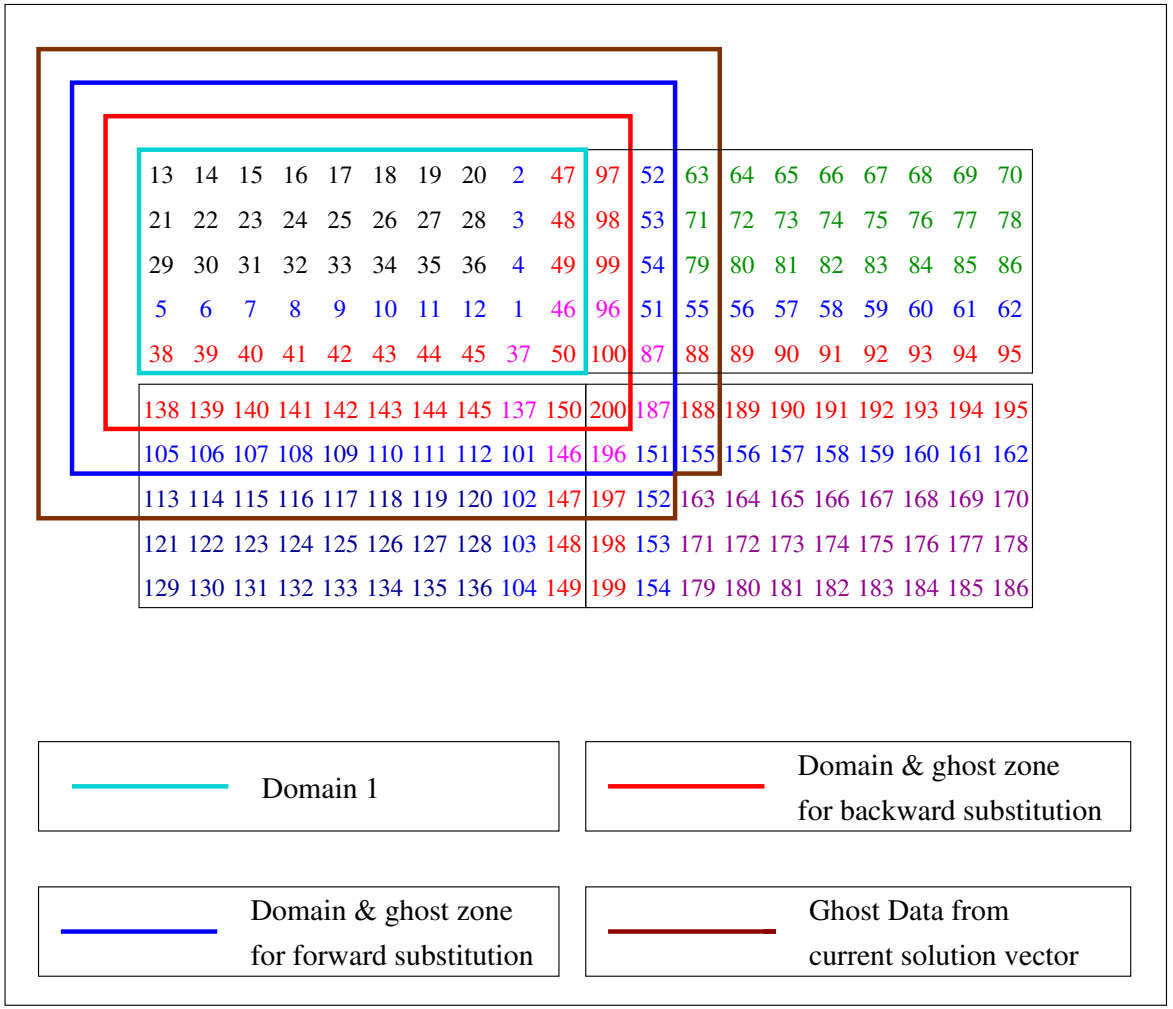

CA-ILU0(s) reordering

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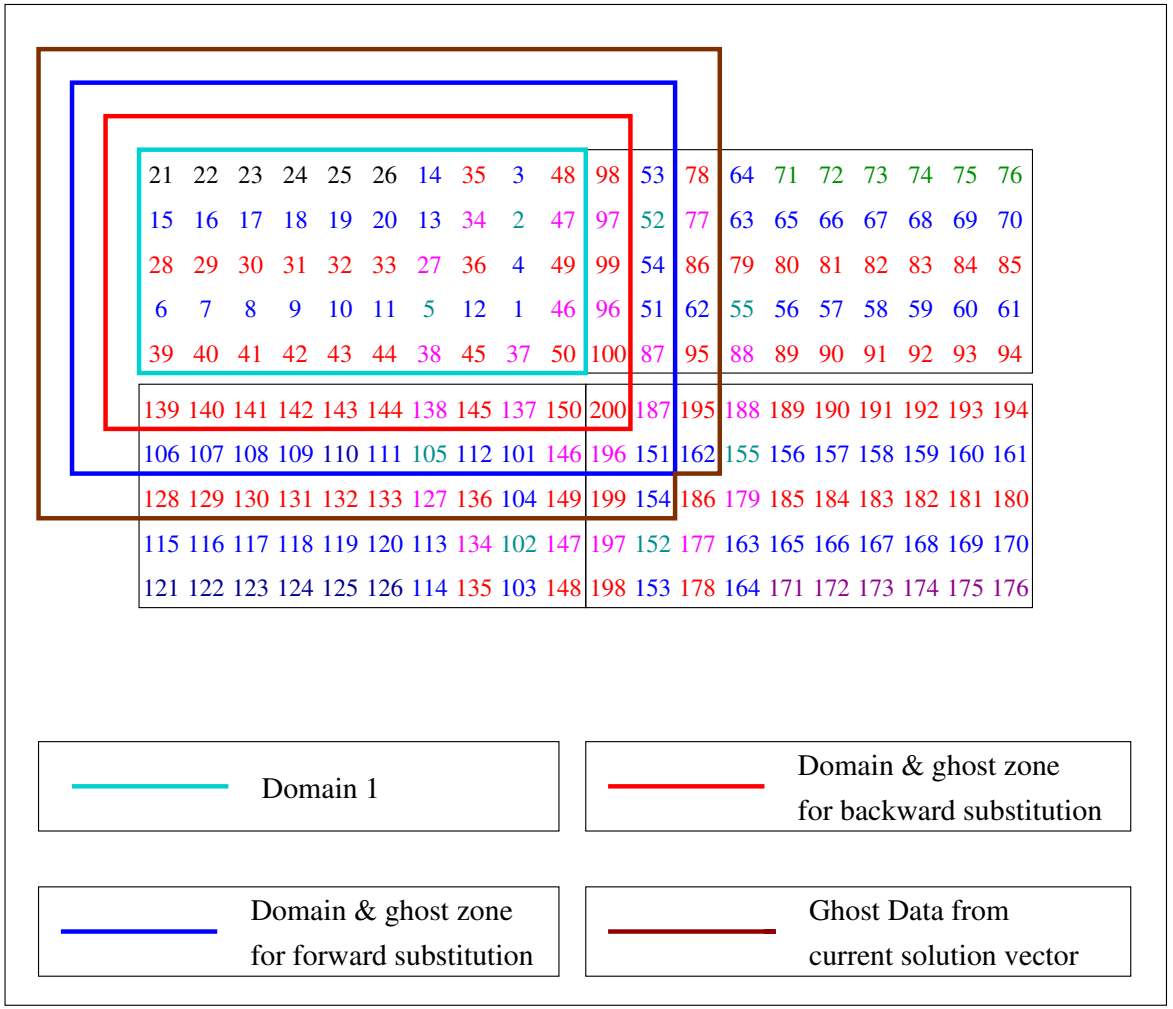

