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Automatic Differentiation and Preconditioning: Myth or Reality?

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Problem

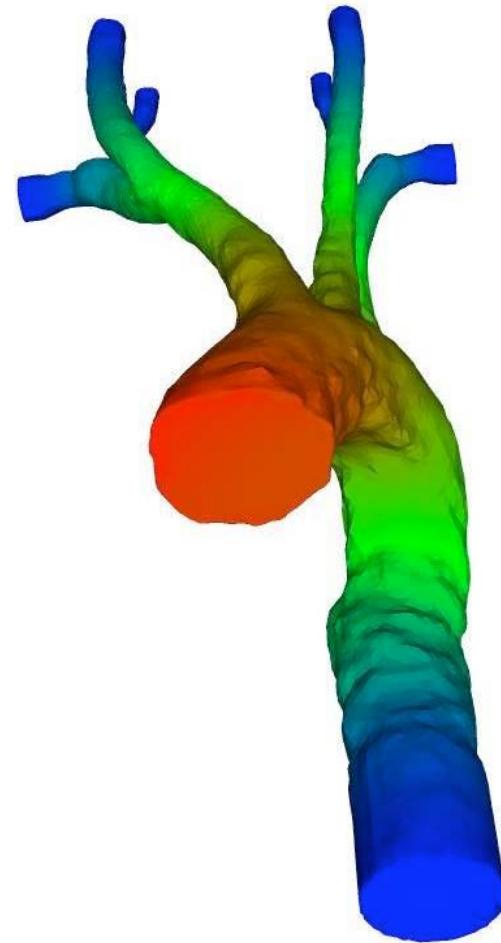
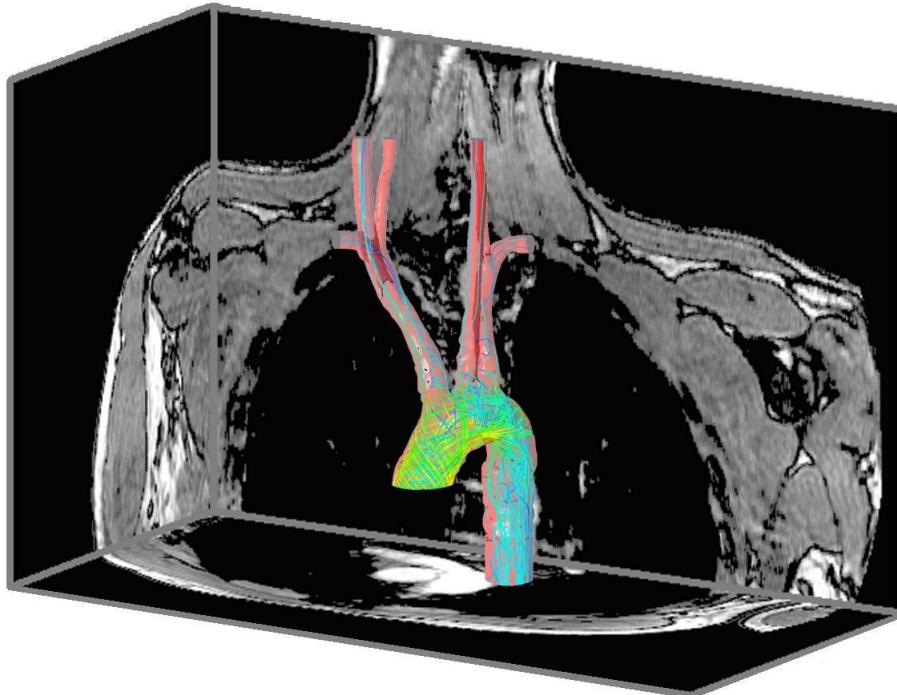
$$A\mathbf{x} = \mathbf{b}$$

$$\mathbf{x}, \mathbf{b} \in \mathbb{R}^N$$

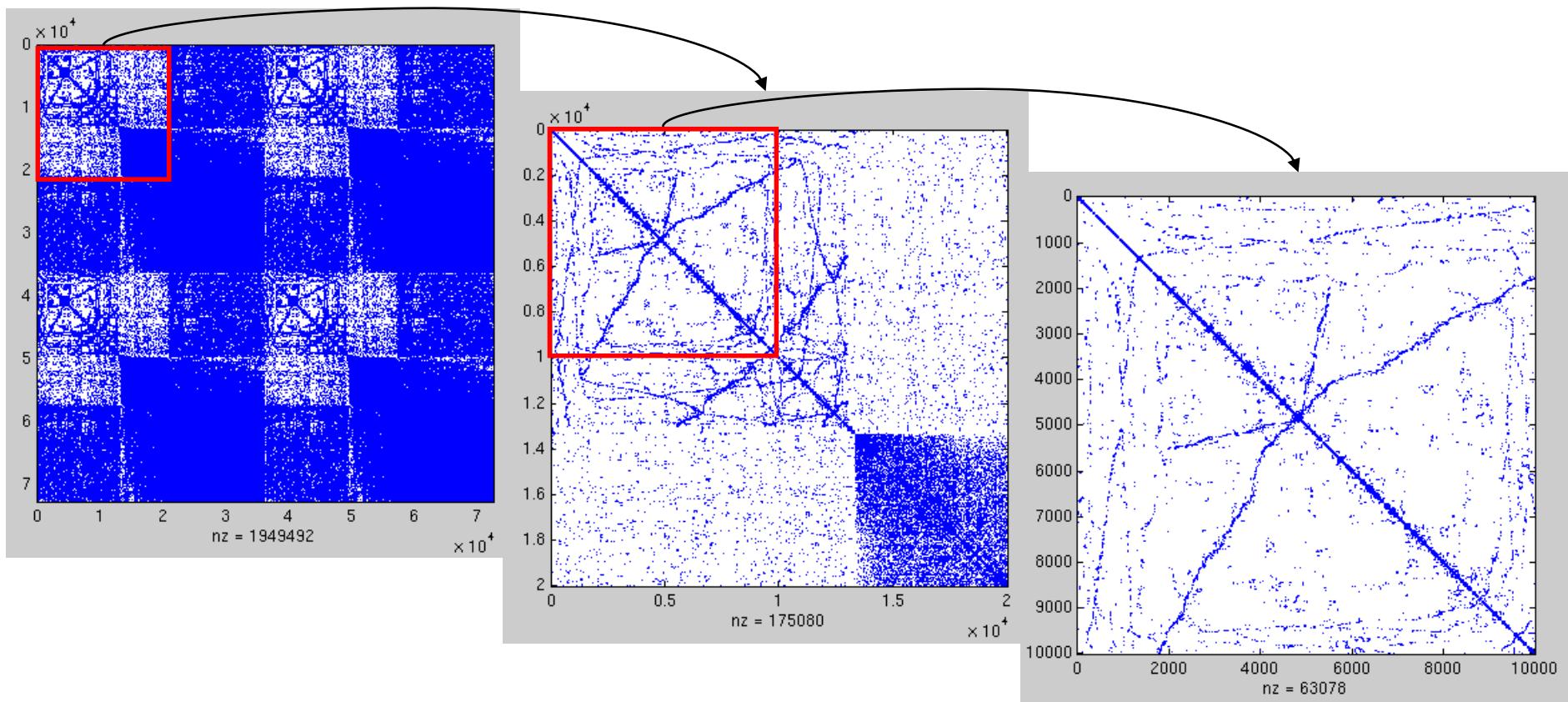
$$A = \frac{\partial \mathbf{f}}{\partial \mathbf{z}} \in \mathbb{R}^{N \times N} \quad \text{Jacobian matrix}$$

large, sparse,
unsymmetric, nonsingular,
a priori known pattern of nonzero elements

