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A tutorial on:
Iterative methods for Sparse Matrix Problems

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CRM Montreal - May 2, 2008

Outline

Part 1

- Sparse matrices and sparsity
- Basic iterative techniques
- Projection methods
- Krylov subspace methods

Part 2

- Preconditioned iterations
- Preconditioning techniques

Part 3

- Parallel implementations
- Multigrid methods

Part 4

- Eigenvalue problems
- Applications

MULTILEVEL PRECONDITIONING

Independent set orderings & ILUM (Background)

Independent set orderings permute a matrix into the form

$$\begin{pmatrix} B & F \\ E & C \end{pmatrix}$$

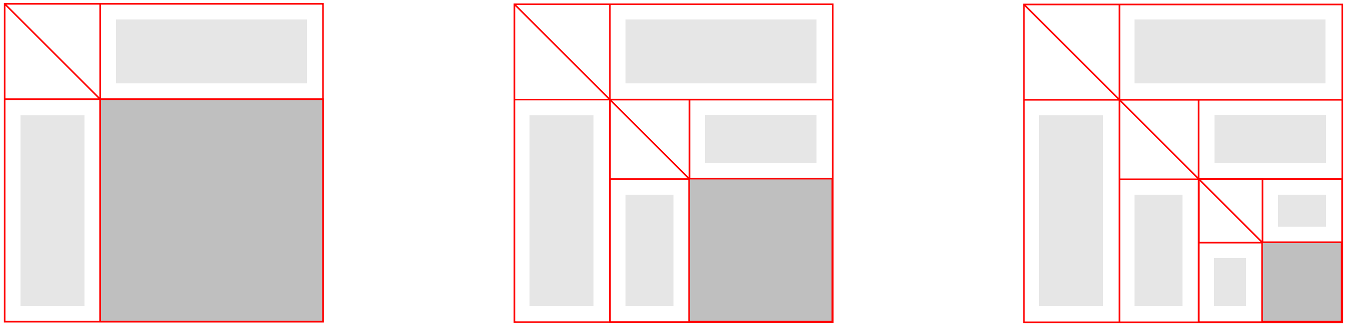
where B is a diagonal matrix.

- Unknowns associated with the B block form an independent set (IS).
- IS is maximal if it cannot be augmented by other nodes to form another IS.
- IS ordering can be viewed as a “simplification” of multicoloring

Main observation: Reduced system obtained by eliminating the unknowns associated with the IS, is still sparse since its coefficient matrix is the Schur complement

$$S = C - EB^{-1}F$$

- Idea: apply IS set reduction recursively.
- When reduced system small enough solve by any method
- Can devise an ILU factorization based on this strategy.



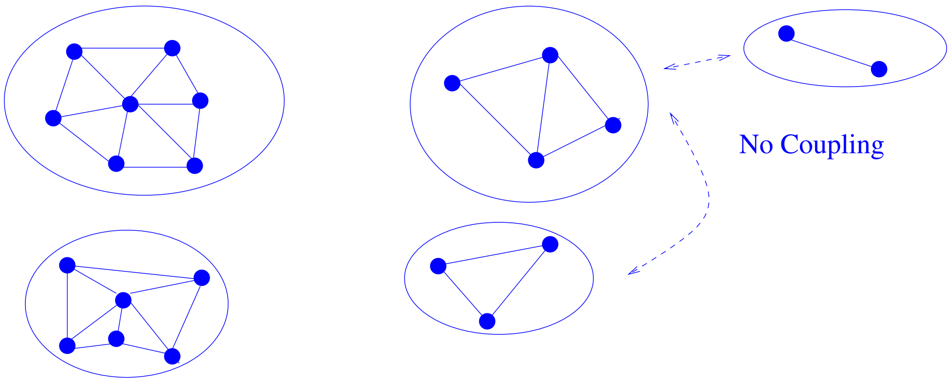
- See work by [Botta-Wubbs '96, '97, YS'94, '96, (ILUM), Leuze '89, ..]

Group Independent Sets / Aggregates

➤ Generalizes (common) Independent Sets

Main goal: to improve robustness

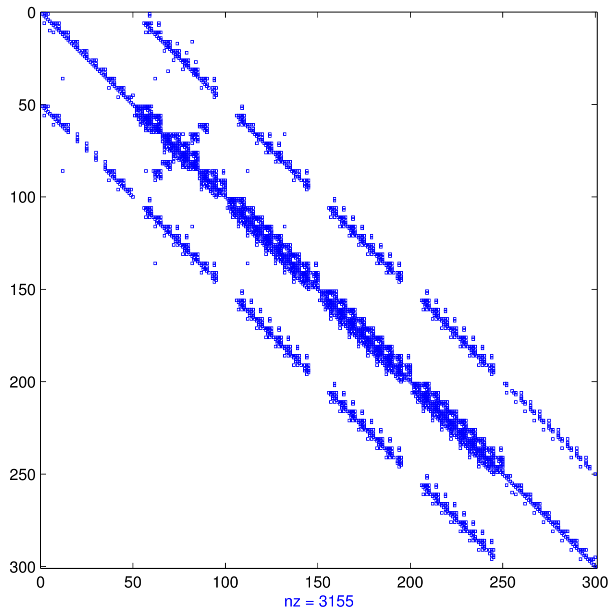
Main idea: use independent sets of "cliques", or "aggregates". There is no coupling between the aggregates.

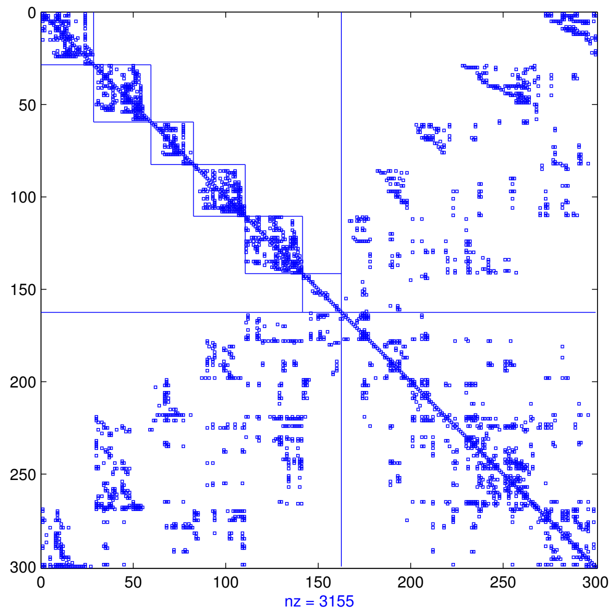


➤ Reorder equations so nodes of independent sets come first

Algebraic Recursive Multilevel Solver (ARMS)

Original matrix, A , and reordered matrix, $A_0 = P_0^T A P_0$.



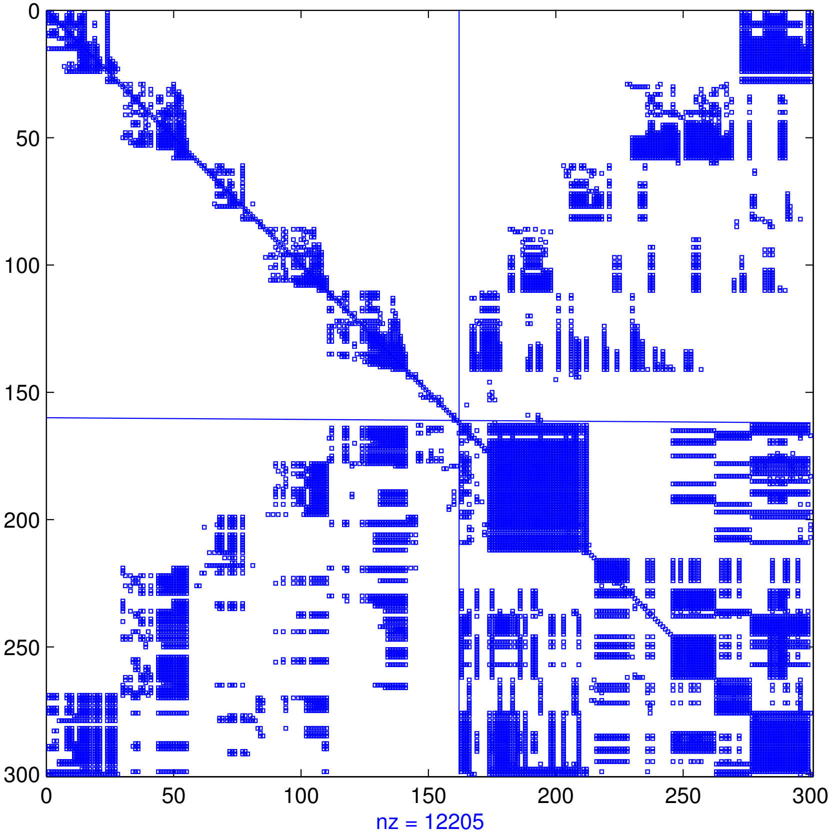


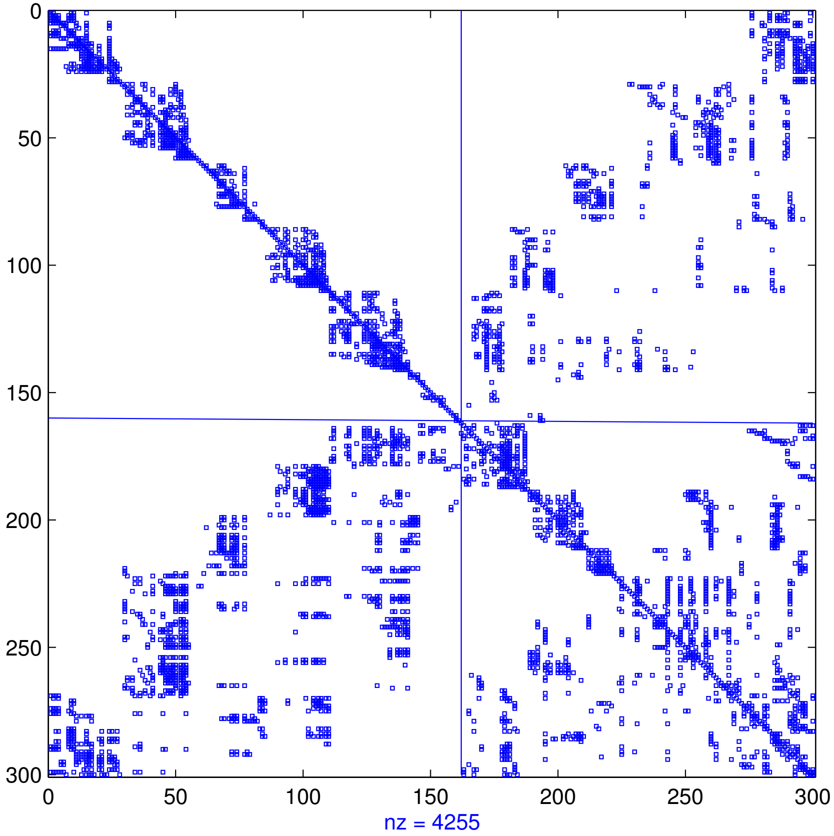
➤ **Block ILU factorization of A_l**

$$\begin{pmatrix} B_l & F_l \\ E_l & C_l \end{pmatrix} \approx \begin{pmatrix} L_l & 0 \\ E_l U_l^{-1} & I \end{pmatrix} \begin{pmatrix} I & 0 \\ 0 & A_{l+1} \end{pmatrix} \begin{pmatrix} U_l & L_l^{-1} F_l \\ 0 & I \end{pmatrix}$$

➤ **Diagonal blocks treated as sparse**

Problem: Fill-in | **Remedy: dropping strategy**





➤ **Next step: treat the Schur complement recursively**

Algebraic Recursive Multilevel Solver (ARMS)

Basic step:

$$\begin{pmatrix} B & F \\ E & C \end{pmatrix} \begin{pmatrix} y \\ z \end{pmatrix} = \begin{pmatrix} f \\ g \end{pmatrix} \qquad \to$$

$$\begin{pmatrix} L & 0 \\ EU^{-1} & I \end{pmatrix} \times \begin{pmatrix} U & L^{-1}F \\ 0 & S \end{pmatrix} \begin{pmatrix} y \\ z \end{pmatrix} = \begin{pmatrix} f \\ g \end{pmatrix}$$

where $S = C - EB^{-1}F$ = Schur complement.