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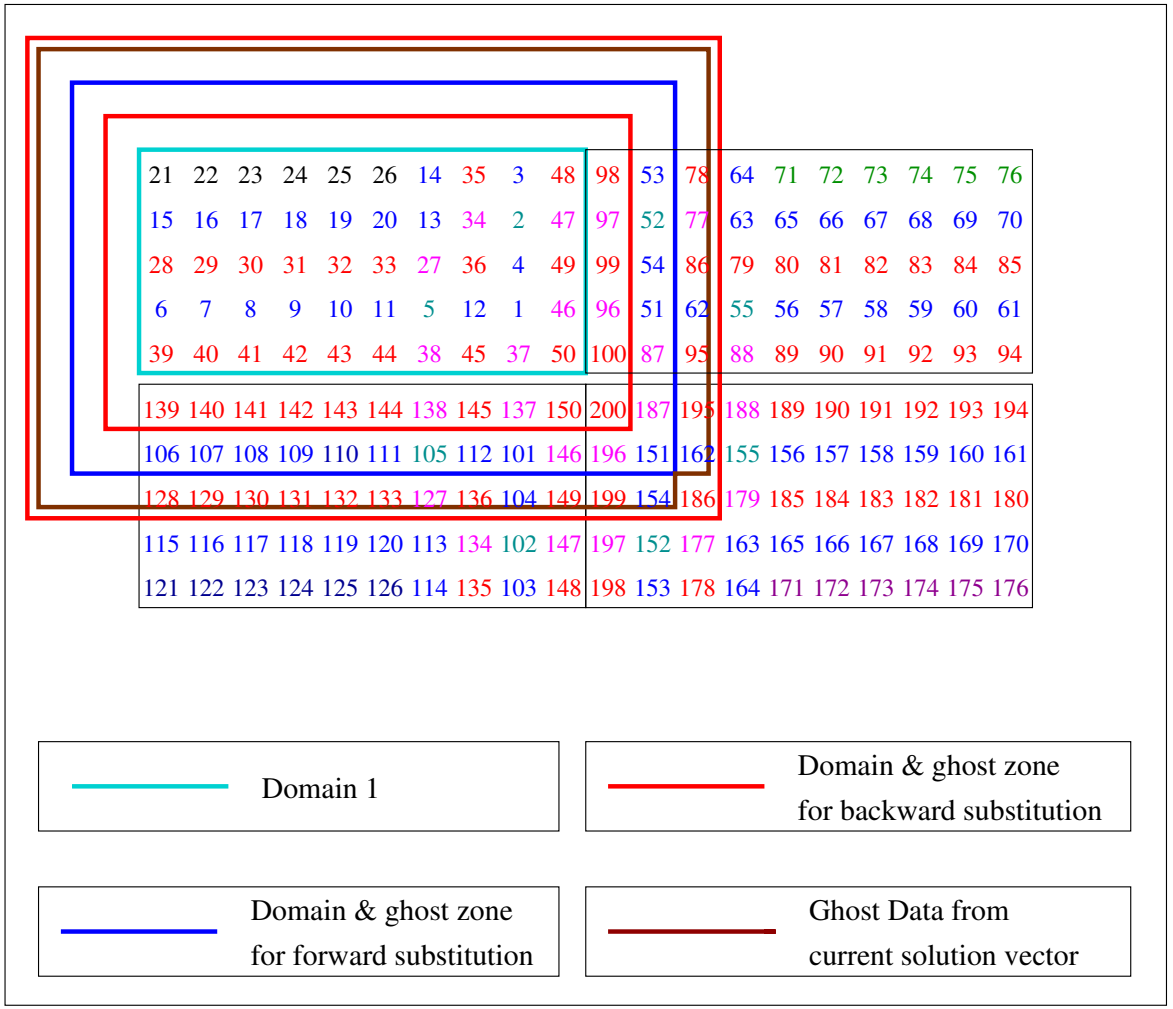

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