Flow through Aorta



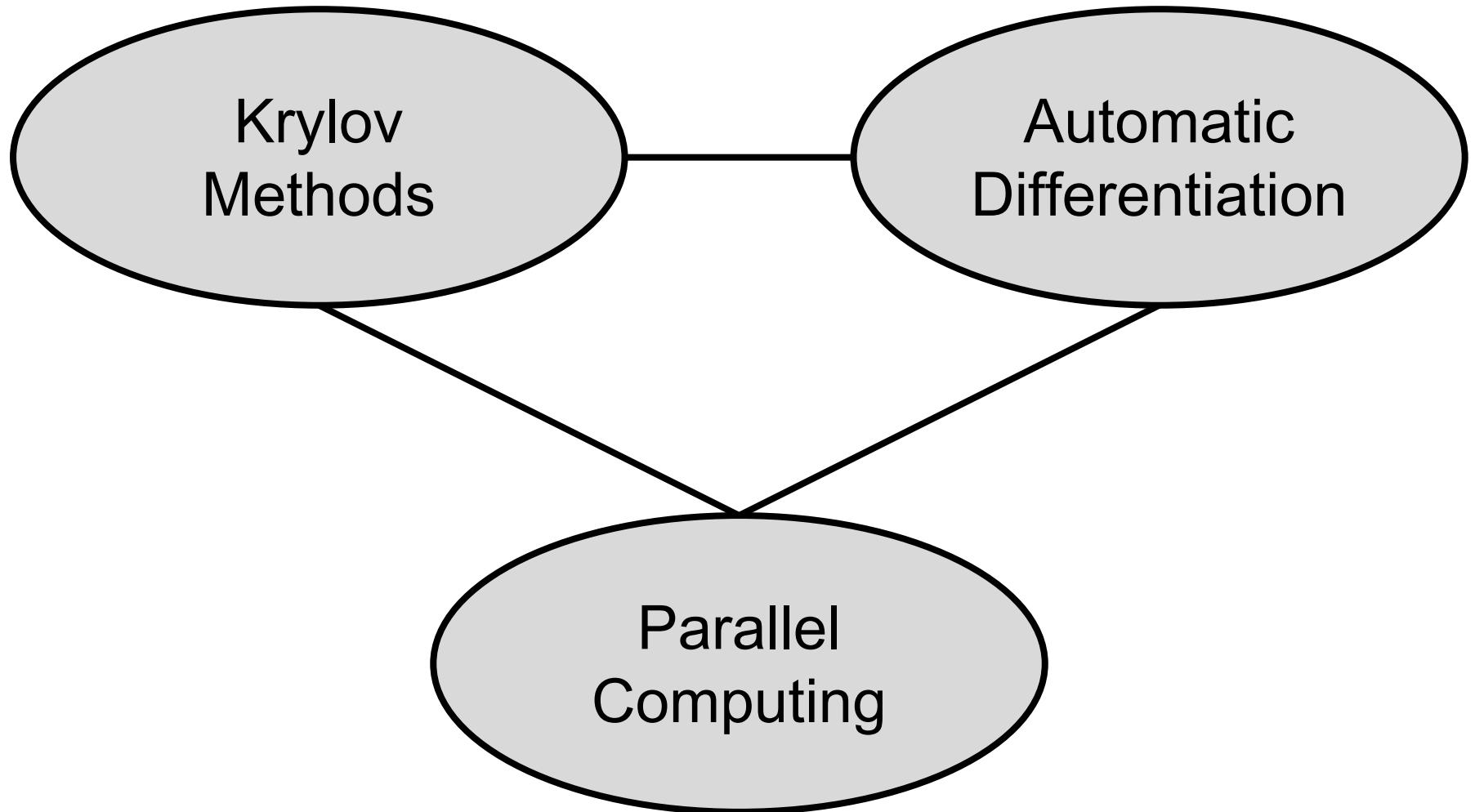
Coefficient Matrix



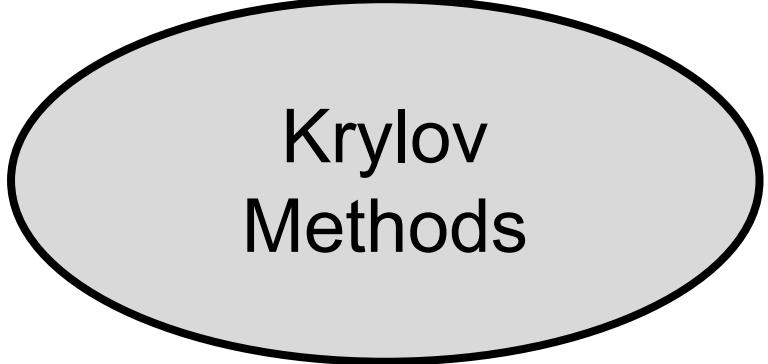
$N = 290,000$ (small problem)

0,04% nonzeros

Research Areas



Research Area



Krylov
Methods

Iterative solution of linear systems

Krylov Subspace Methods

Solve $A\mathbf{x} = \mathbf{b}$ with $A \in \mathbb{R}^{N \times N}$ large, sparse nonsingular
Let $\mathbf{r}_0 := \mathbf{b} - A\mathbf{x}_0$

$$\mathbf{x}_n \in \mathbf{x}_0 + \mathcal{K}_n(A, \mathbf{r}_0)$$

$$\mathbf{r}_n \perp \mathcal{L}_n$$

$$n = 1, 2, \dots$$

$$\mathcal{K}_n(A, \mathbf{r}_0) := \text{span}\{\mathbf{r}_0, A\mathbf{r}_0, \dots, A^{n-1}\mathbf{r}_0\}$$

n th Krylov subspace generated by A and \mathbf{r}_0

Design of Krylov Subspace Methods

- Basis for spaces \mathcal{K}_n and \mathcal{L}_n
- Definition of current iterate

$$\|\mathbf{r}_n\|_1$$

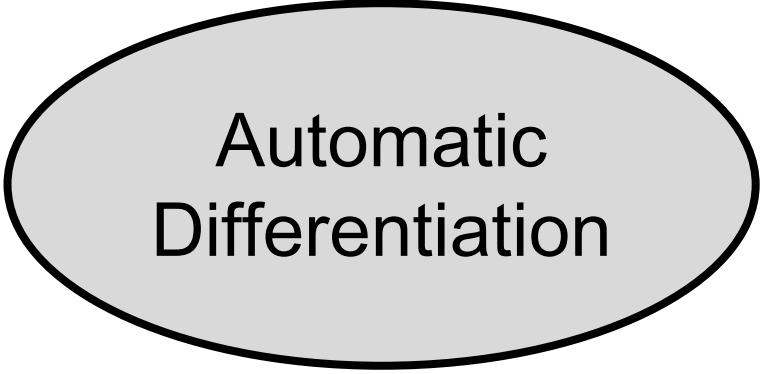
Algorithmic Ingredients

- Preconditioner $M \approx A$

$$M^{-1}A\mathbf{x} = M^{-1}\mathbf{b}$$

- Construction of M with assumption:
Elementwise access to $A(i, j)$ possible
- Solve „simple“ systems $M\mathbf{y} = \mathbf{z}$
- Matrix-vector products $\mathbf{y} = A\mathbf{z}$ $\mathbf{y} = A^T\mathbf{z}$
- Vector-vector operations $\mathbf{y}^T\mathbf{z}$ $\alpha\mathbf{y} + \beta\mathbf{z}$

Research Area



Automatic
Differentiation

Fast computation of exact derivatives

Automatic Differentiation (AD)

- Given: arbitrarily complex computer code evaluating some function
- Generates: new computer code evaluating function and derivatives of selected output w.r.t. selected inputs

Program transformation changing semantics

Example of Program Transformation

x = f(x,y,n)

```
real x,y  
integer n  
do i = 1,n  
    x = x*y  
enddo
```



$$[x, g_x] = [g_f(x, g_x, y, g_y, n)]$$

```
real x,g_x(2),y,g_y(2)  
integer n  
do i = 1,n  
    do j = 1,2  
        g_x = g_x(j)*y + x*g_y[j]  
    enddo  
    x = x*y  
enddo
```

Looking for:

$$\frac{\partial f}{\partial x} \quad \frac{\partial f}{\partial y}$$

Initialization: $g_x = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad g_y = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$

Result: $g_x = \begin{bmatrix} \partial f / \partial x \\ \partial f / \partial y \end{bmatrix}$

AD in a Nutshell

- Code corresponds to composition of few elementary functions (+, -, *, sin, ...)
- Derivatives of elementary functions are known
- Chain rule handles composition
- Accumulation leads to final derivatives without truncation error (in exact arithmetic)

Computation of Jacobian Matrices

- Given: Program evaluating

$$\mathbf{f} : \mathbb{R}^N \longrightarrow \mathbb{R}^N \quad \text{with runtime } T_{\mathbf{f}}(N)$$

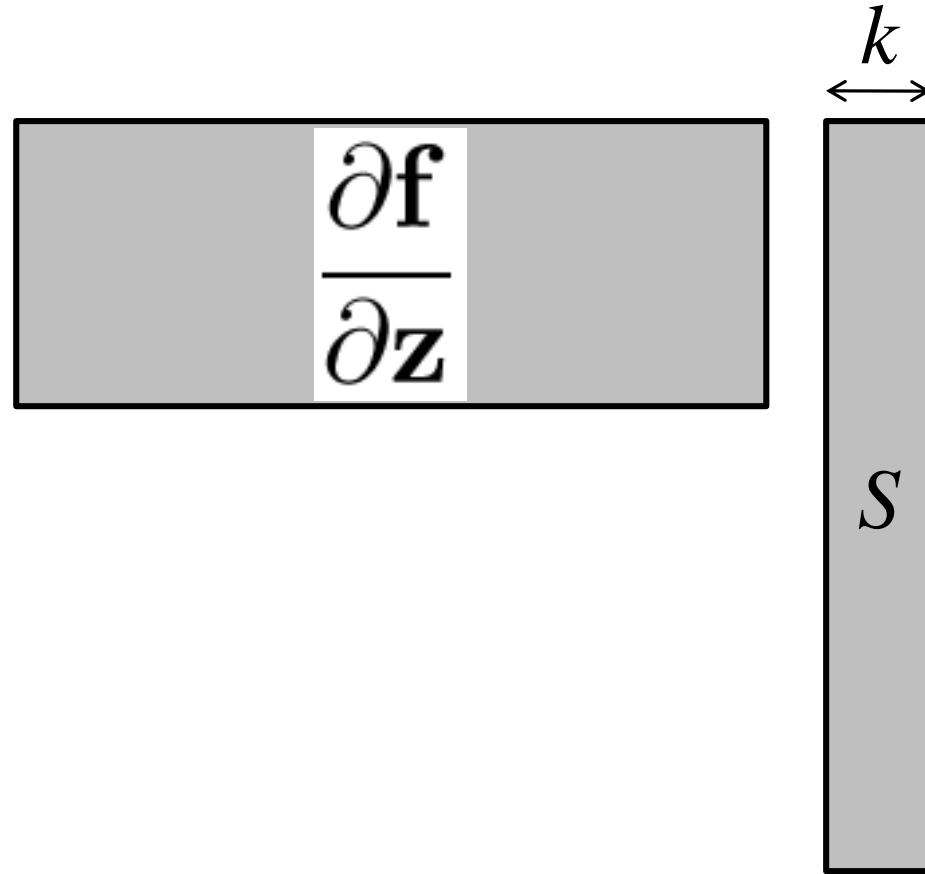
- Options: Program evaluating

a) $\frac{\partial \mathbf{f}}{\partial \mathbf{z}} \cdot S \quad (N \times N) \cdot (N \times k)$

b) $S \cdot \frac{\partial \mathbf{f}}{\partial \mathbf{z}} \quad (k \times N) \cdot (N \times N)$

Runtimes: $T(N, k) \approx k \cdot T_{\mathbf{f}}(N)$

Try to minimize k



Try to minimize k



Exploitation of Sparsity

$$\begin{bmatrix} 2 & 0 & 0 & 0 & 4 \\ 0 & 1 & 0 & 5 & 0 \\ 3 & 0 & 6 & 0 & 7 \end{bmatrix} \cdot \begin{array}{c} \xleftarrow{k=3} \\ \begin{bmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{bmatrix} \end{array} = \begin{bmatrix} 2 & 0 & 4 \\ 1 & 0 & 5 \\ 3 & 6 & 7 \end{bmatrix}$$

$$\frac{\partial \mathbf{f}}{\partial \mathbf{z}} \cdot S$$

Exploitation of Sparsity

$$k = 2 \uparrow \begin{bmatrix} 1 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} 2 & 0 & 0 & 0 & 4 \\ 0 & 1 & 0 & 5 & 0 \\ 3 & 0 & 6 & 0 & 7 \end{bmatrix} = \begin{bmatrix} 2 & 1 & 0 & 5 & 4 \\ 3 & 0 & 6 & 0 & 7 \end{bmatrix}$$

$$S \cdot \frac{\partial \mathbf{f}}{\partial \mathbf{z}}$$

In particular, AD allows:

- Efficient exploitation of sparsity
- Efficient ($k = 1$) matrix-vector products

$$\mathbf{y} = A\mathbf{z}$$

$$\mathbf{y} = A^T \mathbf{z}$$

- Access to complete rows and columns

Missing Connections: PC and AD

Preconditioning:

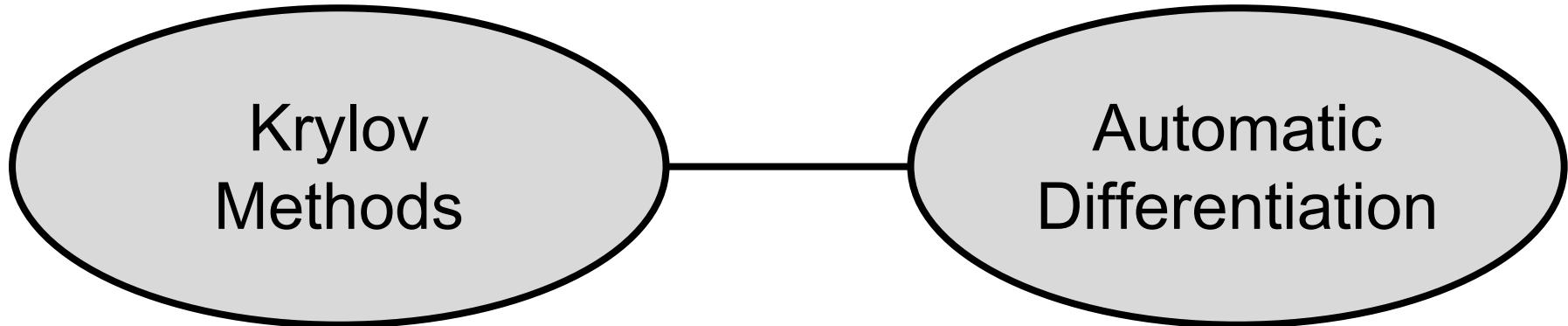
- Access to elements $A(i, j)$
- Access to chunks of rows/columns

Automatic Differentiation:

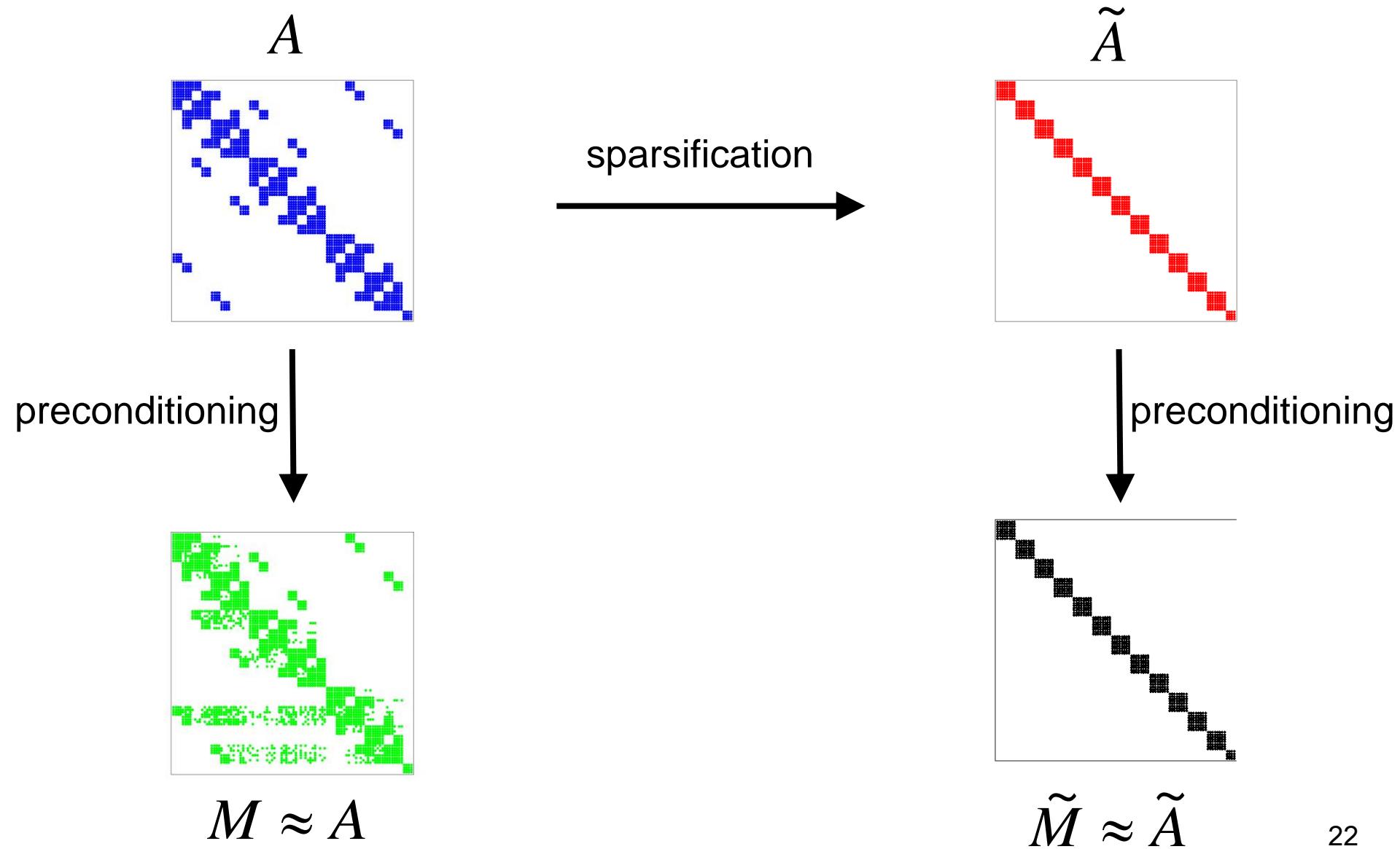
- Access to complete rows/columns
- Access to groups of complete rows/columns

⇒ No work on preconditioning with AD

Connections between Areas

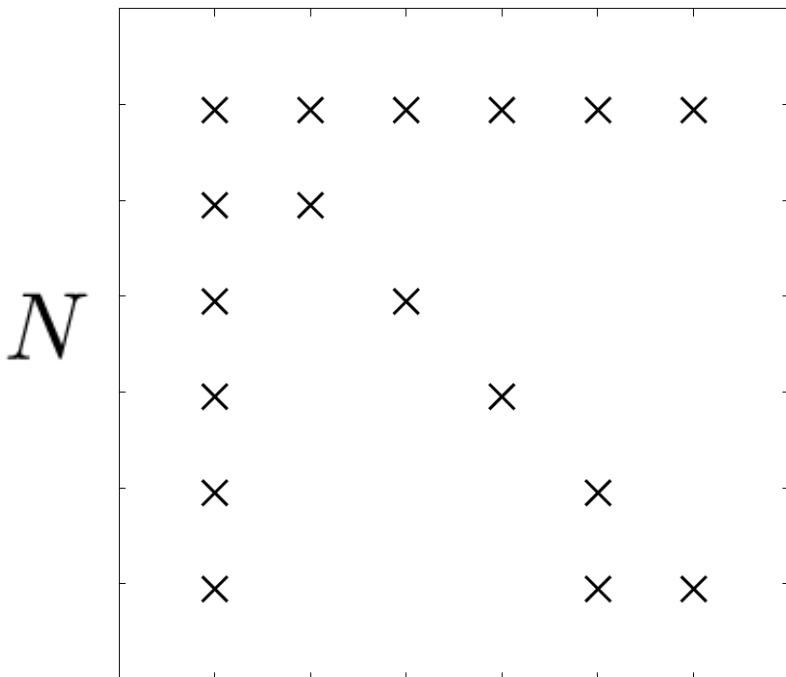


Main Idea



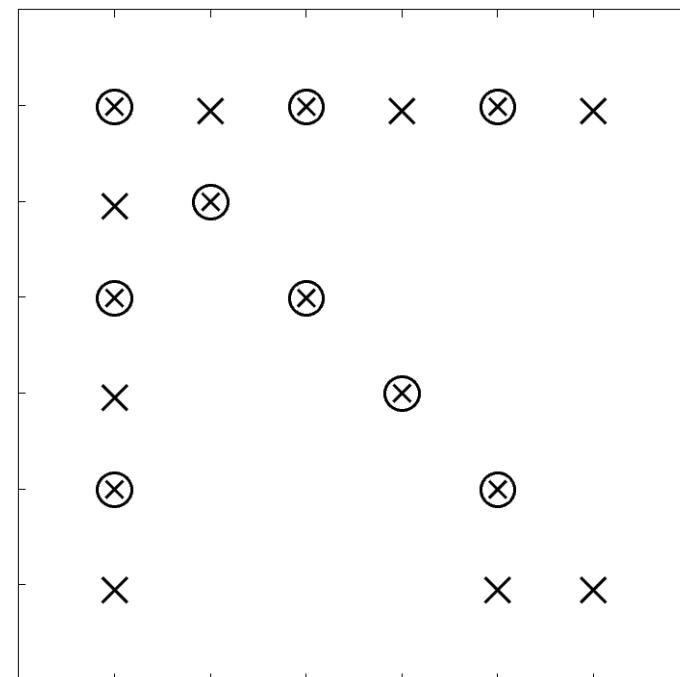
Subset of Nonzeros

Full



N

Partial



N

\otimes , „Required Elements“

Minimal Number of Colors

Uni-directional
Bi-directional

Full

×	×	×	×	×	×	×
×	×					
×		×				
×			×			
×				×		
×					×	×

$$k = N$$

Partial

\otimes	×	\otimes	×	\otimes	×	
×	\otimes					
\otimes		\otimes				
×			\otimes			
\otimes				\otimes		
×					×	×