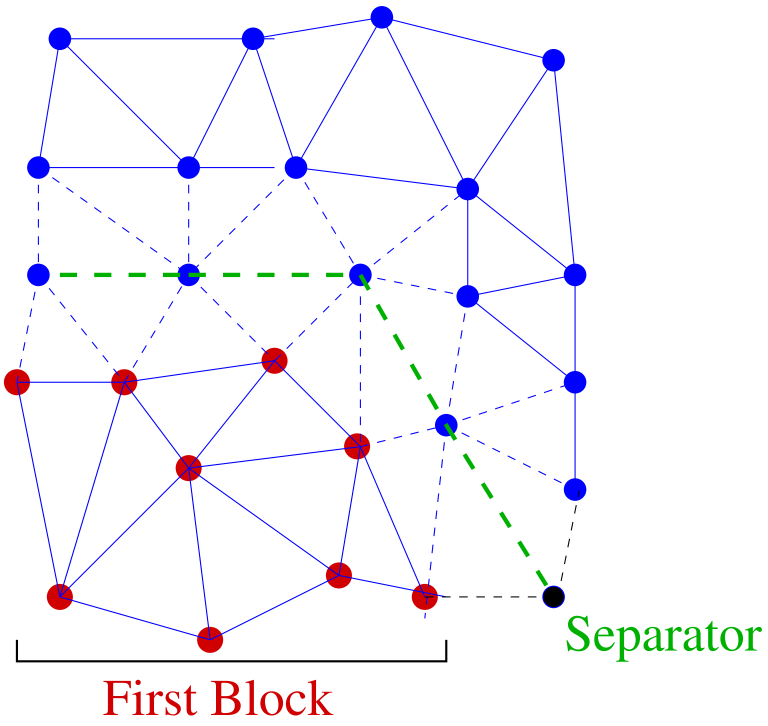
- **Perform block factorization recursively on S**
- **L, U Blocks: sparse**
- **Exploit recursivity**

Factorization: at level l $\quad P_l^T A_l P_l =$

$$\begin{pmatrix} B_l & F_l \\ E_l & C_l \end{pmatrix} \approx \begin{pmatrix} L_l & 0 \\ E_l U_l^{-1} & I \end{pmatrix} \begin{pmatrix} I & 0 \\ 0 & A_{l+1} \end{pmatrix} \begin{pmatrix} U_l & L_l^{-1} F_l \\ 0 & I \end{pmatrix}$$

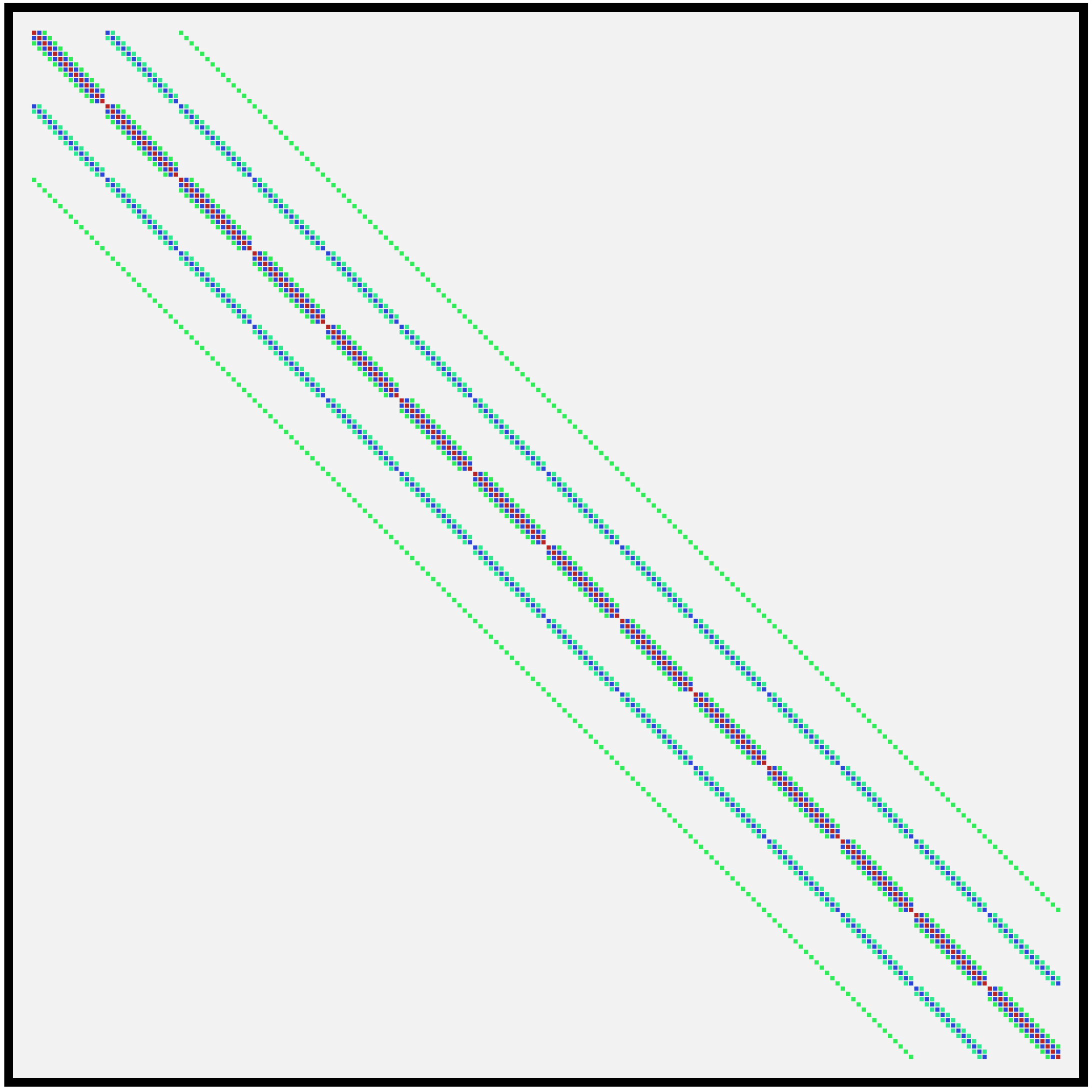
- L-solve $\sim$ restriction. U-solve $\sim$ prolongation.
- Solve Last level system with, e.g., ILUT+GMRES

Group Independent Set reordering

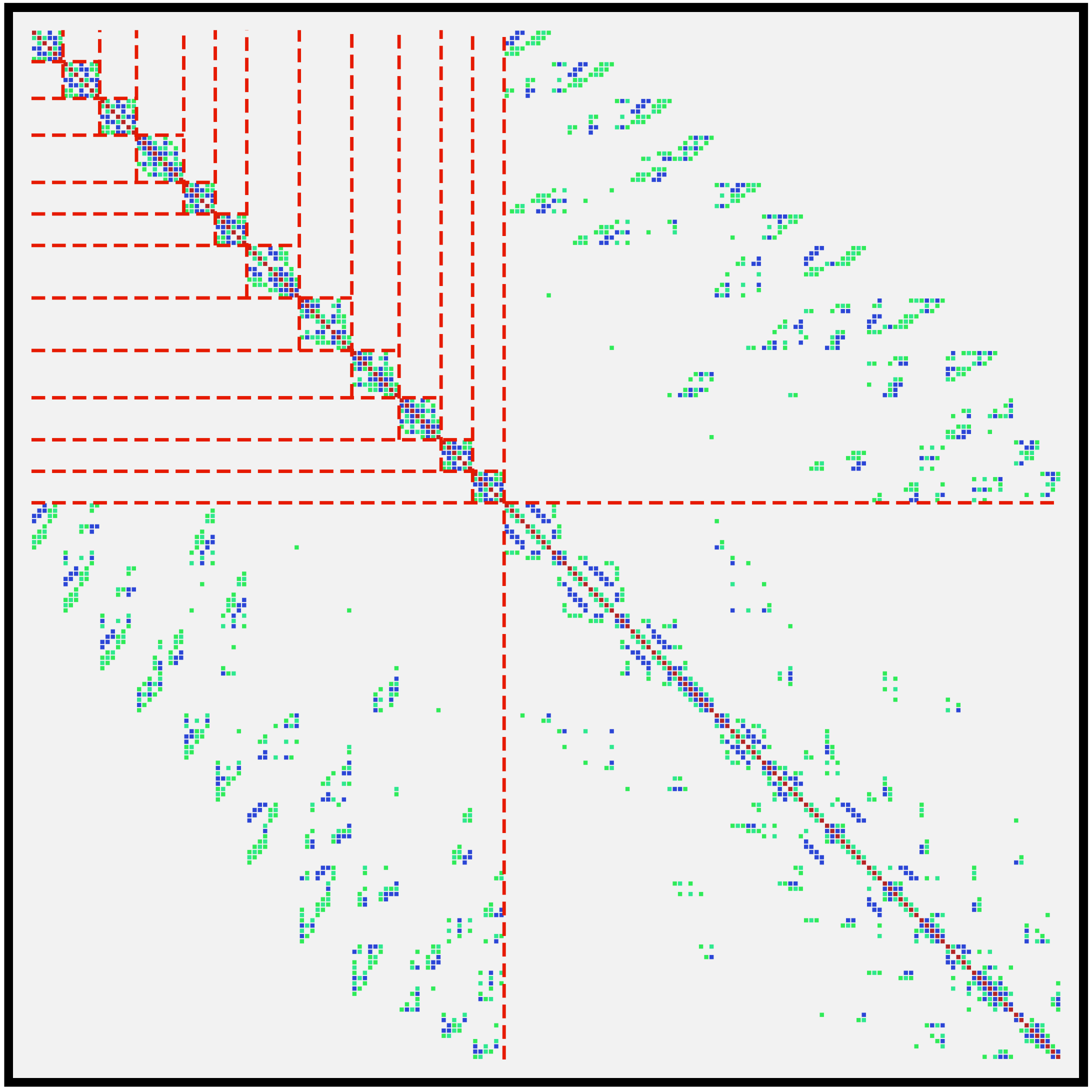


Simple strategy used: Do a Cuthill-MKee ordering until there are enough points to make a block. Reverse ordering. Start a new block from a non-visited node. Continue until all points are visited. Add criterion for rejecting "not sufficiently diagonally dominant rows."