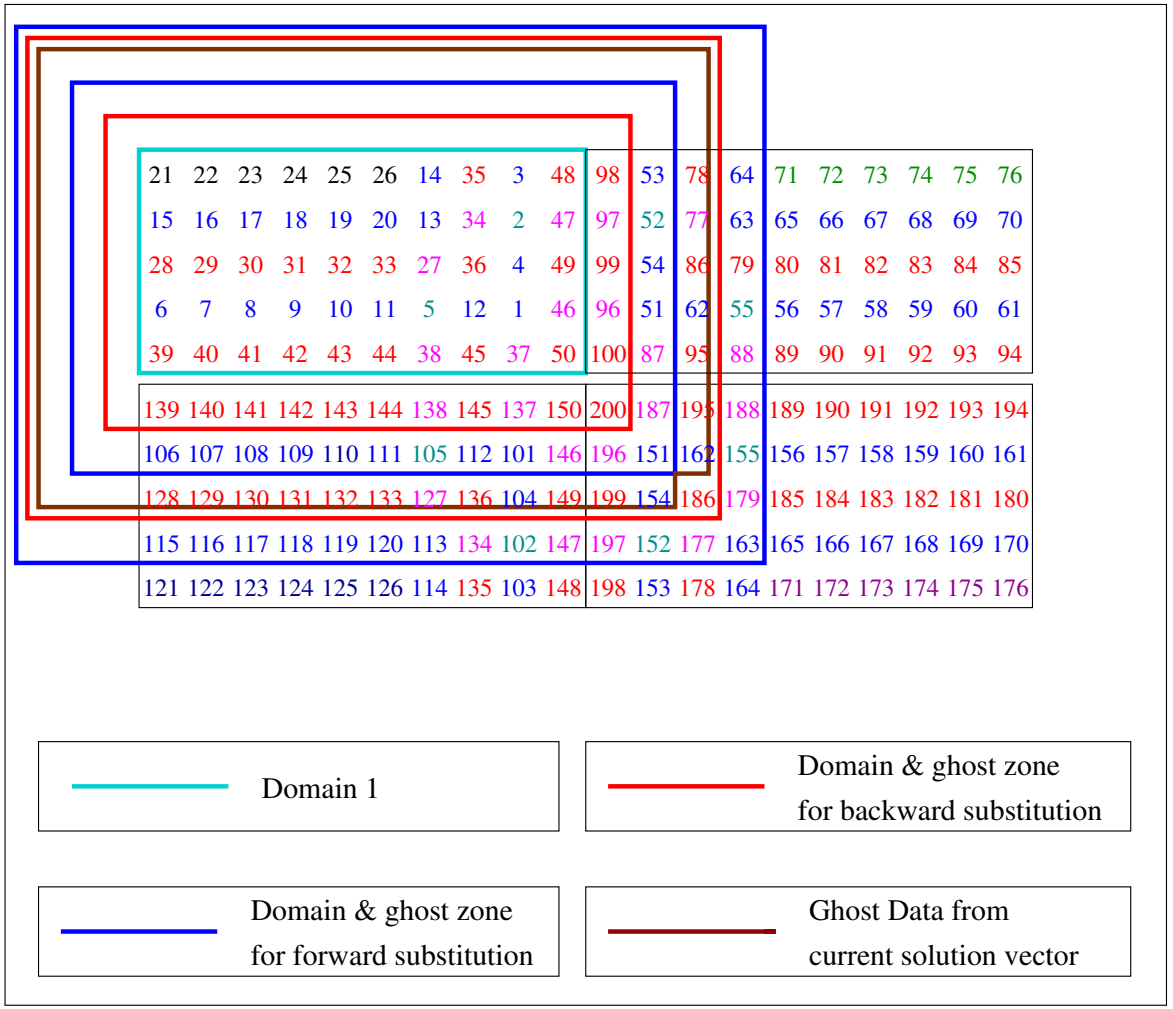

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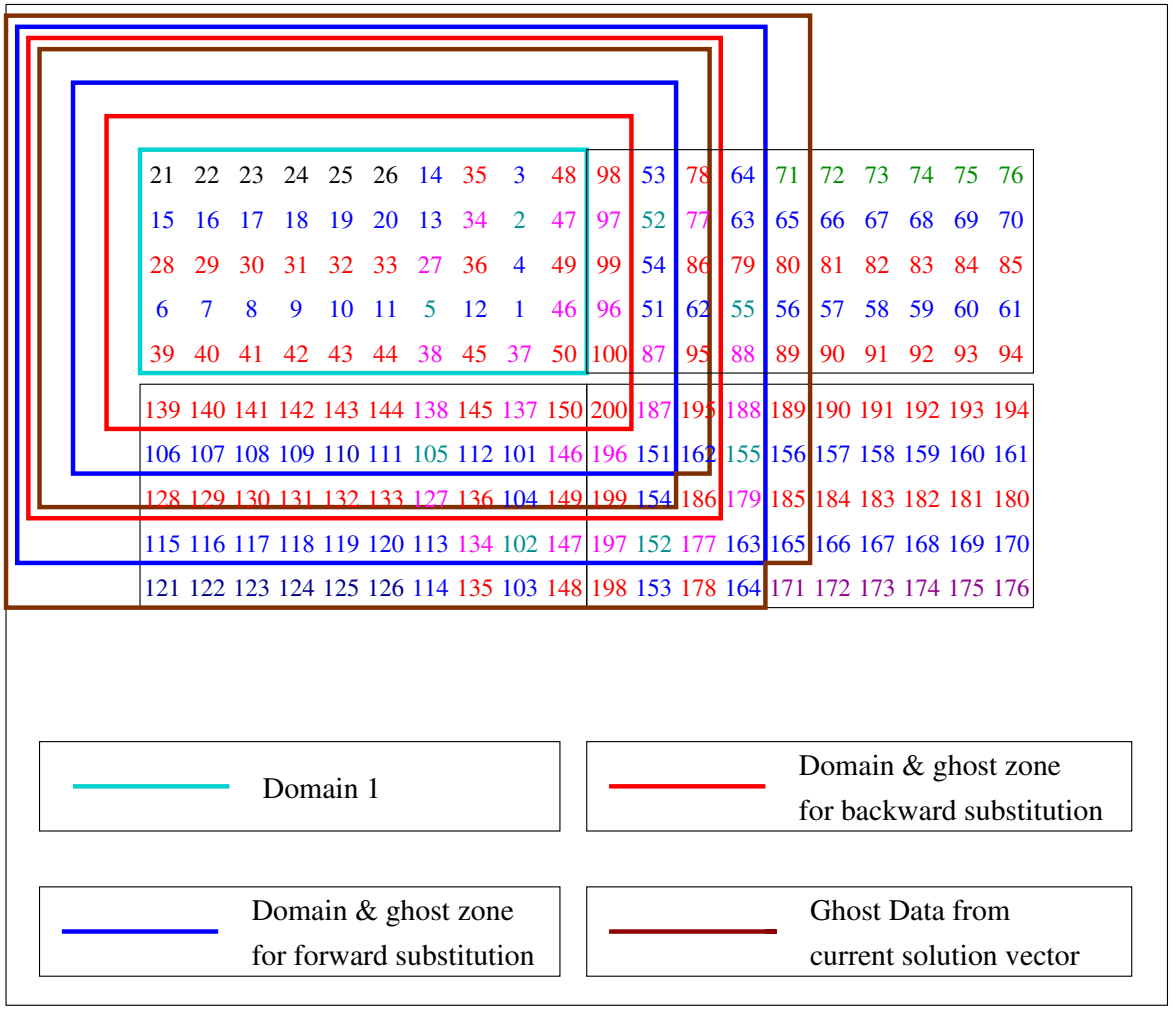