$$k = N/2 + 1$$

×	×	×	×	×	×	×
×	×					
×		×				
×			×			
×				×		
×					×	×

$$k = 4$$

\otimes	×	\otimes	×	\otimes	×	
×	\otimes					
\otimes		\otimes				
×			\otimes			
\otimes				\otimes		
×					×	×

$$k = 3$$

Bipartite Graph

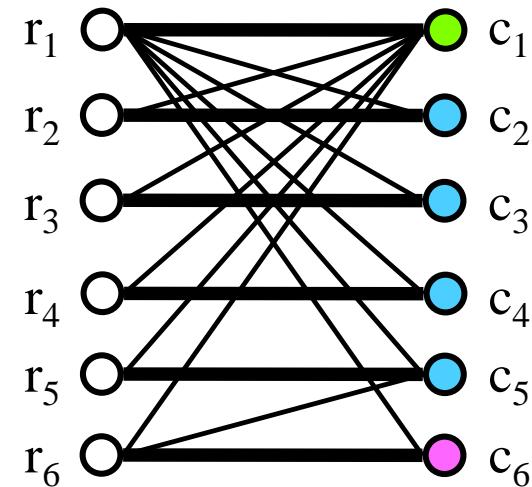
$$G(A) = (V_r, V_c, E)$$

$$V_r = \{r_i \mid 1 \leq i \leq N\}$$

$$V_c = \{c_i \mid 1 \leq i \leq N\}$$

$$E = \{(r_i, c_j) \mid A(i, j) \neq 0\}$$

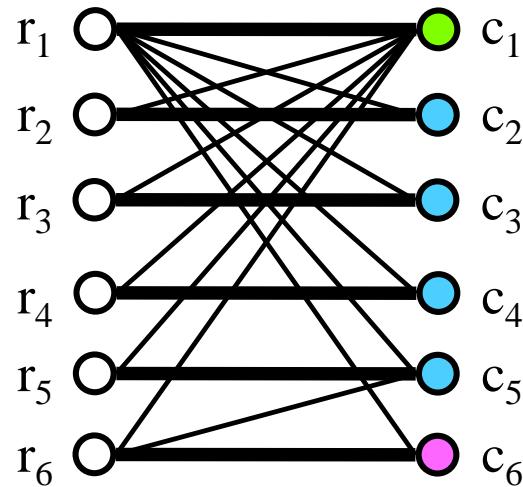
⊗	×	×	×	×	×
×	⊗				
×		⊗			
×			⊗		
×				⊗	
×				×	⊗



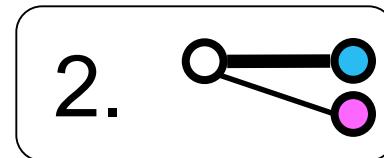
[Gebremedhin, Manne, Pothen] *SIAM Review* 2005

Diagonal Preconditioning

$$E_D = \{(1, 1), \dots, (N, N)\}$$



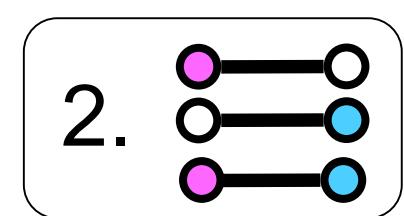
Restricted Distance-2 Coloring

- $G(A) = (V_r, V_c, E)$, Required Elements:
Diagonal $E_D = \{(1, 1), \dots, (N, N)\}$
- Mapping $\phi_c : V_c \longrightarrow \{1, \dots, k\}$ is called *distance-2 coloring restricted to E_D*
 1. $\forall (r_i, c_i) \in E_D$ gilt $\phi_c(c_i) \neq 0$ 
 2. Distance-2 neighbors c_i and c_j have different colors, if \exists path of length 2 with at least one edge in E_D 

Restricted Star Bicoloring

(i)

- $G(A) = (V_r, V_c, E)$, Required Elements:
Diagonal $E_D = \{(1, 1), \dots, (N, N)\}$
- Mapping $\phi : V_r \cup V_c \longrightarrow \{1, \dots, k\}$ is called
star bicoloring restricted to E_D
 1. Different colors for
nodes from V_r and V_c (except 0)

 2. At least one node incident
to $(r_i, c_i) \in E_D$ is colored
different from zero


Restricted Star Bicoloring

(ii)

3. $\forall (r_i, c_i) \in E_D:$

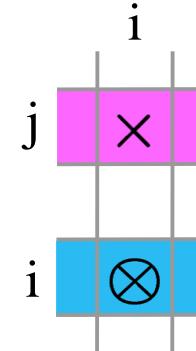
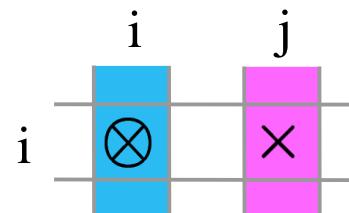
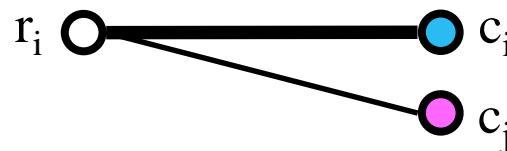
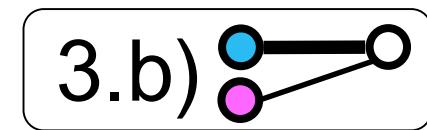
a) If $\phi(r_i) = 0$, then

$\phi(c_i) \neq \phi(c_j) \quad \forall (c_i, r_i, c_j)$



b) If $\phi(c_i) = 0$, then

$\phi(r_i) \neq \phi(r_j) \quad \forall (r_i, c_i, r_j)$



Restricted Star Bicoloring

(iii)

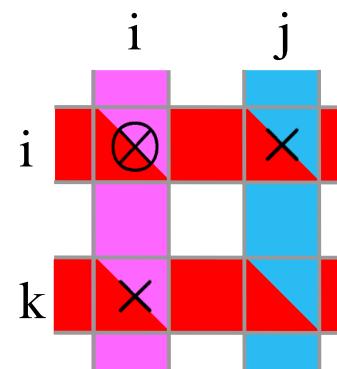
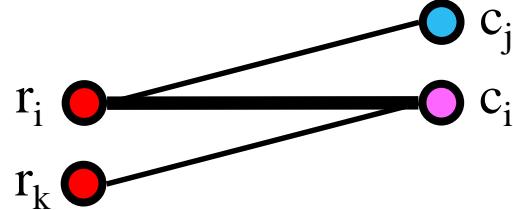
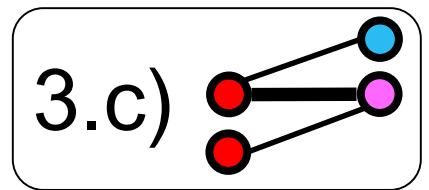
3. $\forall (r_i, c_i) \in E_D:$

c) If $\phi(r_i) \neq 0$ and $\phi(c_i) \neq 0$, then

$\forall (c_j, r_i, c_i, r_k)$

either $\phi(r_i) \neq \phi(r_k)$

or $\phi(c_i) \neq \phi(c_j)$



Bi- is no better than Unidirectional

Theorem (B, Lülfesmann, Wolf):

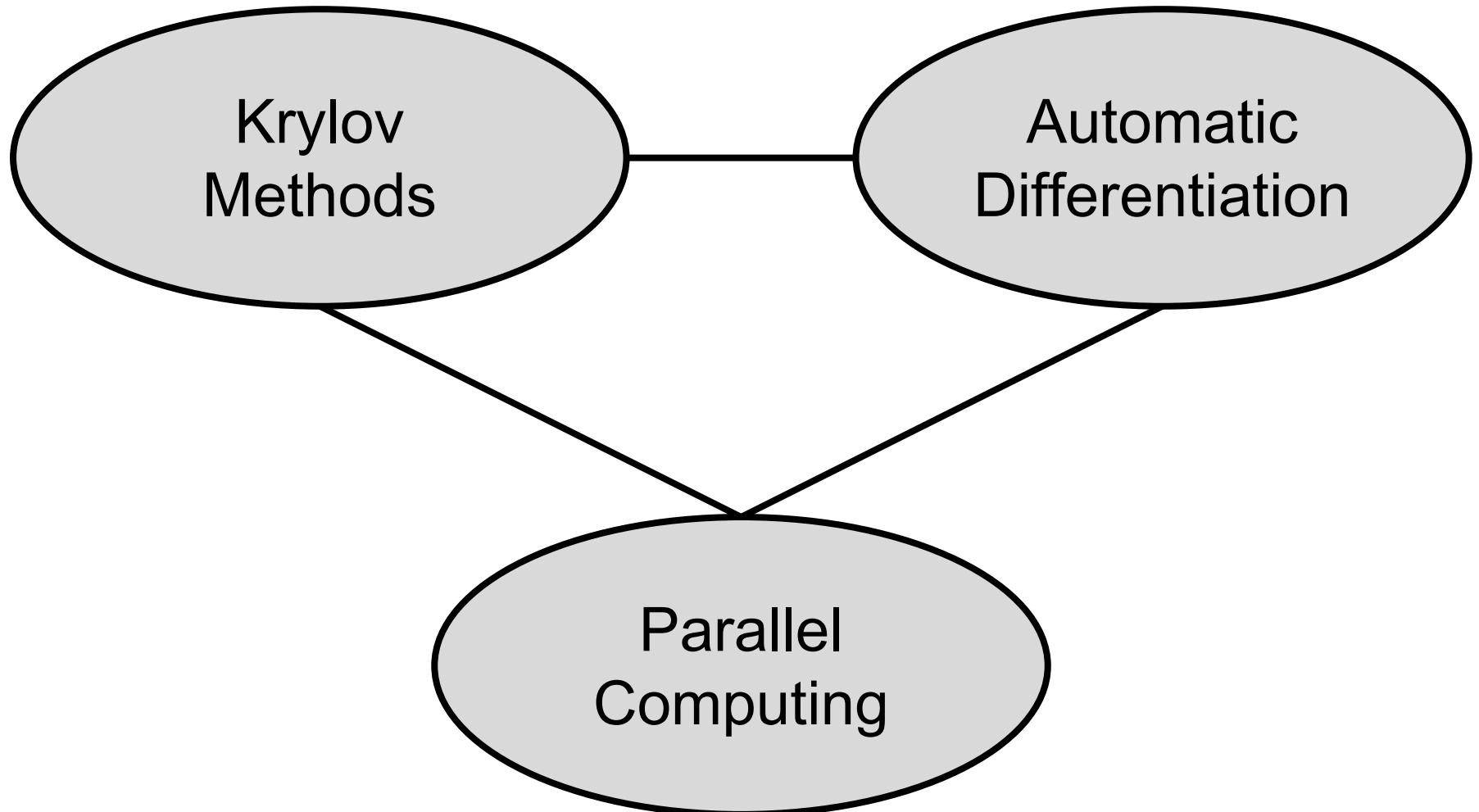
Let $G(A) = (V_r, V_c, E)$

with $E_D = \{(1, 1), \dots, (N, N)\}$.