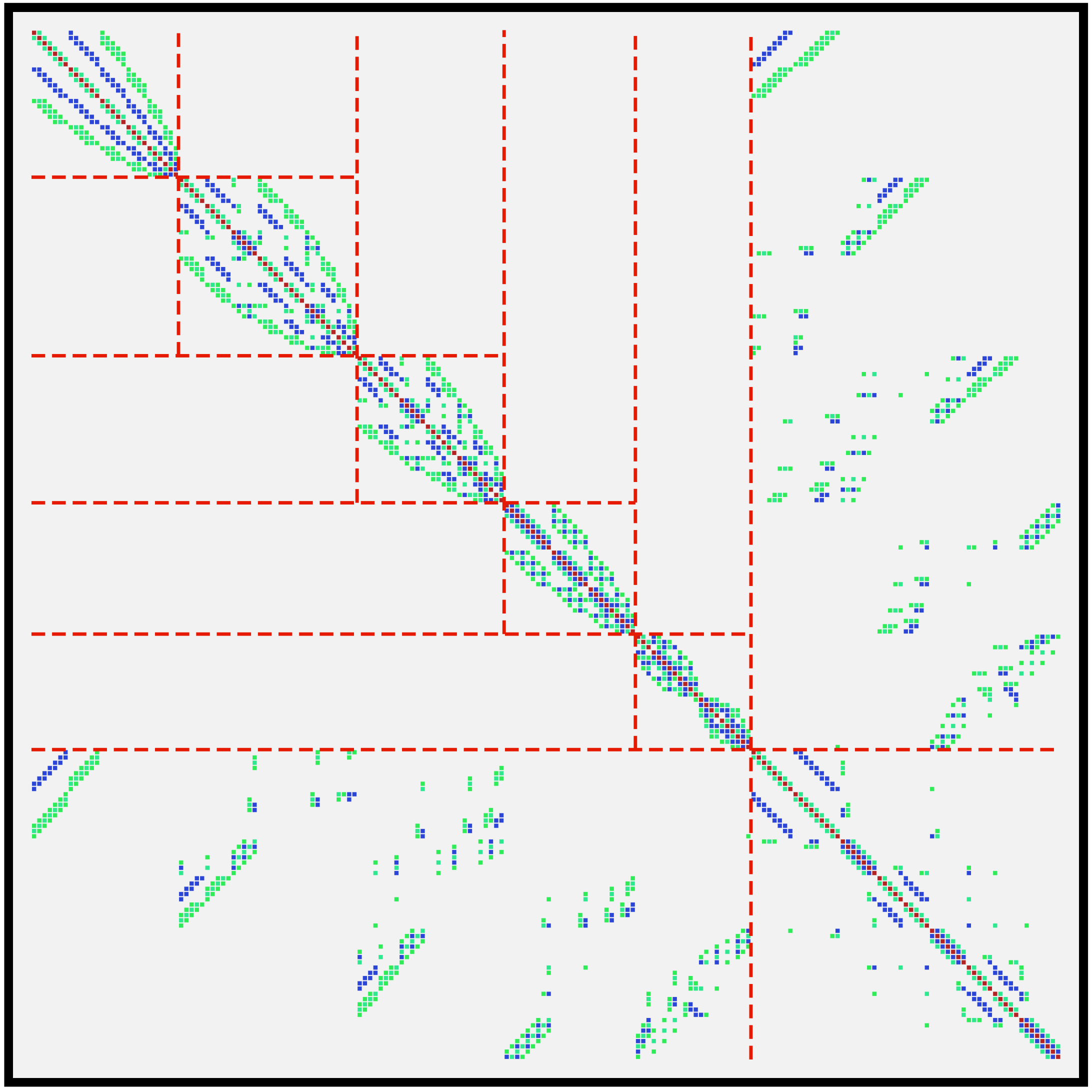
Original matrix



Block size of 6



Block size of 20



ARMS with permutations for diagonal dominance

Idea: ARMS + exploit nonsymmetric permutations

- No particular structure or assumptions for B block

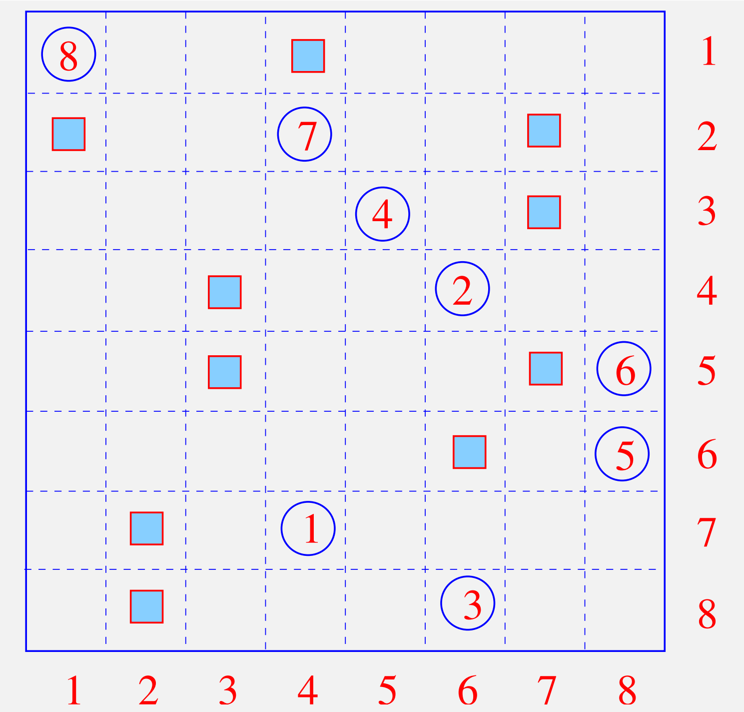
- Permute rows * and * columns of A. Use two permutations P (rows) and Q (columns) to transform A into

$$PAQ^T = \begin{pmatrix} B & F \\ E & C \end{pmatrix}$$

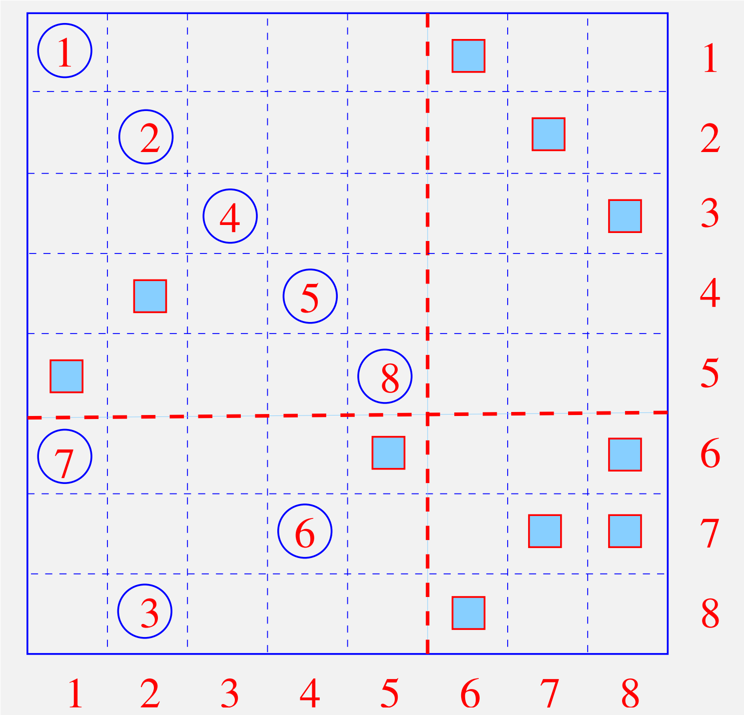
P, Q is a pair of permutations (rows, columns) selected so that the B block has the 'most diagonally dominant' rows (after nonsym perm) and few nonzero elements (to reduce fill-in).

Matching: Greedy algorithm

- Simple algorithm: scan pairs (i_k, j_k) in the given order.
- If i_k and j_k not already assigned, assign them to $\mathcal{M}$.



Matrix after preselection



Matrix after Matching perm.

Numerical illustration

Matrix	order	nonzeros	Application (Origin)
barrier2-9	115,625	3,897,557	Device simul. (Schenk)
matrix_9	103,430	2,121,550	Device simul. (Schenk)
mat-n_3*	125,329	2,678,750	Device simul. (Schenk)
ohne2	181,343	11,063,545	Device simul. (Schenk)
para-4	153,226	5,326,228	Device simul. (Schenk)
cir2a	482,969	3,912,413	circuit simul.
scircuit	170998	958936	circuit simul. (Hamm)
circuit_4	80209	307604	Circuit simul. (Bomhof)
wang3.rua	26064	177168	Device simul. (Wang)
wang4.rua	26068	177196	Device simul. (Wang)

Parameters

		Drop tolerance				$Fill_{max}$			
$nlev_{max}$	tol_{DD}	LU-B	GW	S	LU-S	LU-B	GW	S	LU-S
40	0.1	0.01	0.01	0.01	1.e-05	3	3	3	20

Matrix	Fill Factor	Set-up Time	GMRES(60) Its.	GMRES(60) Time	GMRES(100) Its.	GMRES(100) Time
barr2-9	0.62	4.01e+00	113	3.29e+01	93	3.02e+01
mat-n_3	0.89	7.53e+00	40	1.02e+01	40	1.00e+01
matrix_9	1.77	5.53e+00	160	4.94e+01	82	2.70e+01
ohne2	0.62	4.34e+01	99	6.35e+01	80	5.43e+01
para-4	0.62	5.70e+00	49	1.94e+01	49	1.93e+01
wang3	2.33	8.90e-01	45	2.09e+00	45	1.95e+00
wang4	1.86	5.10e-01	31	1.25e+00	31	1.20e+00
scircuit	0.90	1.86e+00	Fail	7.08e+01	Fail	8.80e+01
circuit_4	0.75	1.60e+00	199	1.69e+01	96	1.07e+01
circ2a	0.76	2.19e+02	18	1.08e+01	18	1.03e+01

Results for the 10 systems - ARMS-ddPQ + GMRES(60) & GMRES(100)

	Fill Factor	Set-up Time	GMRES(60) Its.	GMRES(60) Time	GMRES(100) Its.	GMRES(100) Time
Same param's	0.89	1.81	400	9.13e+01	297	8.79e+01
Droptol = .001	1.00	1.89	98	2.23e+01	82	2.27e+01

Solution of the system `scircuit` – no scaling + two different sets of parameters.

PARALLEL IMPLEMENTATION

Introduction

- Thrust of parallel computing techniques in most applications areas.
- Programming model: Message-passing seems (MPI) dominates
- Open MP and threads for small number of processors
- Important new reality: parallel programming has penetrated the 'applications' areas [Sciences and Engineering + industry]
- Problem 1: algorithms lagging behind somewhat
- Problem 2: Message passing is painful for large applications. 'Time to solution' up.

Parallel preconditioners: A few approaches

“Parallel matrix computation” viewpoint:

- Local preconditioners: Polynomial (in the 80s), Sparse Approximate Inverses, [M. Benzi-Tuma & al ’99., E. Chow ’00]
- Distributed versions of ILU [Ma & YS ’94, Hysom & Pothen ’00]
- Use of multicoloring to unaravel parallelism

Domain Decomposition ideas:

- Schwarz-type Preconditioners [e.g. Widlund, Bramble-Pasciak-Xu, X. Cai, D. Keyes, Smith, ...]

- Schur-complement techniques [Gropp & Smith, Ferhat et al. (FETI), T.F. Chan et al., YS and Sosonkina '97, J. Zhang '00, ...]

Multigrid / AMG viewpoint:

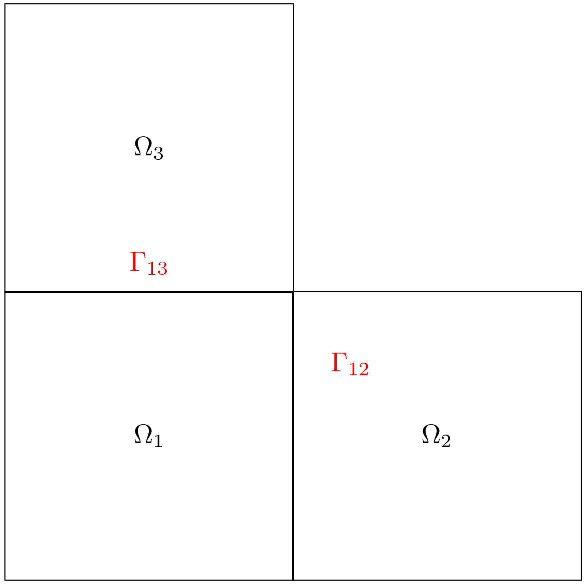
- Multi-level Multigrid-like preconditioners [e.g., Shadid-Tuminaro et al (Aztec project), ...]

➤ In practice: Variants of additive Schwarz very common (simplicity)

Standard Domain Decomposition

Problem:

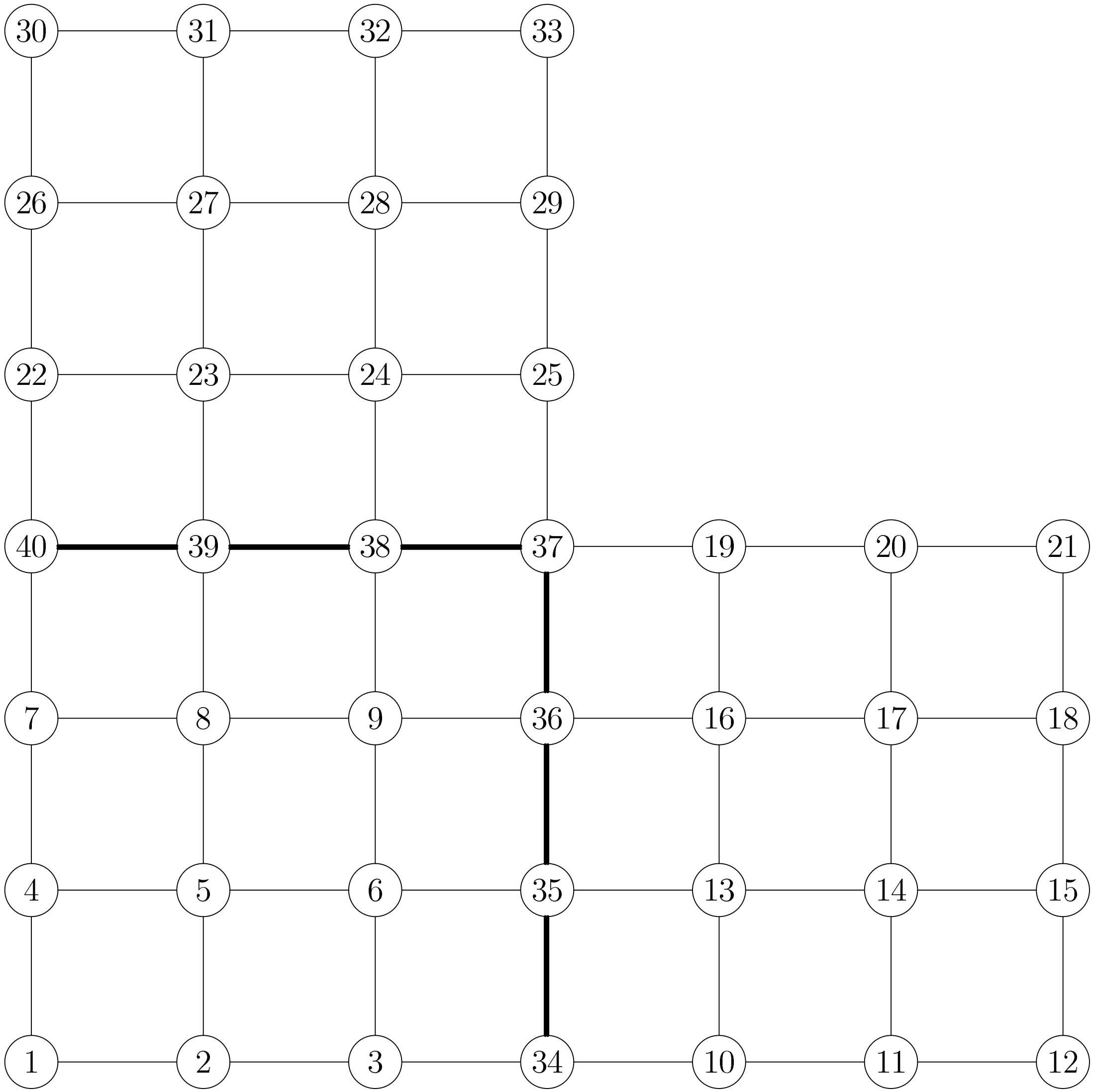
$$\begin{cases} \Delta u = f \text{ in } \Omega \\ u = u_\Gamma \text{ on } \Gamma = \partial\Omega. \end{cases}$$