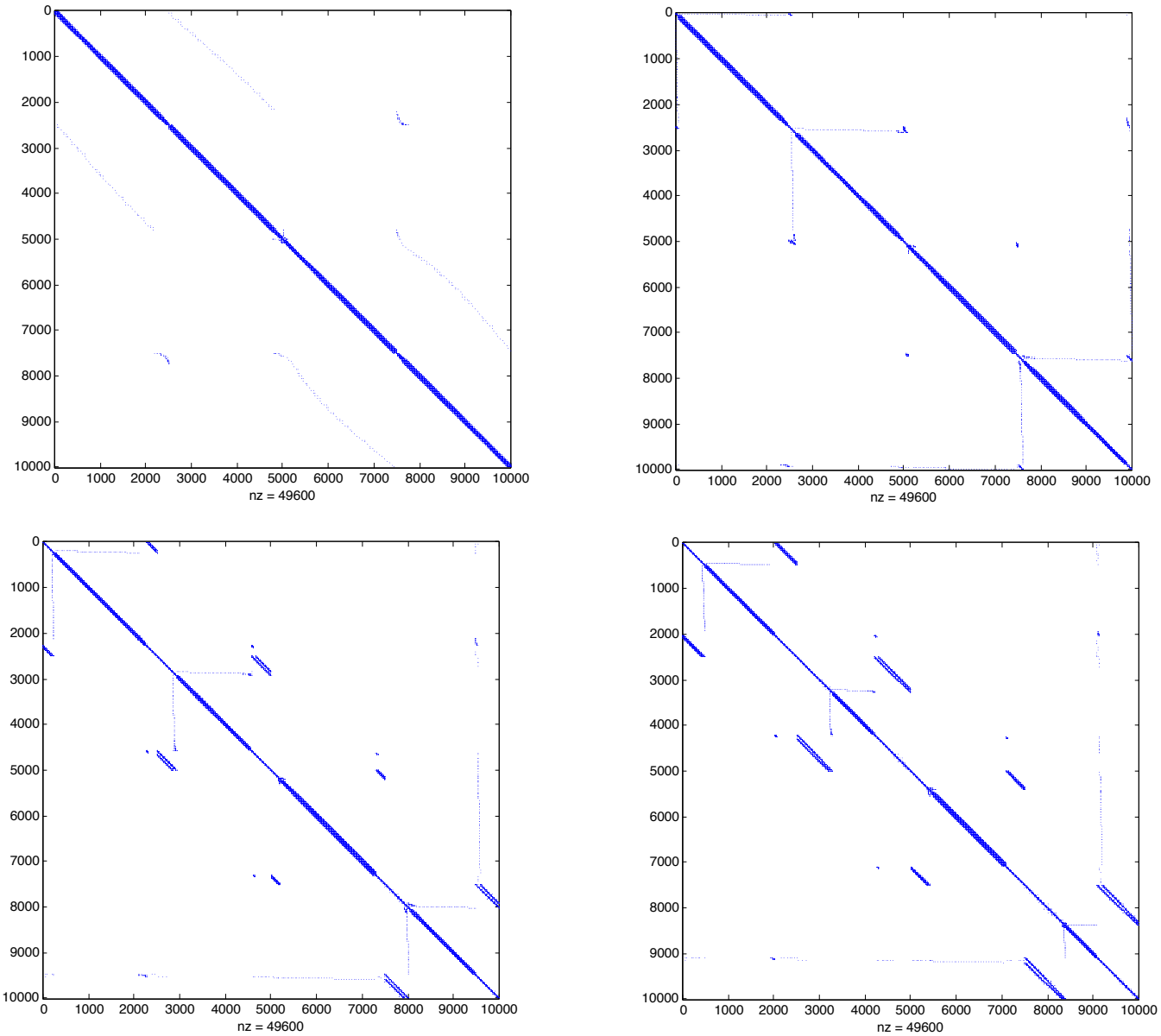
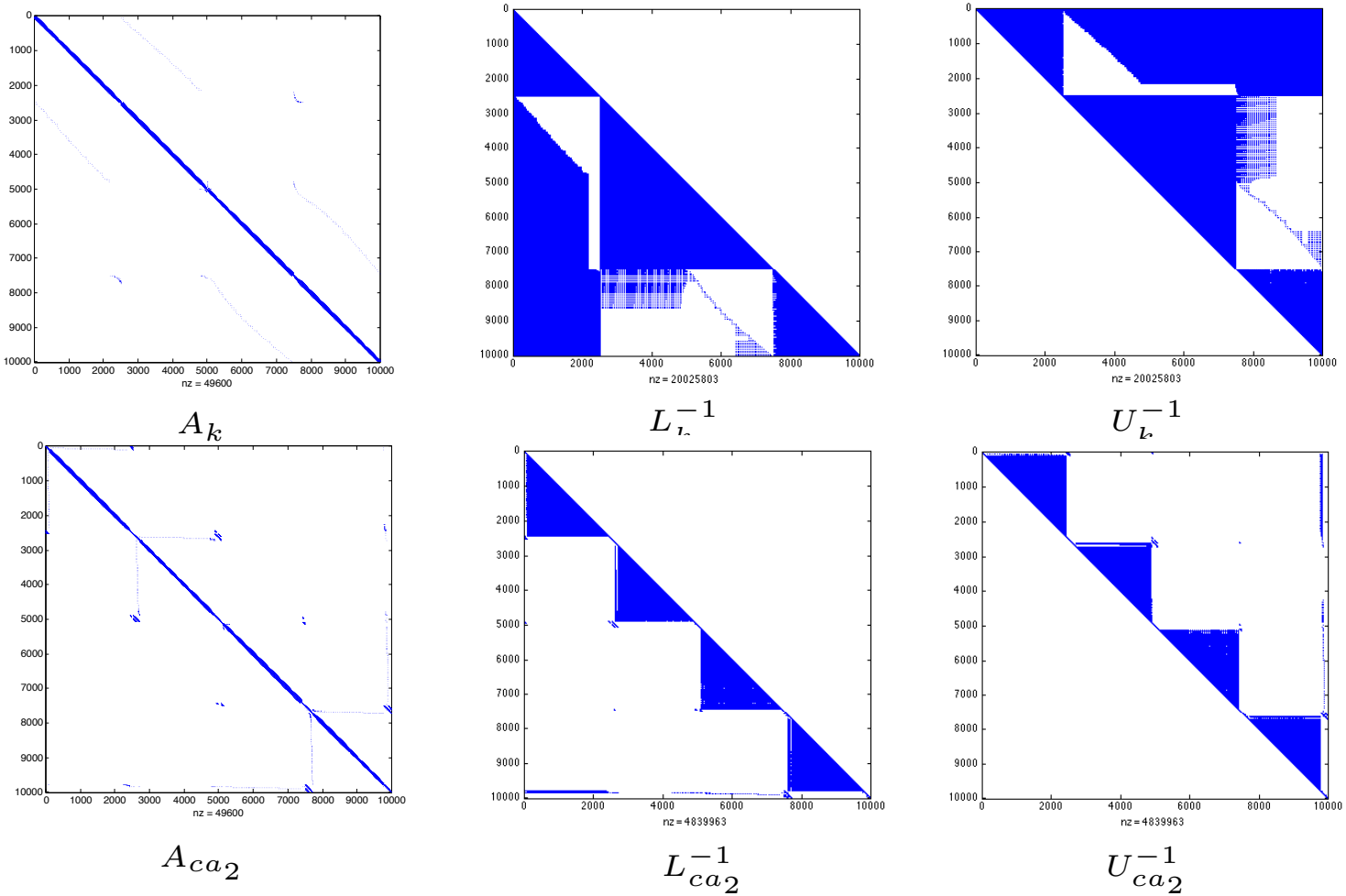


Figure:
Comparison of the sparsity patterns of the