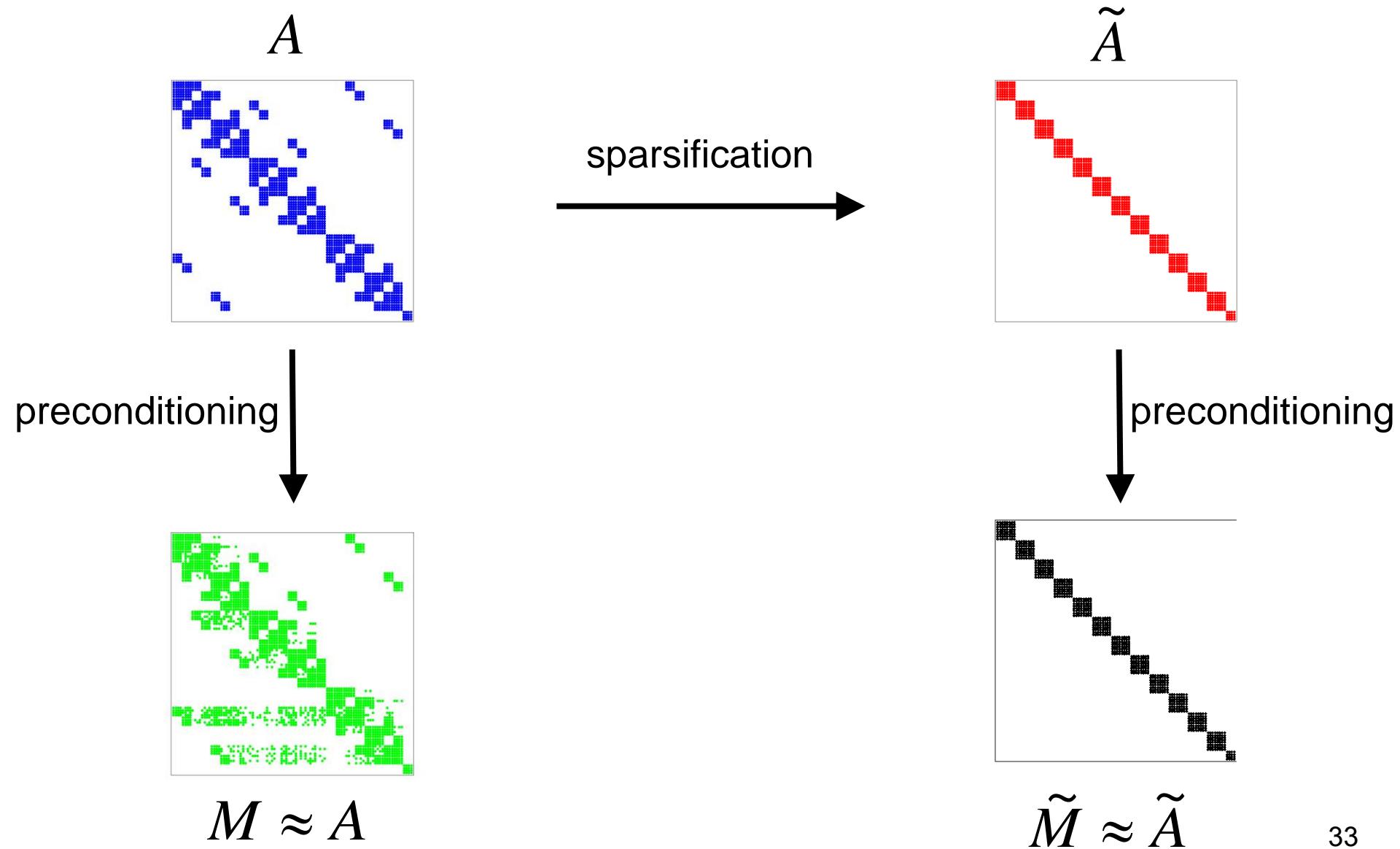
Minimal number of colors is equal for

- Distance-2 coloring restricted to E_D
- Star bicoloring restricted to E_D

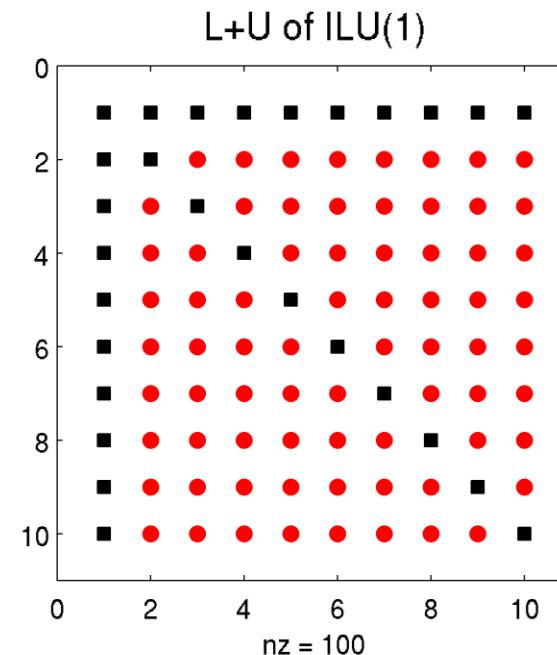
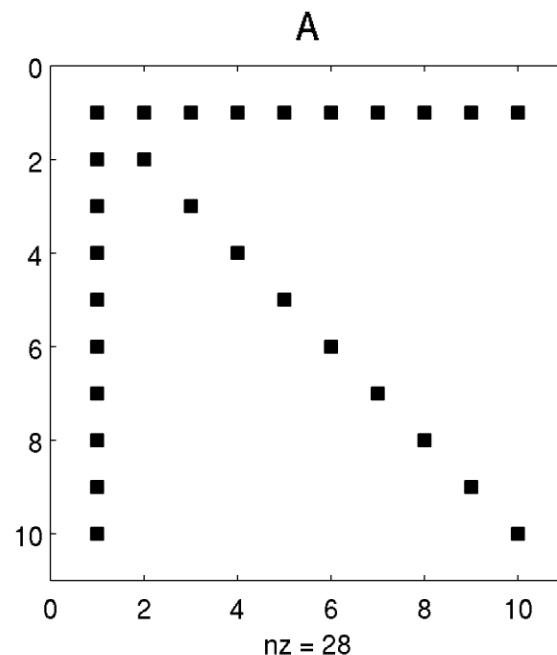
Research Areas



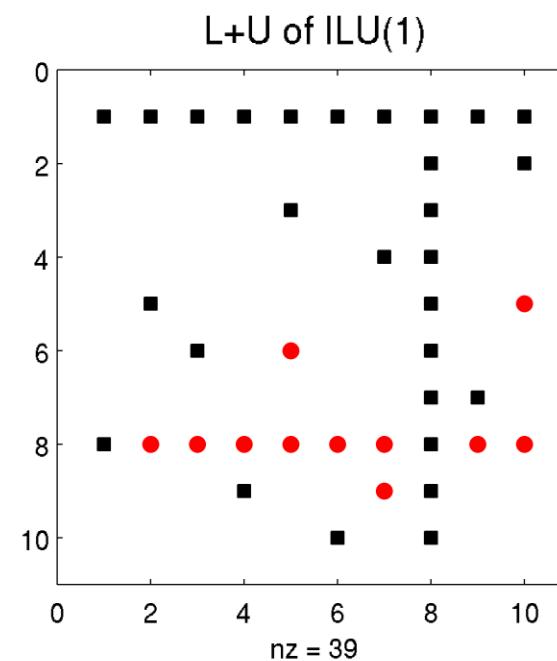
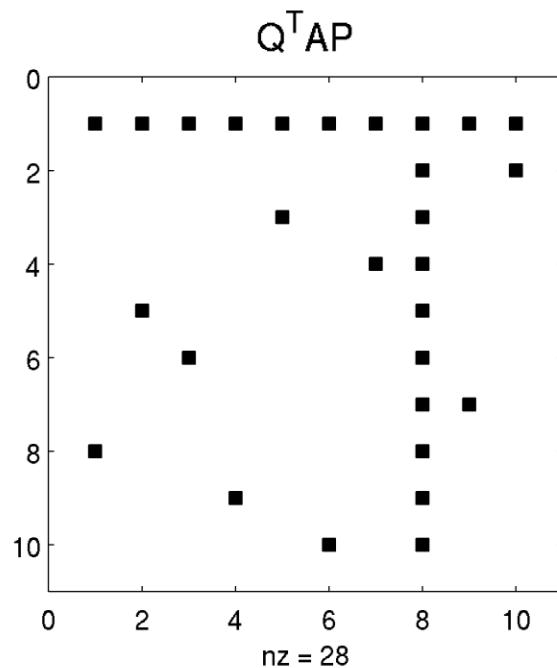
Main Idea