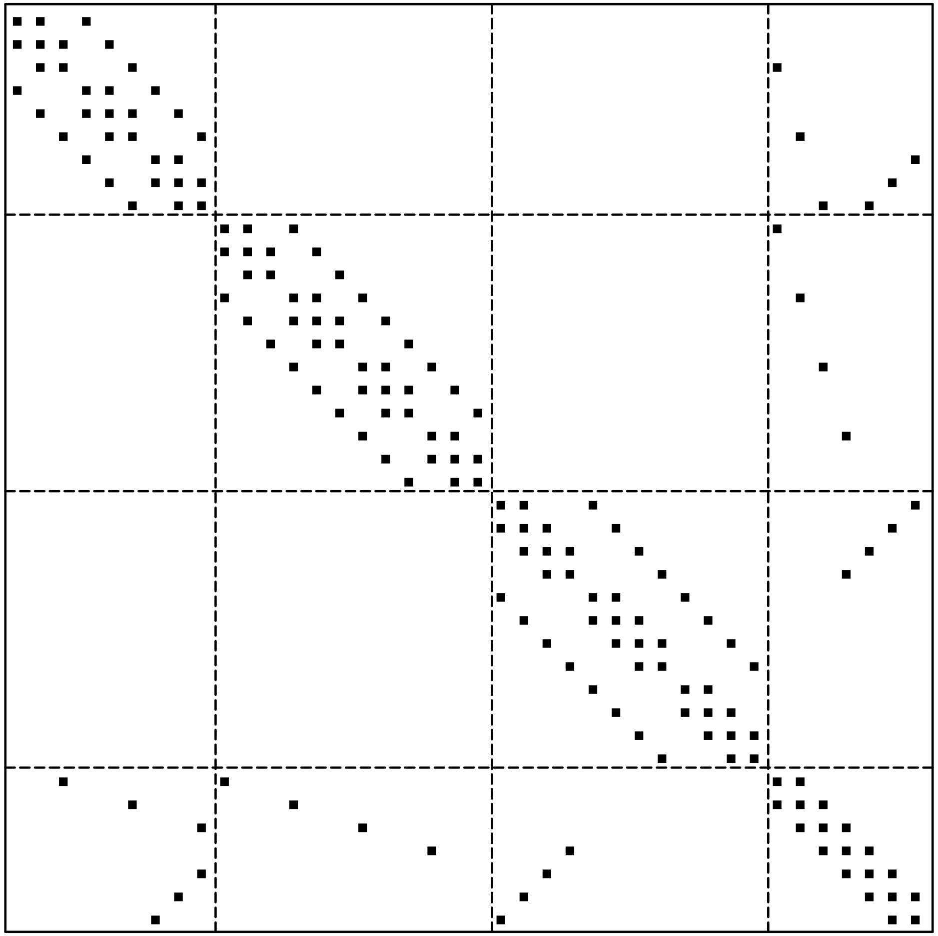
Domain:

$$\Omega = \bigcup_{i=1}^{s} \Omega_i,$$

- **Domain decomposition or substructuring methods attempt to solve a PDE problem (e.g.) on the entire domain from problem solutions on the subdomains Ω_i.**

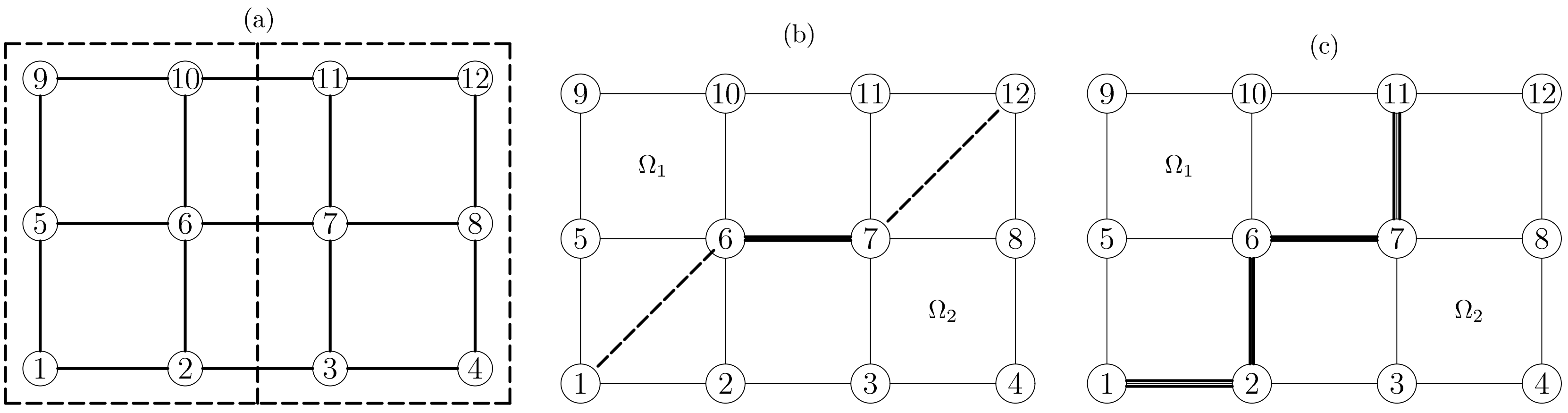


Discretization of domain



Coefficient Matrix

Types of mappings



(a) Vertex-based; (b) edge-based; and (c) element-based partitioning

- **Can adapt PDE viewpoint to general sparse matrices**
- **Will use the graph representation and 'vertex-based' viewpoint**

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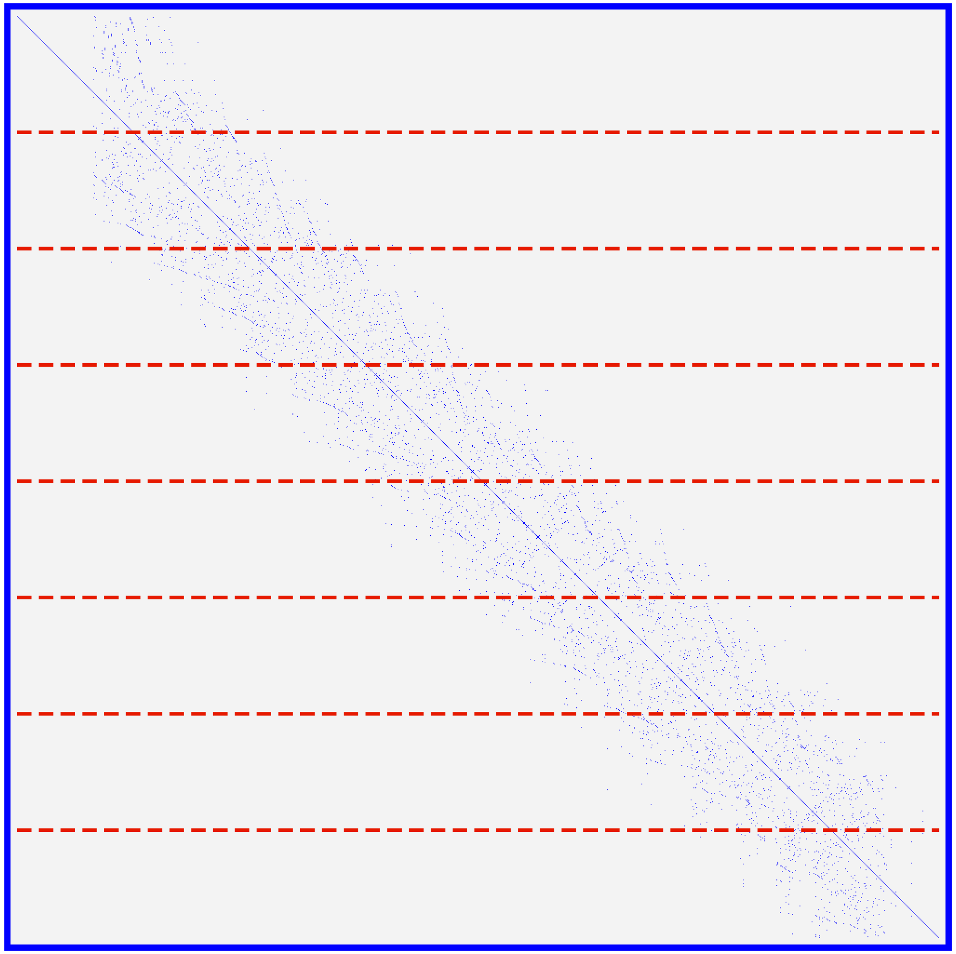
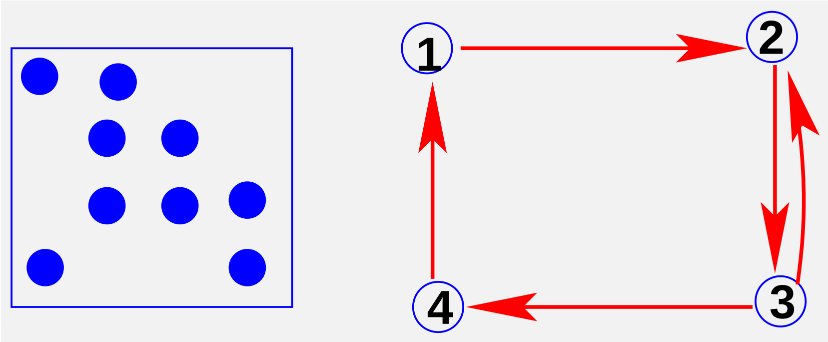
DISTRIBUTED SPARSE MATRICES

Generalization: Distributed Sparse Systems

- Simple illustration: Block assignment. Assign equation i and unknown i to a given 'process'
- Naive partitioning - won't work well in practice



➤ Best idea is to use the adjacency graph of A:



Vertices = $\{1, 2, \cdots, n\}$;

Edges: $i \rightarrow j$ iff $a_{ij} \neq 0$

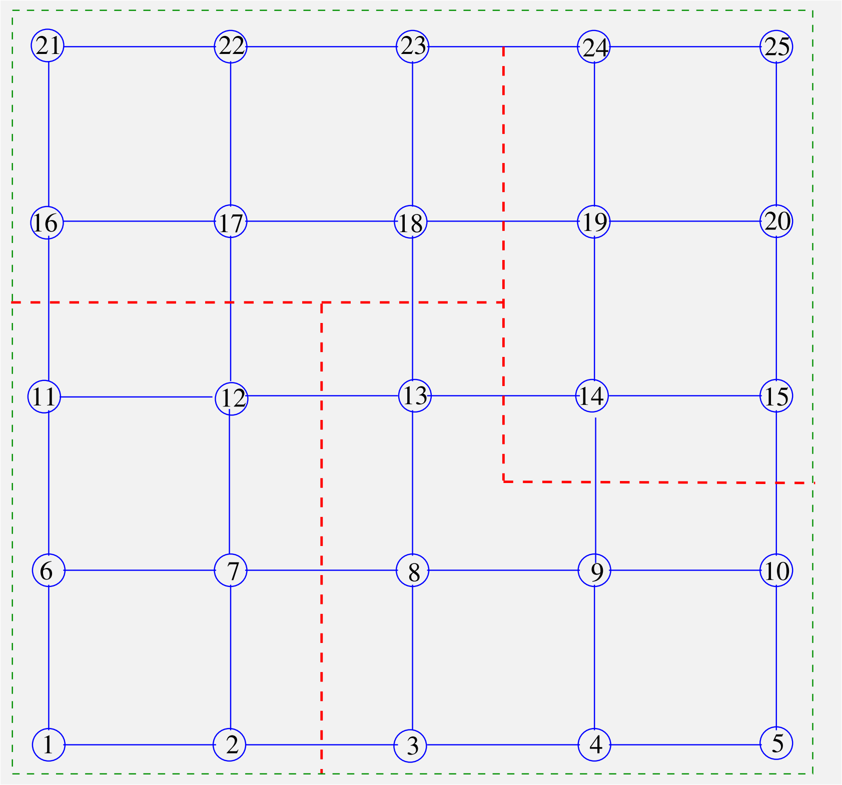
Graph partitioning problem:

- Want a partition of the vertices of the graph so that

(1) partitions have $\sim$ the same sizes

(2) interfaces are small in size

General Partitioning of a sparse linear system



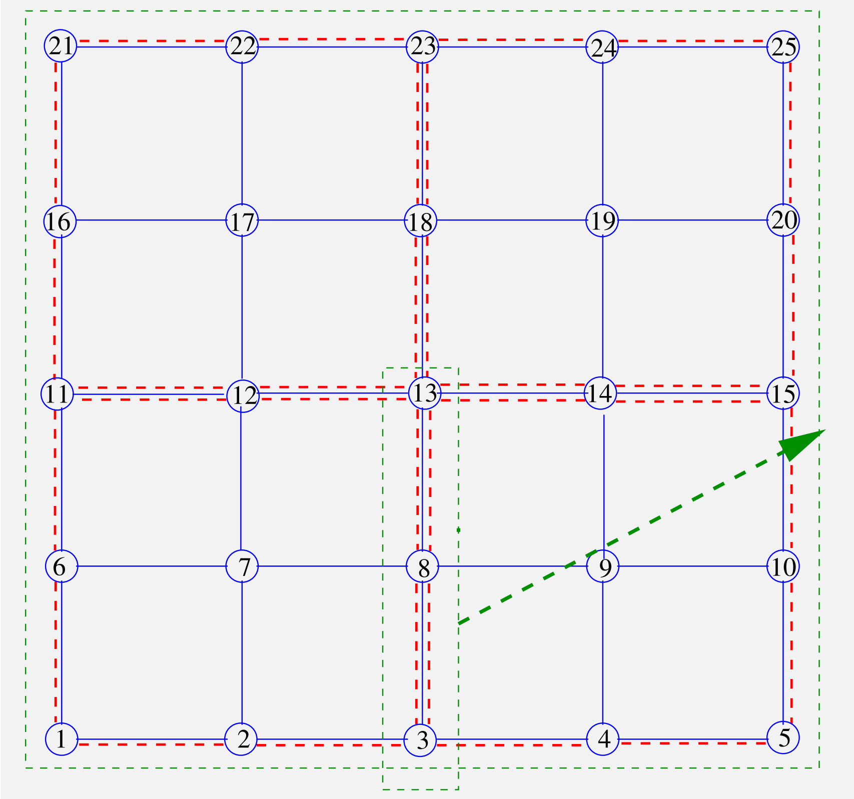
$S_1 = \{1, 2, 6, 7, 11, 12\}$: This means equations and unknowns 1, 2, 3, 6, 7, 11, 12 are assigned to Domain 1.

$S_2 = \{3, 4, 5, 8, 9, 10, 13\}$

$S_3 = \{16, 17, 18, 21, 22, 23\}$

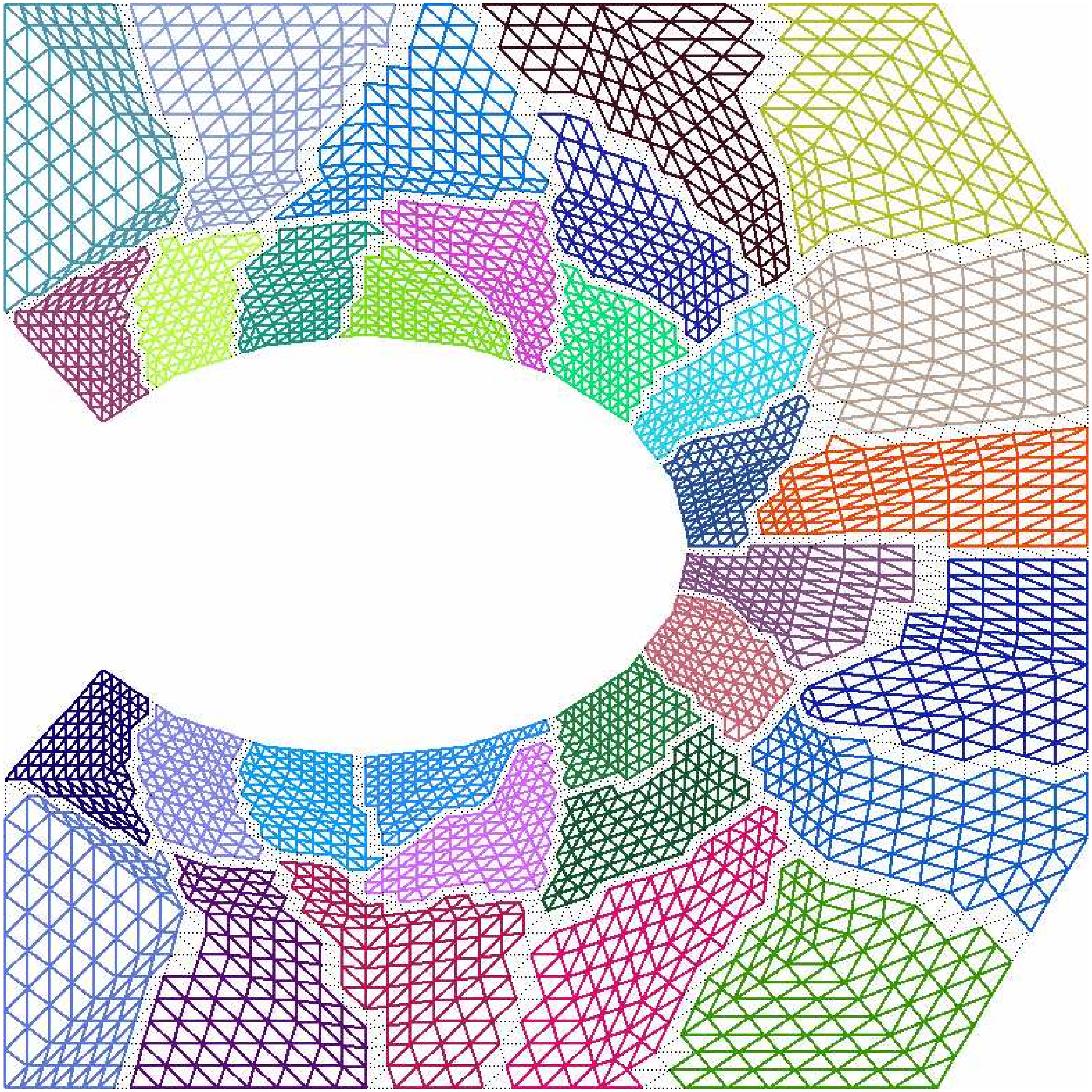
$S_4 = \{14, 15, 19, 20, 24, 25\}$

Alternative: Map elements / edges rather than vertices



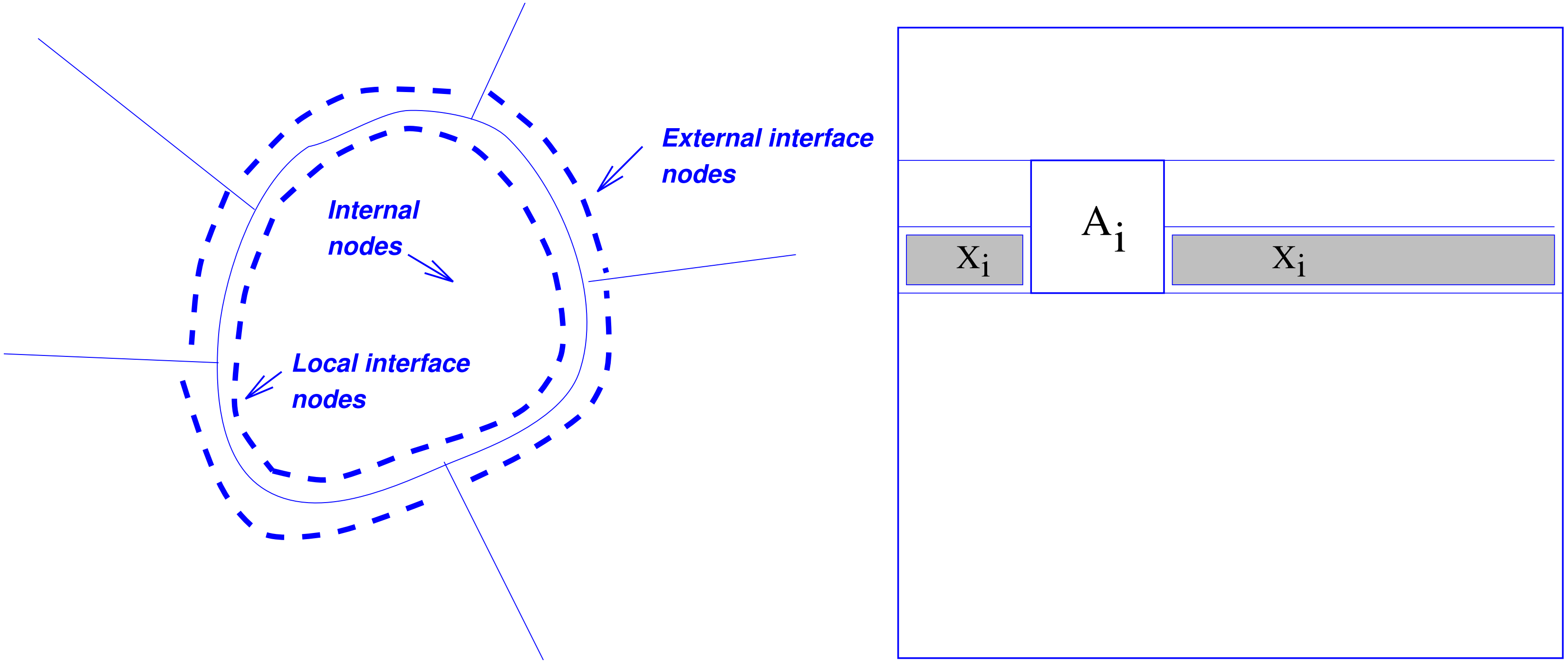
Equations/unknowns 3, 8, 12 shared by 2 domains. From distributed sparse matrix viewpoint this is an overlap of one layer

- **Partitioners : Metis, Chaco, Scotch, ..**
- **More recent: Zoltan, H-Metis, PaToH**



- Standard dual objective: "minimize" communication + "balance" partition sizes
- Recent trend: use of hypergraphs [PaToh, Hmetis,...]
- Hypergraphs are very general.. Ideas borrowed from VLSI work
- Main motivation: to better represent communication volumes when partitioning a graph. Standard models face many limitations
- Hypergraphs can better express complex graph partitioning problems and provide better solutions. Example: completely nonsymmetric patterns.

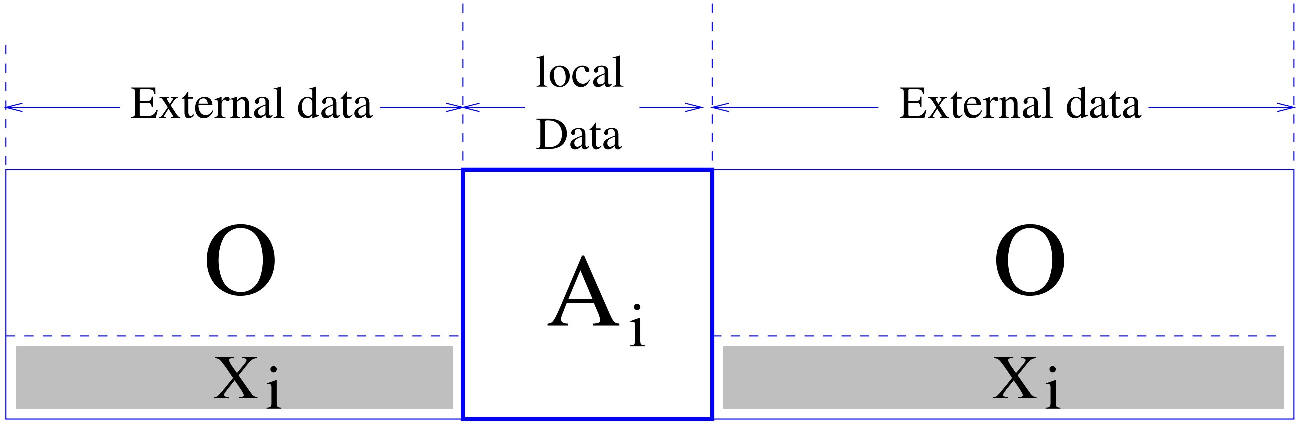
Two views of a distributed sparse matrix



- Local interface variables always ordered last.