k-way, CR-ILU0, CA-ILU0(5) and CA-ILU0(10) reordered matrix matvf2DNH100100 of size $10^4 \times 10^4$ with P=4



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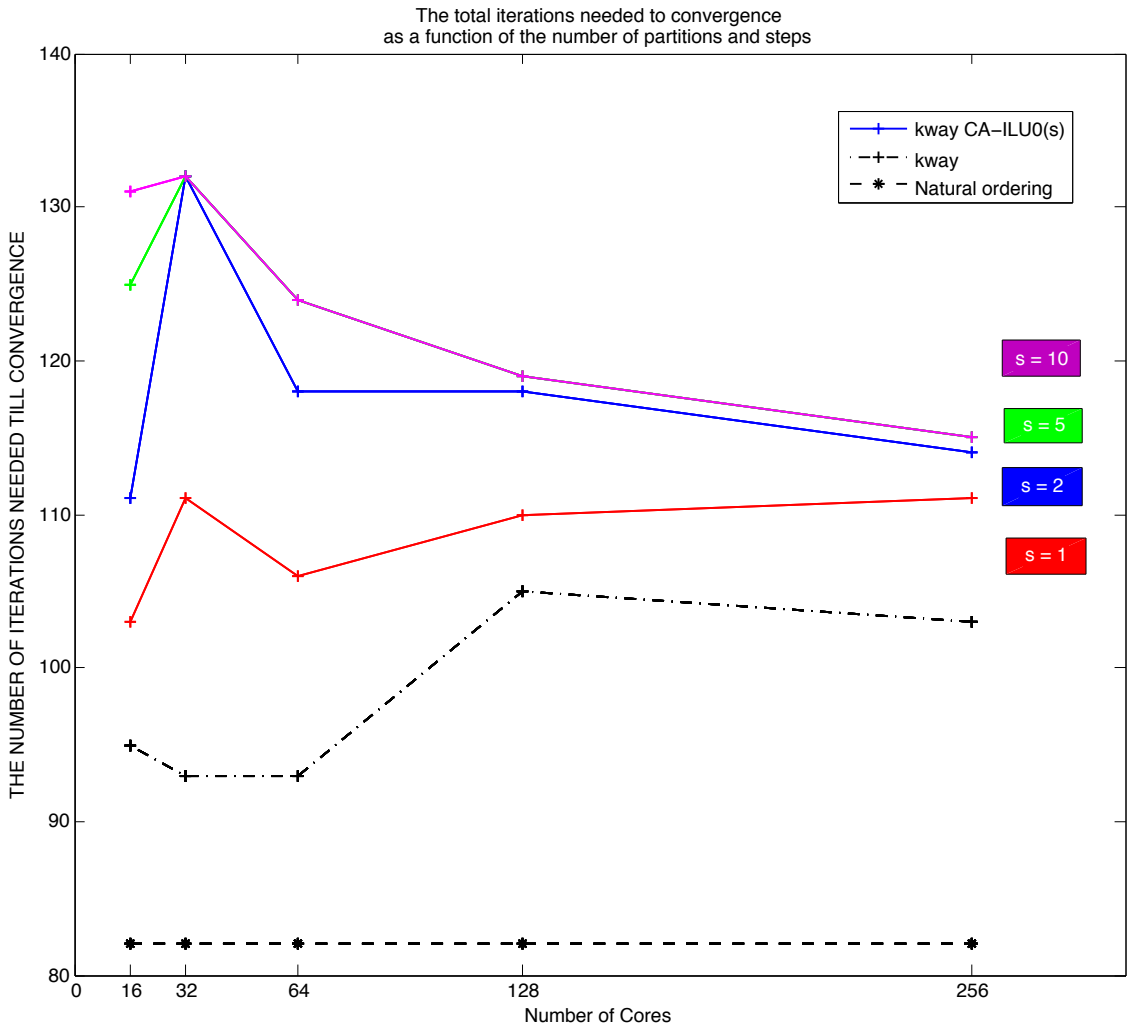
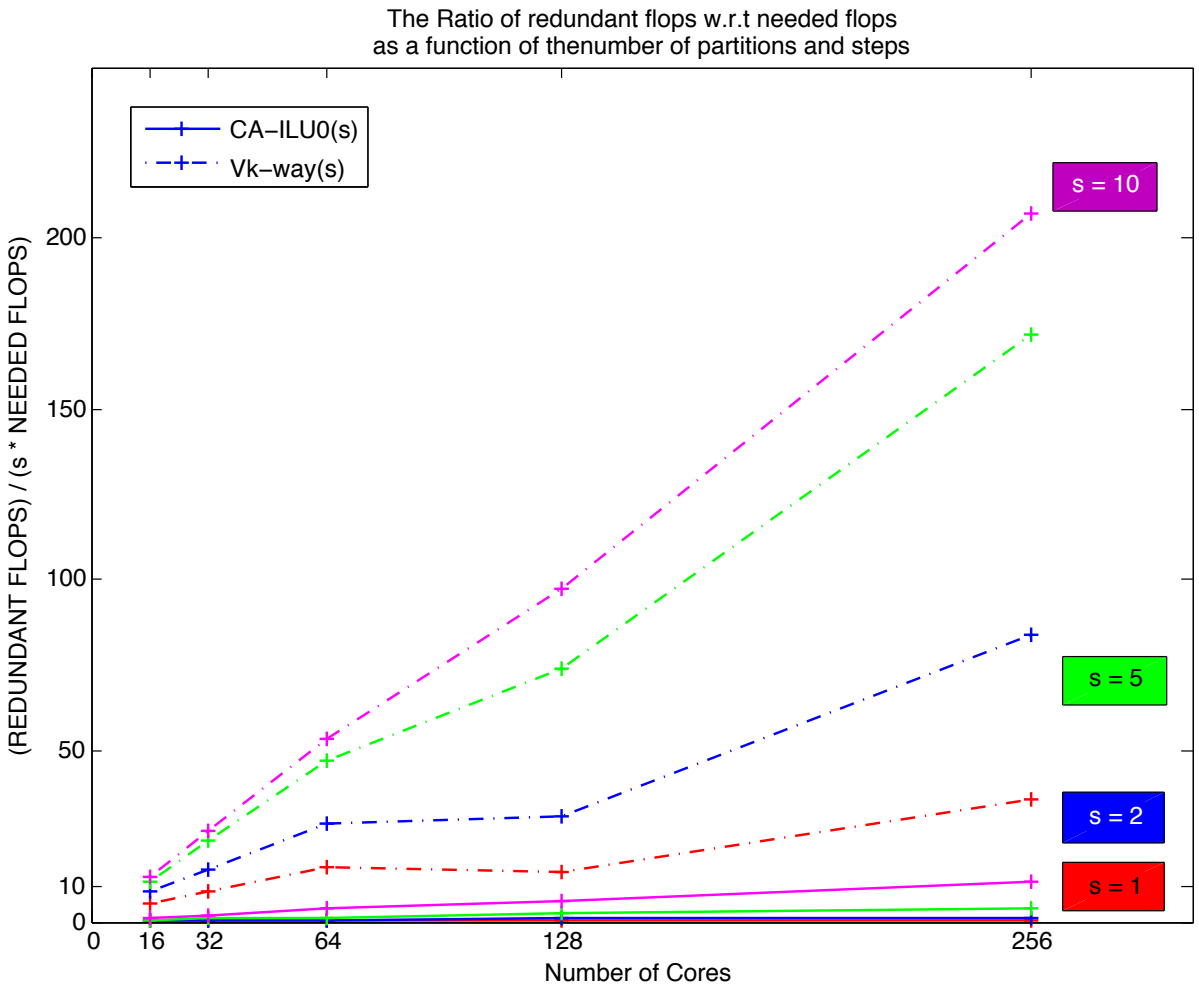


Redundant Flops in ILU-Matrix Powers Kernel