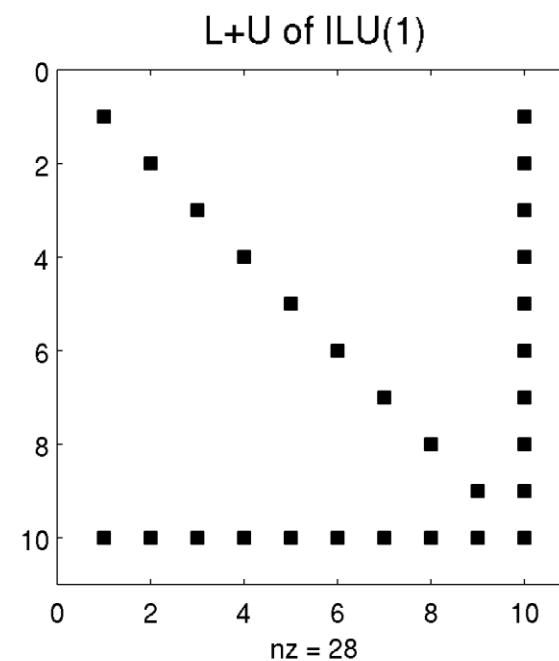
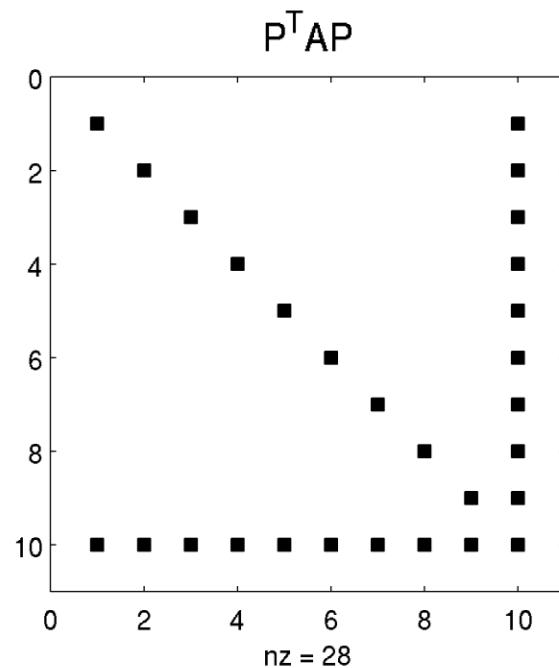
ILU(L): Influence of Ordering



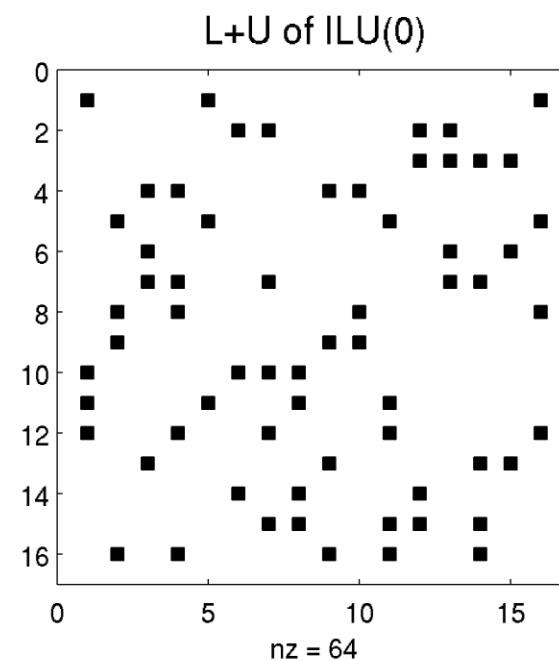
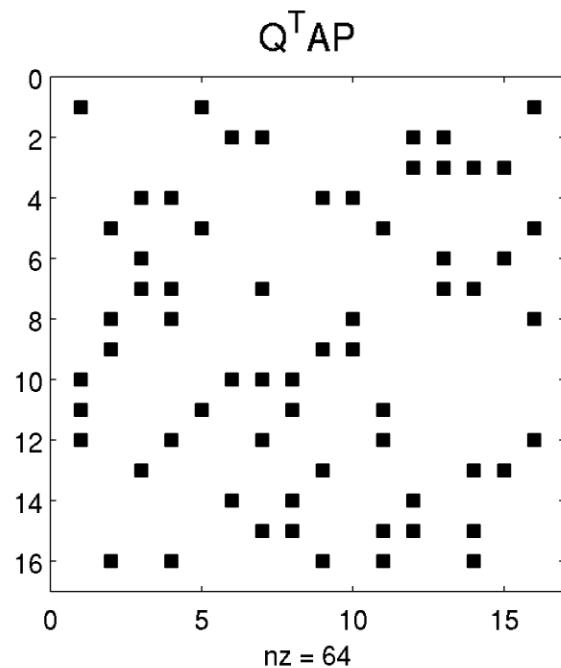
ILU(L): Influence of Ordering



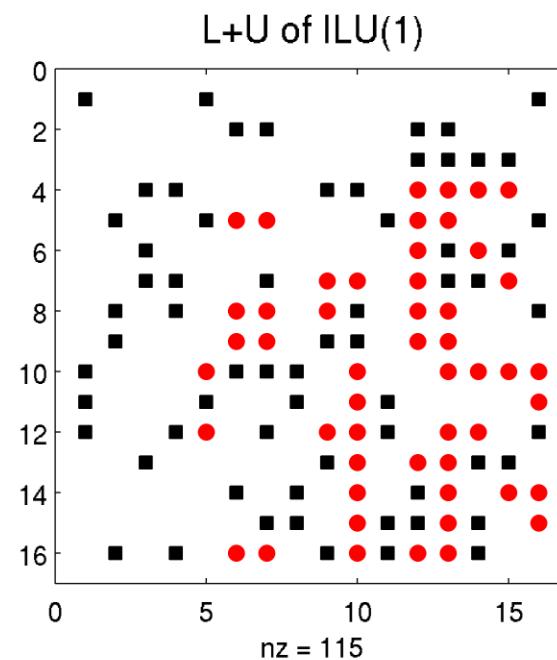
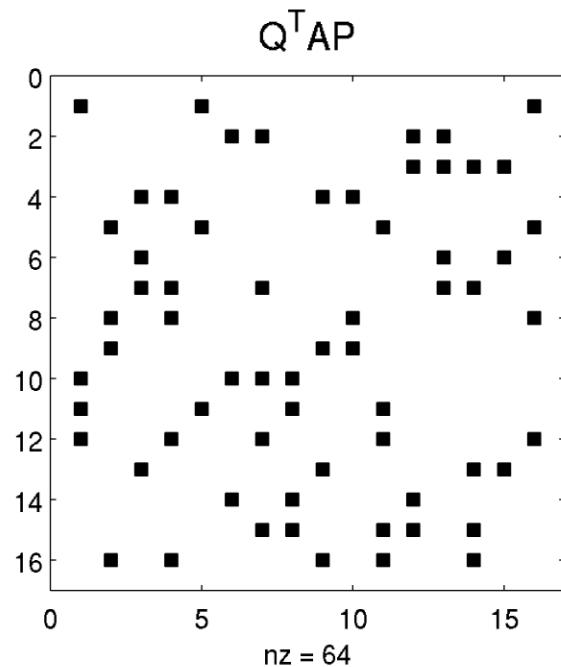
ILU(L): Influence of Ordering



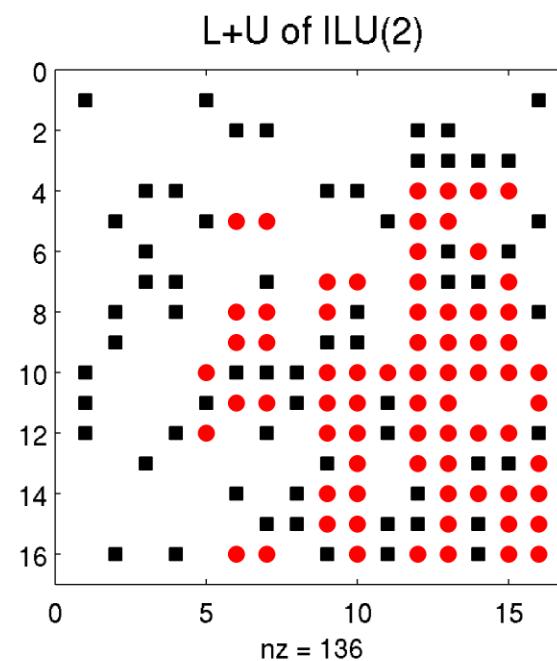
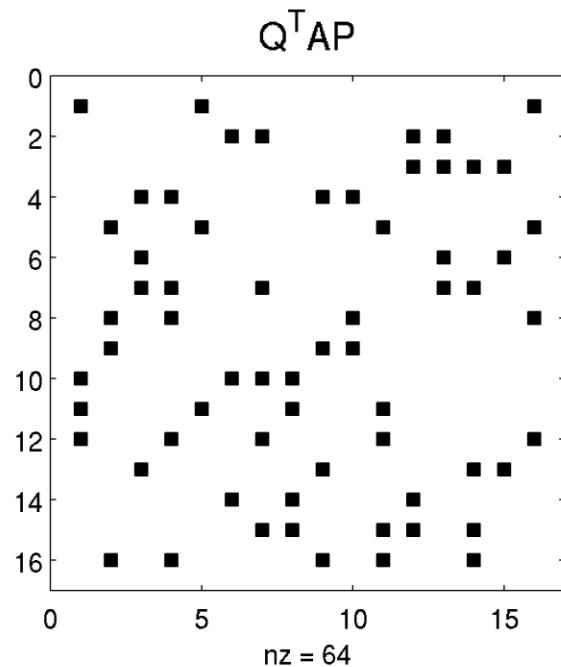
$\text{ILU}(L)$: Influence of Level