- Need: 1) to set up the various "local objects". 2) Preprocessing to prepare for communications needed during iteration?

Local view of distributed matrix:

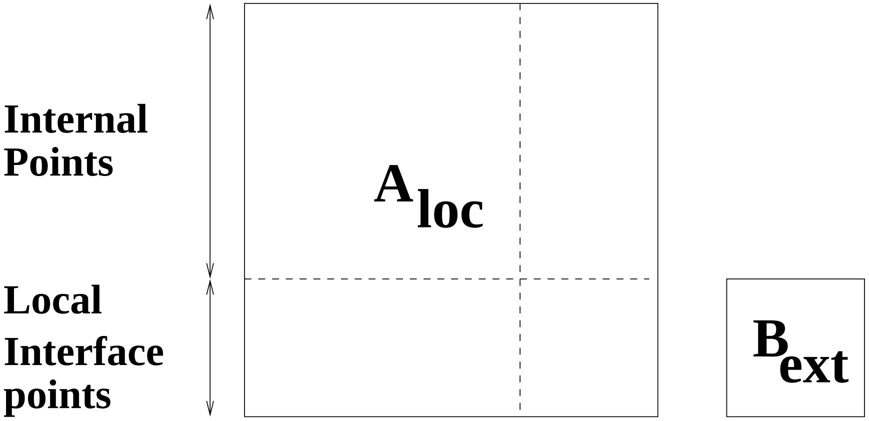


The local system:

$$\underbrace{\begin{pmatrix} B_i & F_i \\ E_i & C_i \end{pmatrix}}_{A_i} \begin{pmatrix} u_i \\ y_i \end{pmatrix} + \underbrace{\begin{pmatrix} 0 \\ \sum_{j \in N_i} E_{ij} y_j \end{pmatrix}}_{y_{ext}} = \begin{pmatrix} f_i \\ g_i \end{pmatrix}$$

- u_i : **Internal variables;** y_i : **Interface variables**

The local matrix:



The local matrix consists of 2 parts: a part ('A_{loc}') which acts on local data and another ('B_{ext}') which acts on remote data.

- Once the partitioning is available these parts must be identified and built locally..
- In finite elements, assembly is a local process.
- How to perform a matrix vector product? [needed by iterative schemes?]

Distributed Sparse Matrix-Vector Product Kernel

Algorithm:

1. Communicate: exchange boundary data.

   Scatter x_{bound} to neighbors - Gather x_{ext} from neighbors

2. Local matrix – vector product

$$y = A_{loc} x_{loc}$$

3. External matrix – vector product

$$y = y + B_{ext} x_{ext}$$

NOTE: 1 and 2 are independent and can be overlapped.

Main Operations in (F) GMRES :

1. Saxpy's – local operation – no communication

2. Dot products – global operation

3. Matrix-vector products – local operation – local communication

4. Preconditioning operations – locality varies.

Distributed Dot Product

```
/*-------------------- call blas1 function
   tloc = DDOT(n, x, incx, y, incy);
/*-------------------- call global reduction
   MPI_Allreduce(&tloc,&ro,1,MPI_DOUBLE,MPI_SUM,comm);
```

A remark: the global viewpoint

$$
\left(\begin{array}{ccccc|cccc}
B_1 & & & & & F_1 & & & \\
& B_2 & & & & & F_2 & & \\
& & \ddots & & & & & \cdot & \\
& & & \ddots & & & & & \cdot \\
& & & & B_p & & & & F_p \\
\hline
E_1 & & & & & C_1 & E_{12} & \cdots & E_{1p} \\
& E_2 & & & & E_{21} & C_2 & \cdots & E_{2p} \\
& & \ddots & & & \vdots & \vdots & \vdots & \\
& & & & E_p & E_{p1} & E_{p2} & \cdots & C_p
\end{array}\right)
\begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ \vdots \\ u_p \\ y_1 \\ y_2 \\ \vdots \\ y_p \end{pmatrix}
=
\begin{pmatrix} f_1 \\ f_2 \\ \vdots \\ \vdots \\ f_p \\ g_1 \\ g_2 \\ \vdots \\ g_p \end{pmatrix}
$$

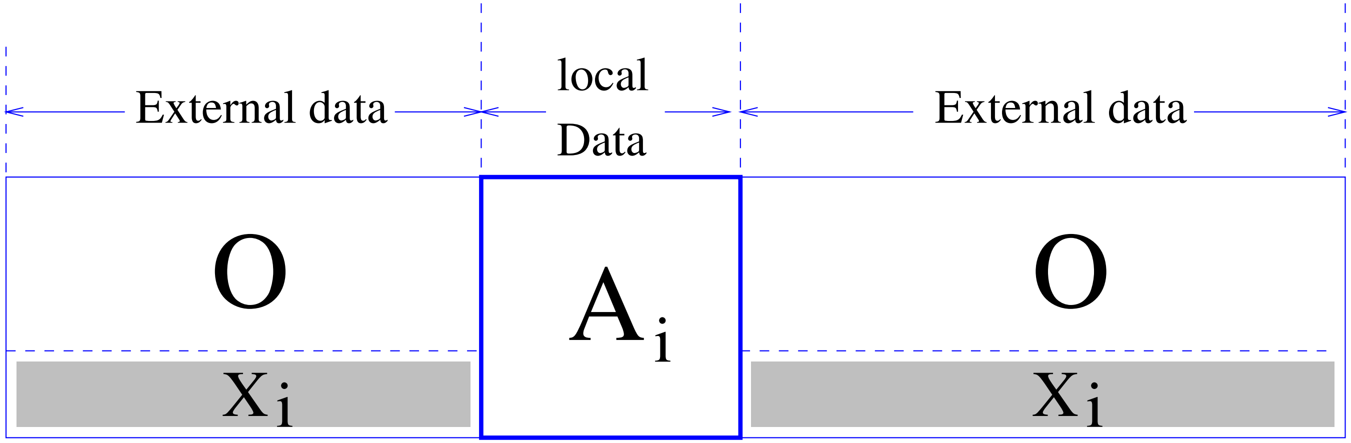
$\longleftarrow$ **Interior variables** $\longrightarrow$ $\longleftarrow$ **Interface variables** $\longrightarrow$

SCHUR COMPLEMENT-BASED PRECONDITIONERS

Schur complement system

Local system can be written as

$$A_i x_i + X_i y_{i,ext} = b_i. \tag{1}$$



x_i= **vector of local unknowns,** $y_{i,ext}$ **= external interface variables, and** b_i **= local part of RHS.**

- **Local equations**

$$\begin{pmatrix} B_i & F_i \\ E_i & C_i \end{pmatrix} \begin{pmatrix} u_i \\ y_i \end{pmatrix} + \begin{pmatrix} 0 \\ \sum_{j \in N_i} E_{ij} y_j \end{pmatrix} = \begin{pmatrix} f_i \\ g_i \end{pmatrix} \tag{2}$$

- **eliminate u_i from the above system:**

$$S_i y_i + \sum_{j \in N_i} E_{ij} y_j = g_i - E_i B_i^{-1} f_i \equiv g_i',$$

where S_i is the "local" Schur complement

$$S_i = C_i - E_i B_i^{-1} F_i. \tag{3}$$

Structure of Schur complement system

Global Schur complement system: $Sy = g'$ **with :**

$$S = \begin{pmatrix} S_1 & E_{12} & \dots & E_{1p} \\ E_{21} & S_2 & \dots & E_{2p} \\ \vdots & & \ddots & \vdots \\ E_{p1} & E_{p-1,2} & \dots & S_p \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_p \end{pmatrix} = \begin{pmatrix} g'_1 \\ g'_2 \\ \vdots \\ g'_p \end{pmatrix}.$$

- E_{ij}'s are sparse = same as in the original matrix
- Can solve global Schur complement system iteratively. Back-substitute to recover rest of variables (internal).
- Can use the procedure as a preconditining to global system.

Simplest idea: Schur Complement Iterations

$$\begin{pmatrix} u_i \\ y_i \end{pmatrix} \quad \begin{matrix} \text{Internal variables} \\ \text{Interface variables} \end{matrix}$$

- Do a global primary iteration (e.g., block-Jacobi)
- Then accelerate only the y variables (with a Krylov method)

Still need to precondition..

Approximate Schur-LU

➤ Two-level method based on induced preconditioner. Global system can also be viewed as

$$\begin{pmatrix} B & F \\ E & C \end{pmatrix} \begin{pmatrix} u \\ y \end{pmatrix} = \begin{pmatrix} f \\ g \end{pmatrix}, \quad B = \left(\begin{array}{cccc|c} B_1 & & & & F_1 \\ & B_2 & & & F_2 \\ & & \ddots & & \vdots \\ & & & B_p & F_p \\ \hline E_1 & E_2 & \cdots & E_p & C \end{array}\right)$$

Block LU factorization of A:

$$\begin{pmatrix} B & F \\ E & C \end{pmatrix} = \begin{pmatrix} B & 0 \\ E & S \end{pmatrix} \begin{pmatrix} I & B^{-1}F \\ 0 & I \end{pmatrix},$$

Preconditioning:

$$L = \begin{pmatrix} B & 0 \\ E & M_S \end{pmatrix} \quad \text{and} \quad U = \begin{pmatrix} I & B^{-1}F \\ 0 & I \end{pmatrix}$$

with M_S = some approximation to S.

➤ Preconditioning to global system can be induced from any preconditioning on Schur complement.

Rewrite local Schur system as

$$y_i + S_i^{-1} \sum_{j \in N_i} E_{ij} y_j = S_i^{-1} \left[g_i - E_i B_i^{-1} f_i \right] .$$

➤ equivalent to Block-Jacobi preconditioner for Schur complement.

➤ Solve with, e.g., a few s (e.g., 5) of GMRES

- **Question: How to solve with S_i?**

- **Can use LU factorization of local matrix** $A_i = \begin{pmatrix} B_i & F_i \\ E_i & C_i \end{pmatrix}$

and exploit the relation:

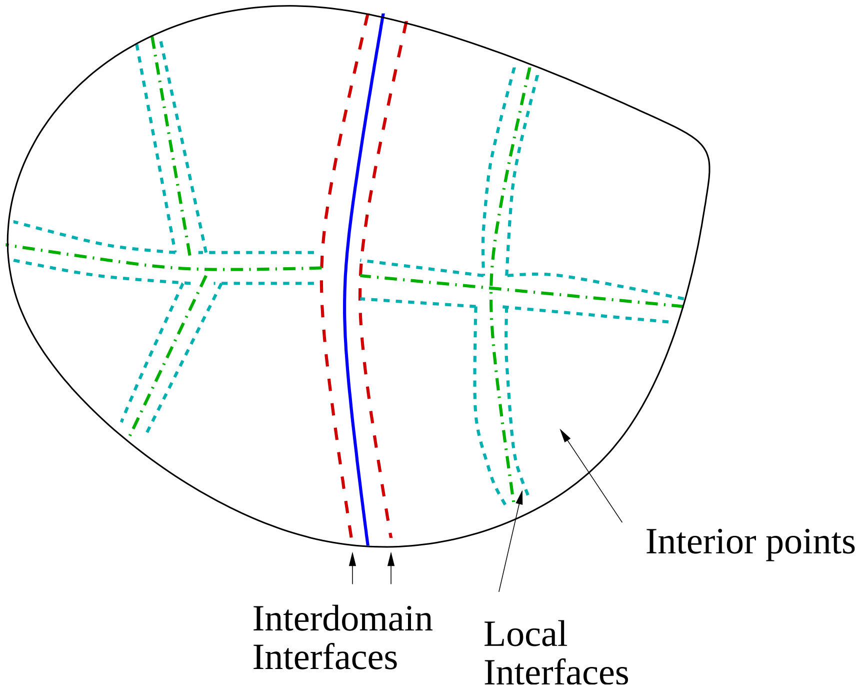
$$A_i = \begin{pmatrix} L_{B_i} & 0 \\ E_i U_{B_i}^{-1} & L_{S_i} \end{pmatrix} \begin{pmatrix} U_{B_i} & L_{B_i}^{-1} F_i \\ 0 & U_{S_i} \end{pmatrix} \quad \rightarrow \quad L_{S_i} U_{S_i} = S_i$$