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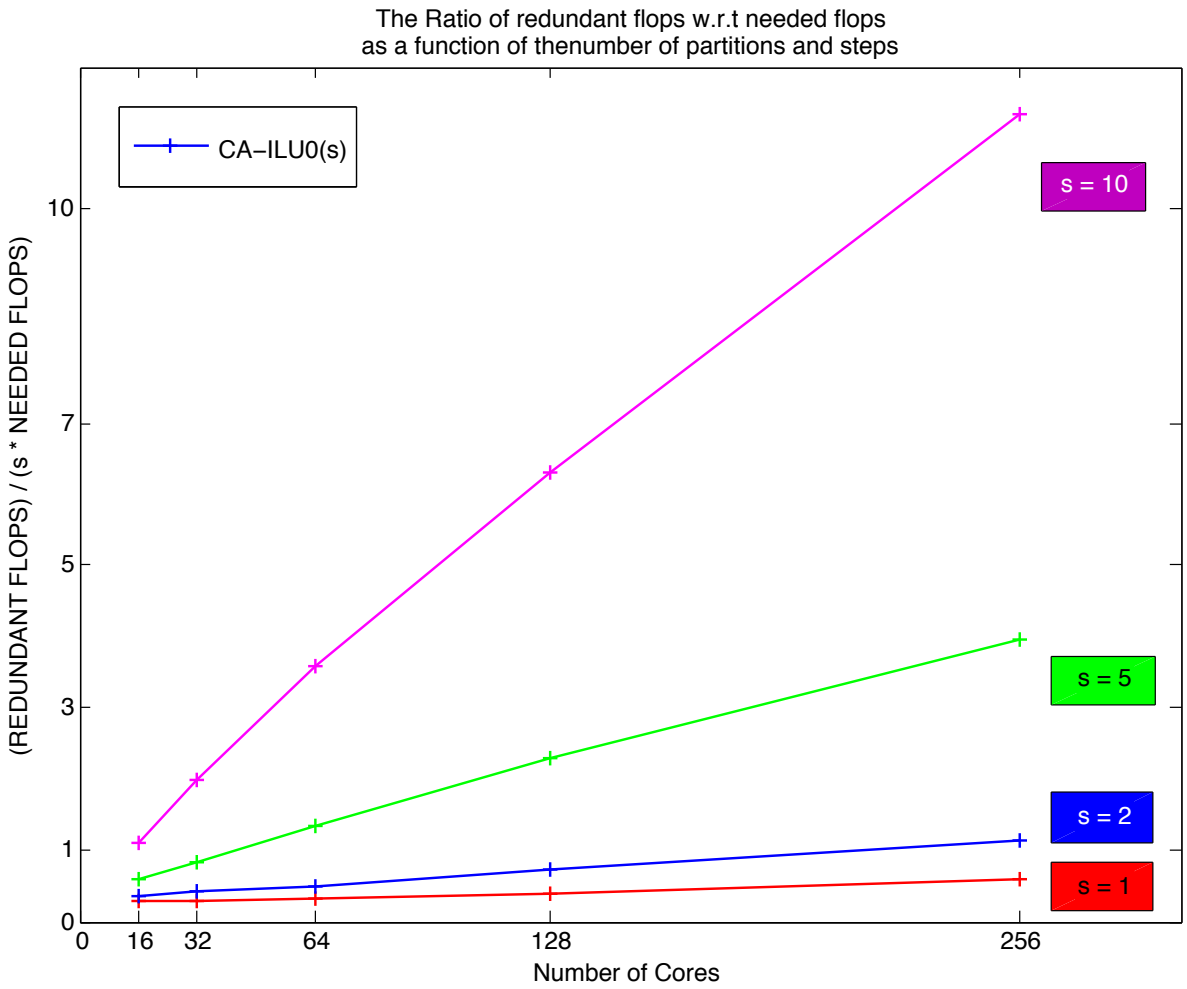

Conclusion

In this talk we have presented:

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Current and Future Work

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Thank you!