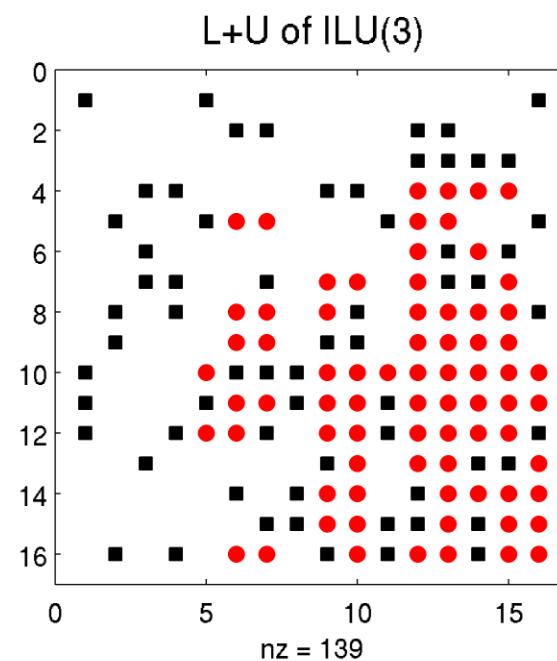
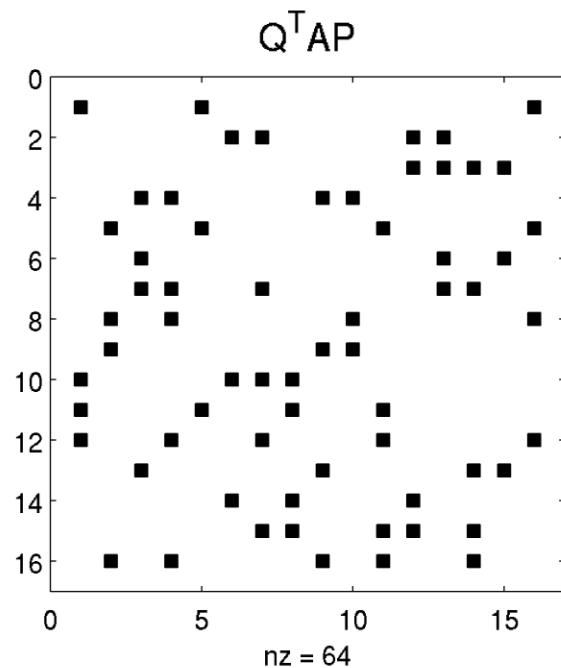
$\text{ILU}(L)$: Influence of Level