- **Need only the (I) LU factorization of the A_i [rest is already available]**

- **Very easy implementation of (parallel) Schur complement techniques for vertex-based partitioned systems : YS-Sosonkina '97; YS-Sosonkina-Zhang '99.**

PARALLEL ARMS

Parallel implementation of ARMS

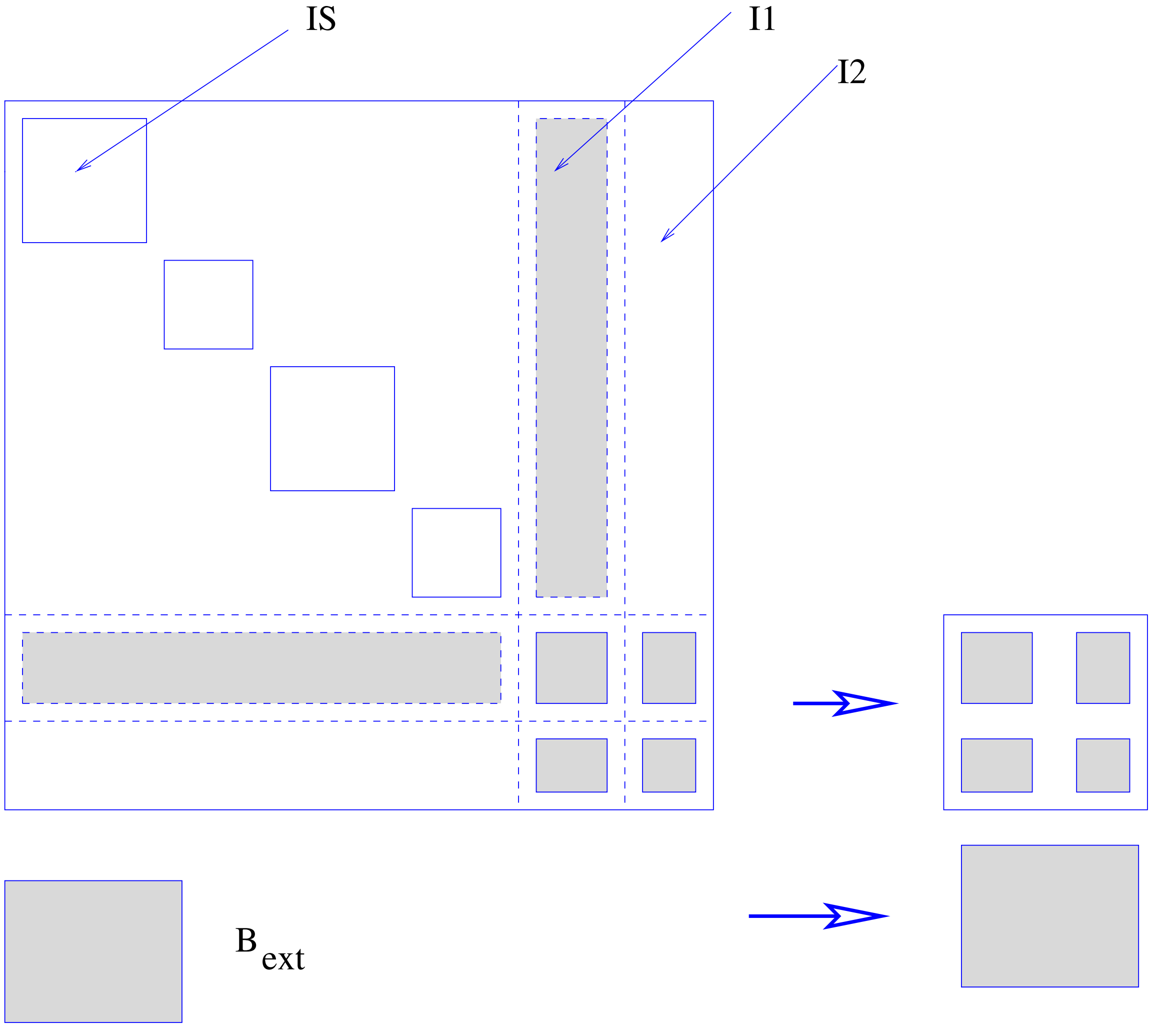


Three types of points:

interior (independent sets), local interfaces, and global interfaces

Main ideas: **(1) exploit recursivity (2) distinguish two phases: elimination of interior points and then interface points.**

Result: **2-part Schur complement: one corresponding to local interfaces and the other to inter-domain interfaces.**



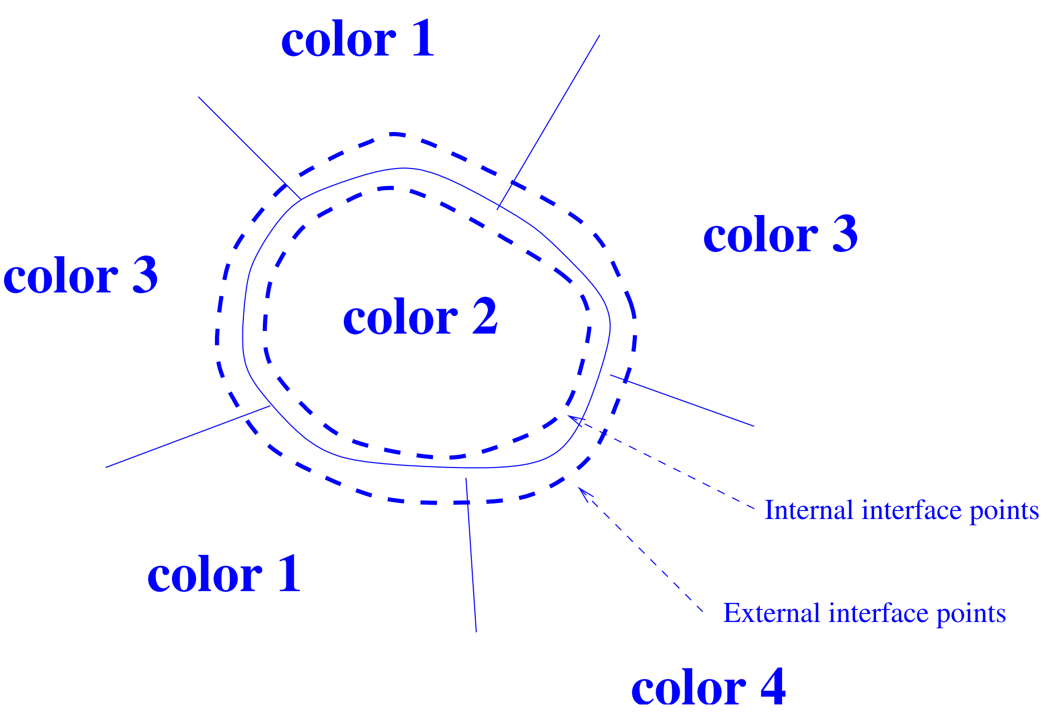
Three approaches

Method 1: Simple additive Schwarz using ILUT or ARMS locally

Method 2: Schur complement approach. Solve Schur complement system (both I1 and I2) with either a block Jacobi (M. Sosonkina and YS, '99) or multicolor ILU(0).

Method 3: Do independent set reduction across subdomains. Requires construction of global group independent sets.

➤ pARMS: Methods 1 and 2. Method 3 : Phidal [w. Pascal Henon]



Algorithm: Multicolor Distributed ILU(0)

1. Eliminate local rows,
2. Receive external interf. rows from PEs s.t. $color(PE) < \texttt{MyColor}$
3. Process local interface rows
4. Send local interface rows to PEs s.t. $color(PE) > \texttt{MyColor}$

Methods implemented in pARMS:

add_x Additive Schwarz with method x for subdomains. With/out overlap. x = one of ILUT, ILUK, ARMS.

sch_x Schur complement technique, with method x = factorization used for local submatrix. Same x as above. Equiv. to Additive Schwarz preconditioner on Schur complement.

sch_sgs Multicolor Multiplicative Schwarz (block Gauss-Seidel) preconditioning is used instead of additive Schwarz for Schur complement.

sch_gilu0 ILU(0) preconditioning to solve global Schur complement system obtained from ARMS reduction.

Test problem

1. Scalability experiment: sample finite difference problem.

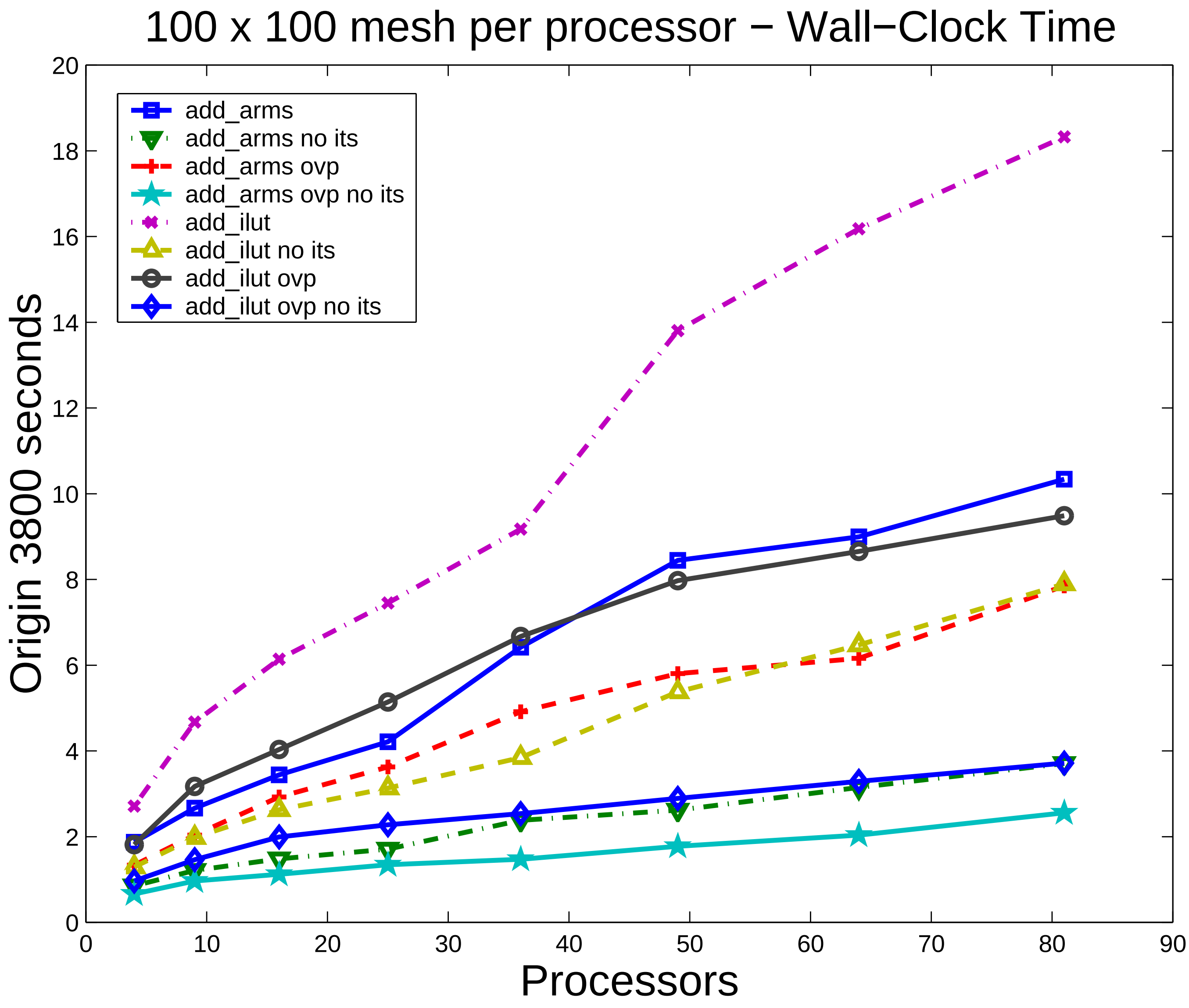
$$-\Delta u + \gamma \left(e^{xy}\frac{\partial u}{\partial x} + e^{-xy}\frac{\partial u}{\partial y} \right) + \alpha u = f \ ,$$

Dirichlet Boundary Conditions ; $\gamma = 100, \alpha = -10$; centered differences discretization.

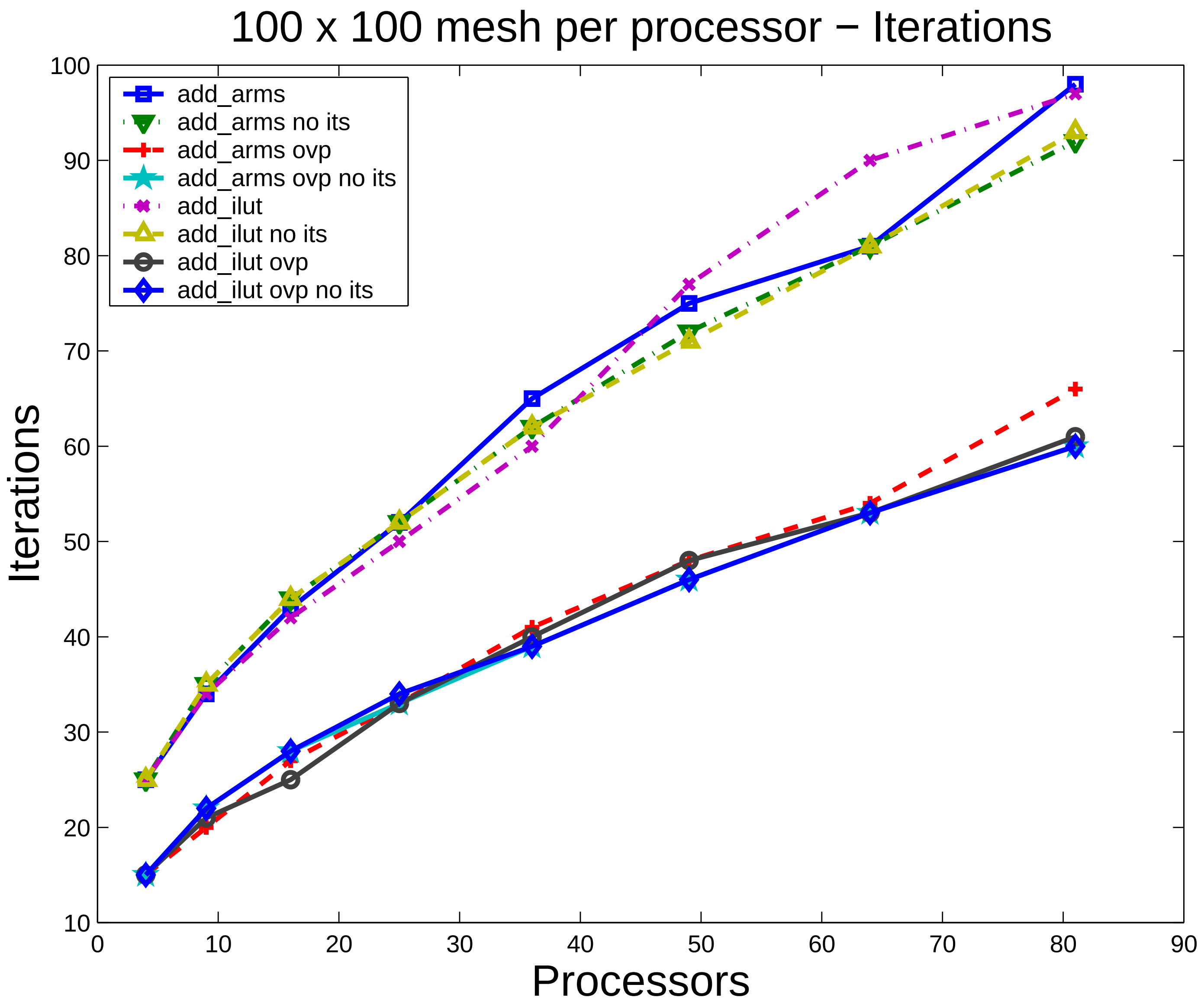
➤ Keep size constant on each processor $[100 \times 100]$ ➤ Global linear system with $10,000 * nproc$ unknowns.

2. Comparison with a parallel direct solver – symmetric problems

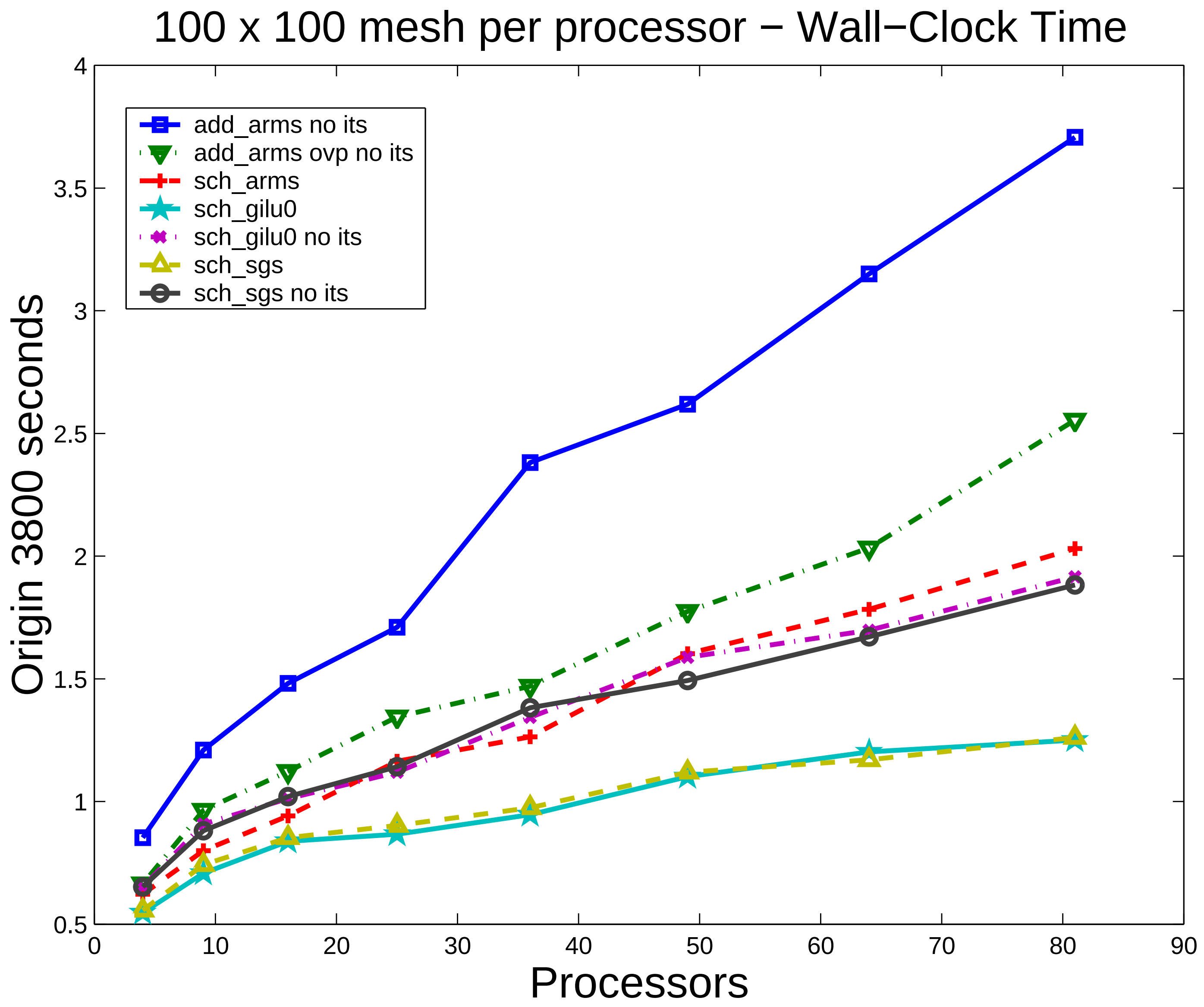
3. Large irregular matrix example arising from magneto hydrodynamics.



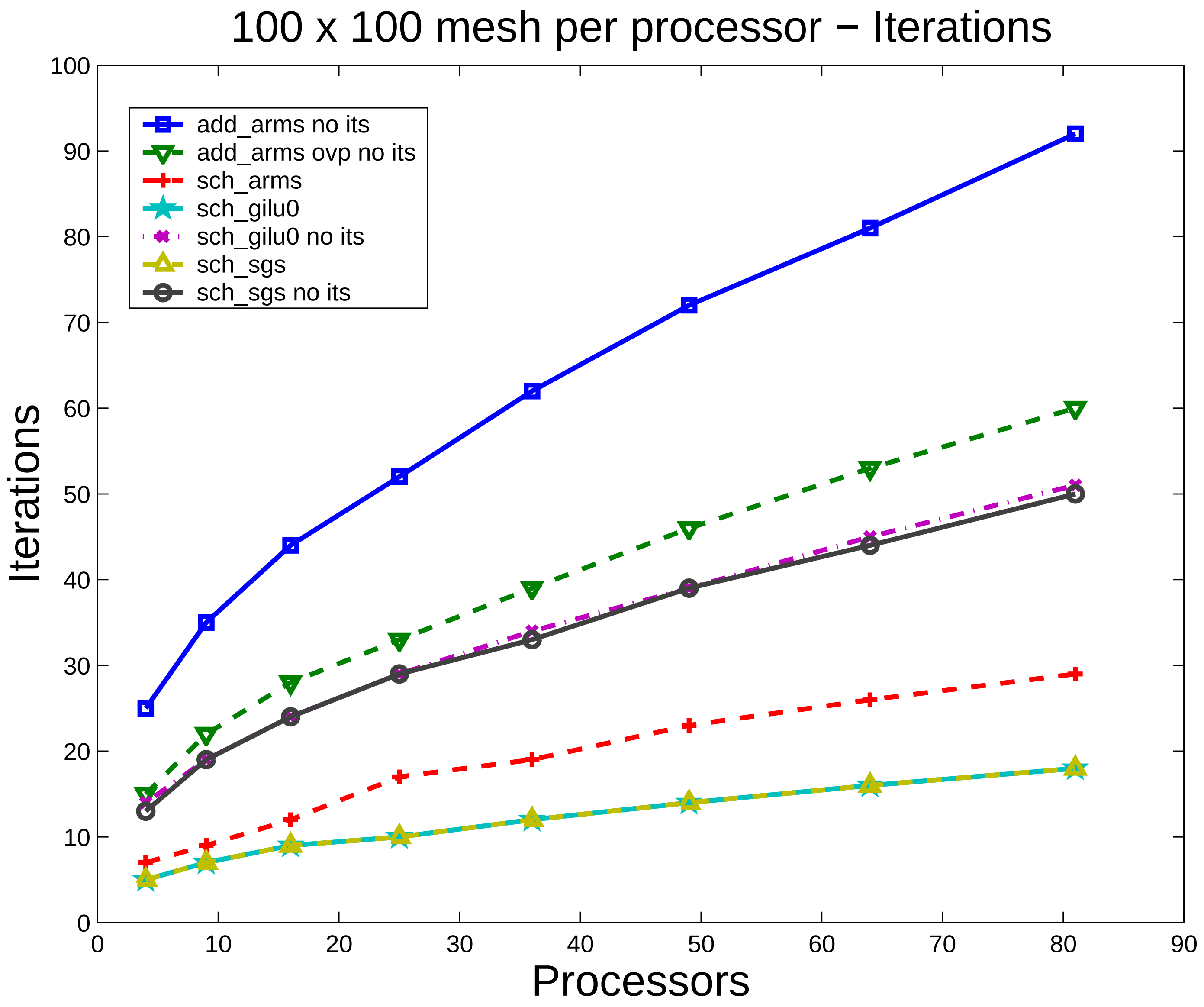
Times for 2D PDE problem with fixed subproblem size



Iterations for 2D PDE problem with fixed subproblem size



Times for 2D PDE problem with fixed subproblem size


100 x 100 mesh per processor − Iterations
Iterations
Processors
add_arms no its
add_arms ovp no its
sch_arms
sch_gilu0
sch_gilu0 no its
sch_sgs
sch_sgs no its
0
10
20
30
40
50
60
70
80
90
100

Iterations

Software

Direct solvers:

- **SUPERLU**

  `http://crd.lbl.gov/ xiaoye/SuperLU/`

- **MUMPS: [cerfacs]**

- **Univ. Minn. / IBM's PSPASES [SPD matrices]**

  `http://www-users.cs.umn.edu/ mjoshi/pspases/`

- **UMFPACK**

Iterative solvers:

- **PETSc**

  `http://acts.nersc.gov/petsc/`

and Trilinos (more recent)

`http://trilinos.sandia.gov/`

... are very comprehensive packages..

- **PETSc includes few preconditioners...**
- **Hypre, ML, ..., all include interfaces to PETSc or trilinos**
- **pARMS:**

  `http://www.cs.umn.edu∼saad/software`

is a more modest effort -