$\text{ILU}(L)$: Influence of Level



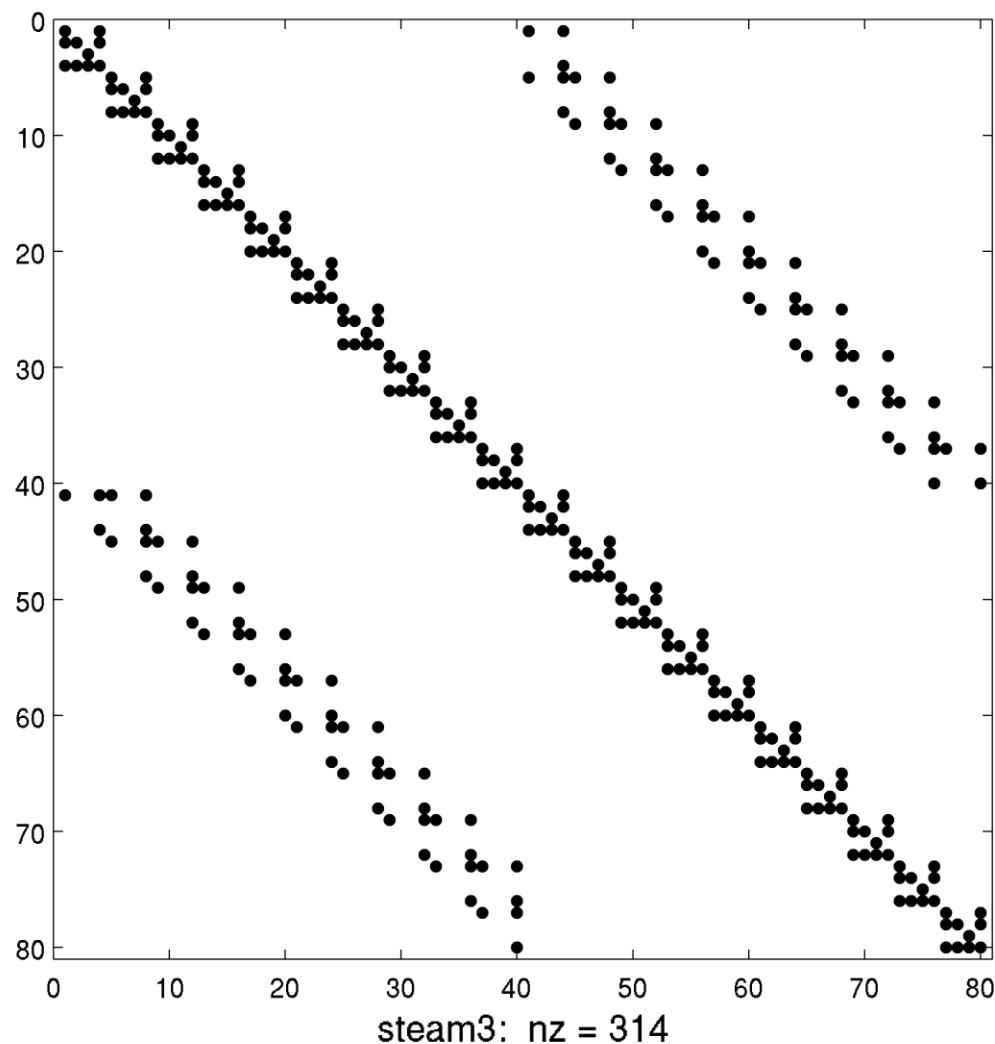
$\text{ILU}(L)$: Influence of Level

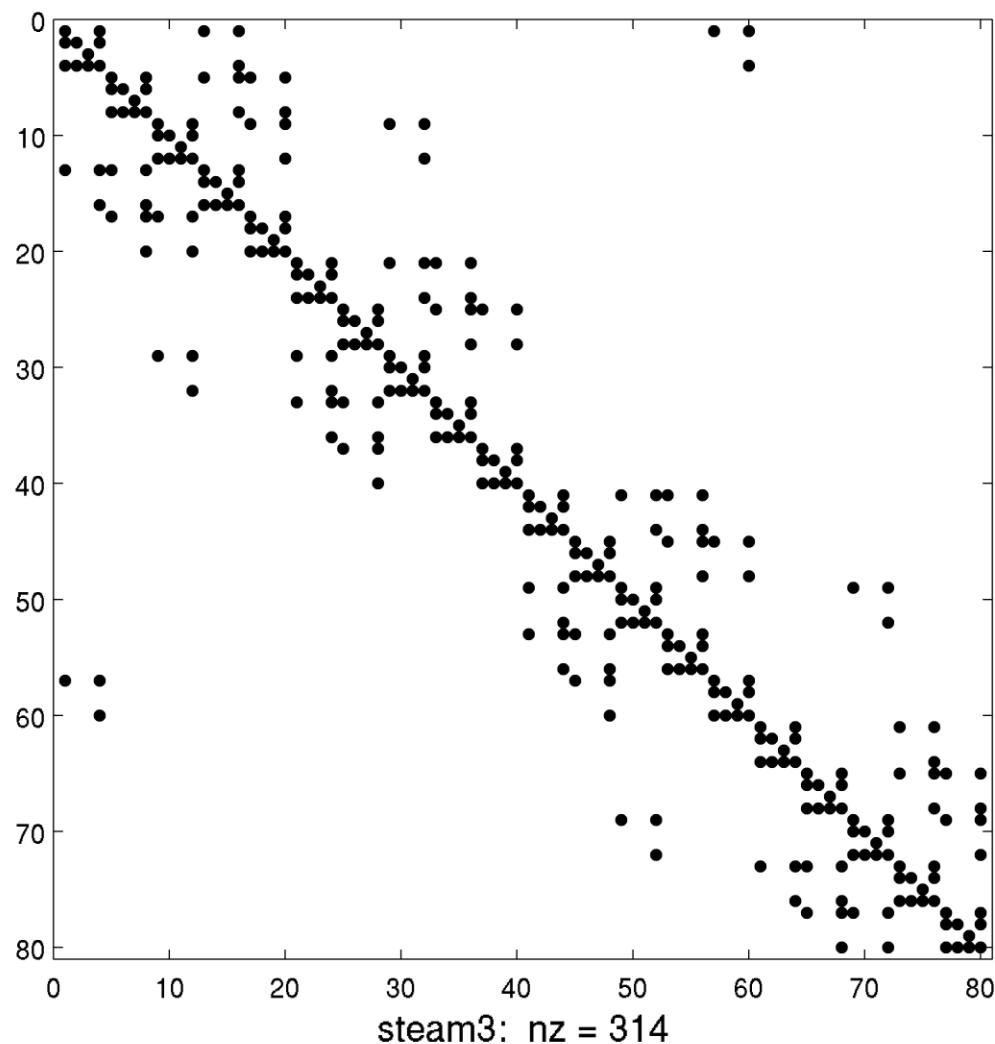


Sparsification & Parallel

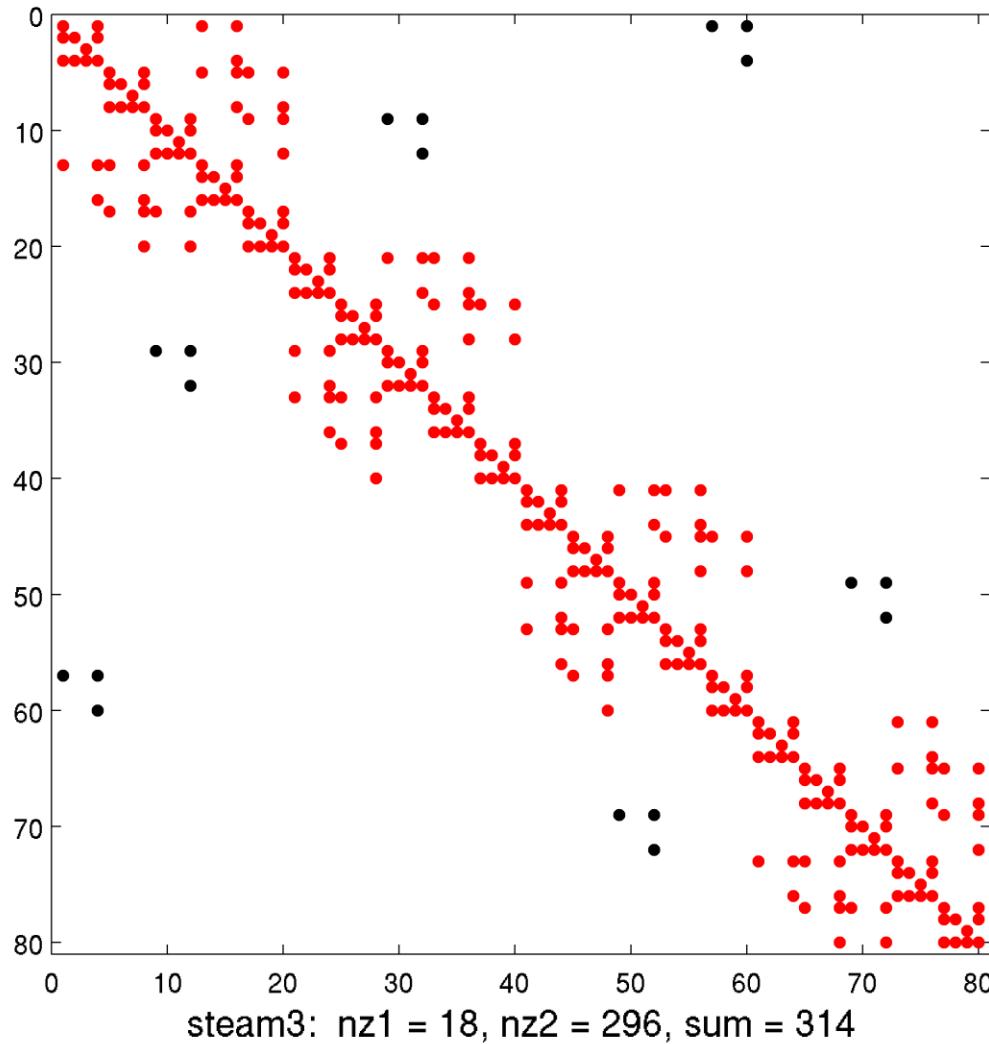
- Permute such that many nonzeros gather around diagonal
- Sparsify in form of block diagonal
- Apply ILU(L) to each block
- Advantages:
 - ◆ Parallel construction of M
 - ◆ Parallel application $M\mathbf{y} = \mathbf{z}$

A

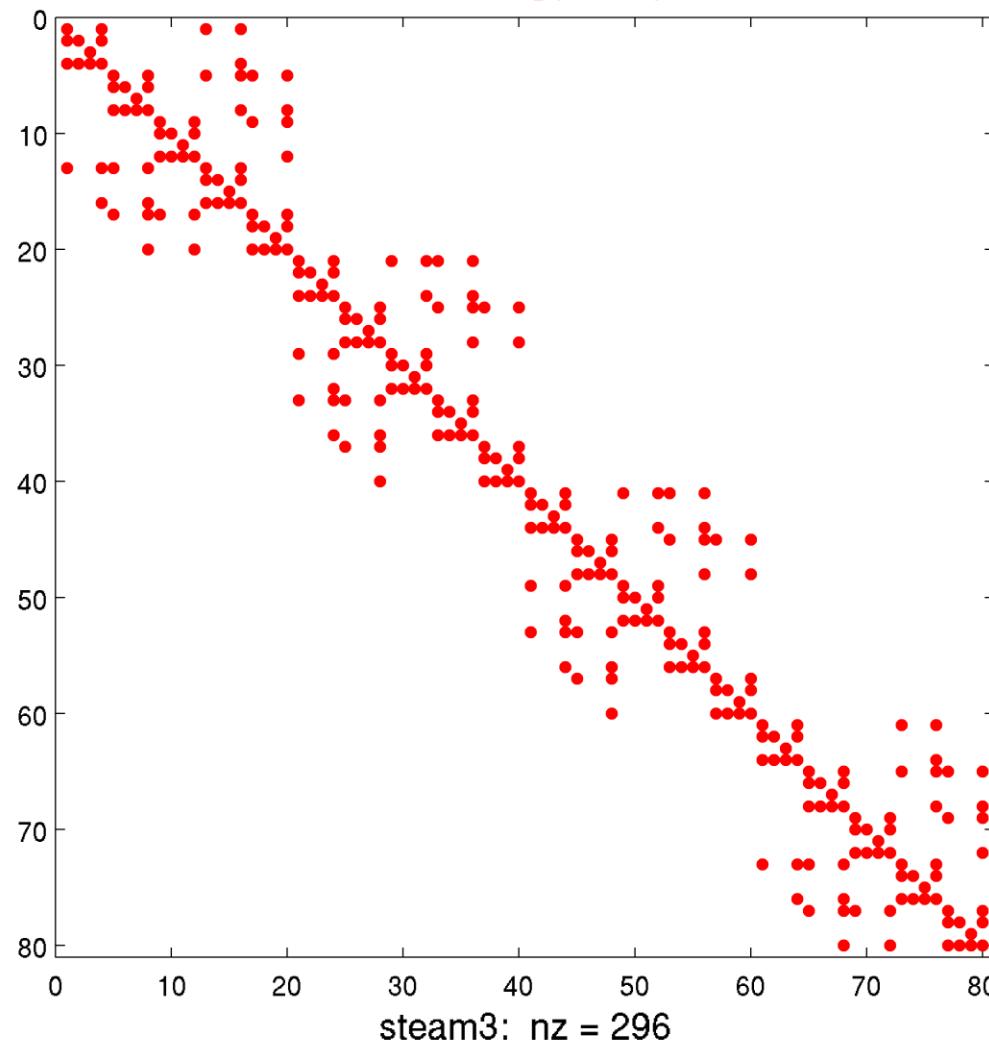


$P^T A P$ 

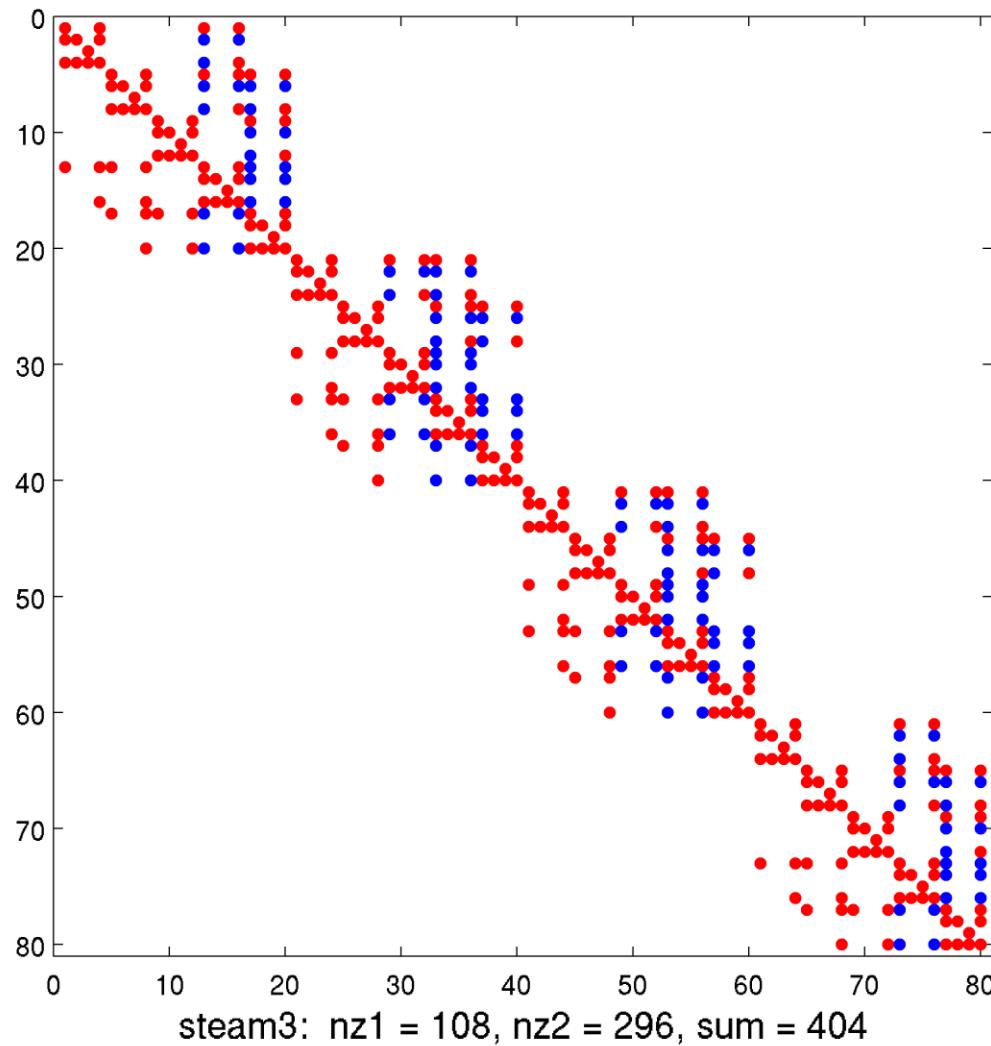
$P^T AP$ including BlockDiag($P^T AP$)



BlockDiag($P^T AP$)



ILU(BlockDiag($P^T AP$)) including BlockDiag($P^T AP$)



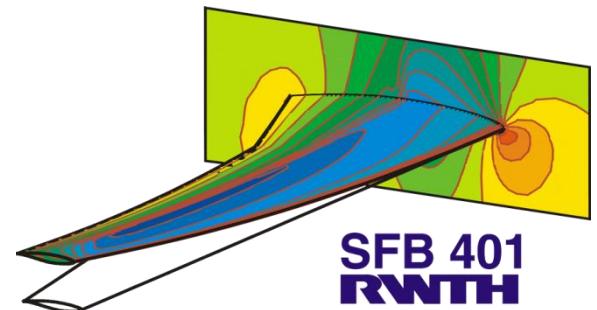
QUADFLOW

Josef Ballmann
Mechanik



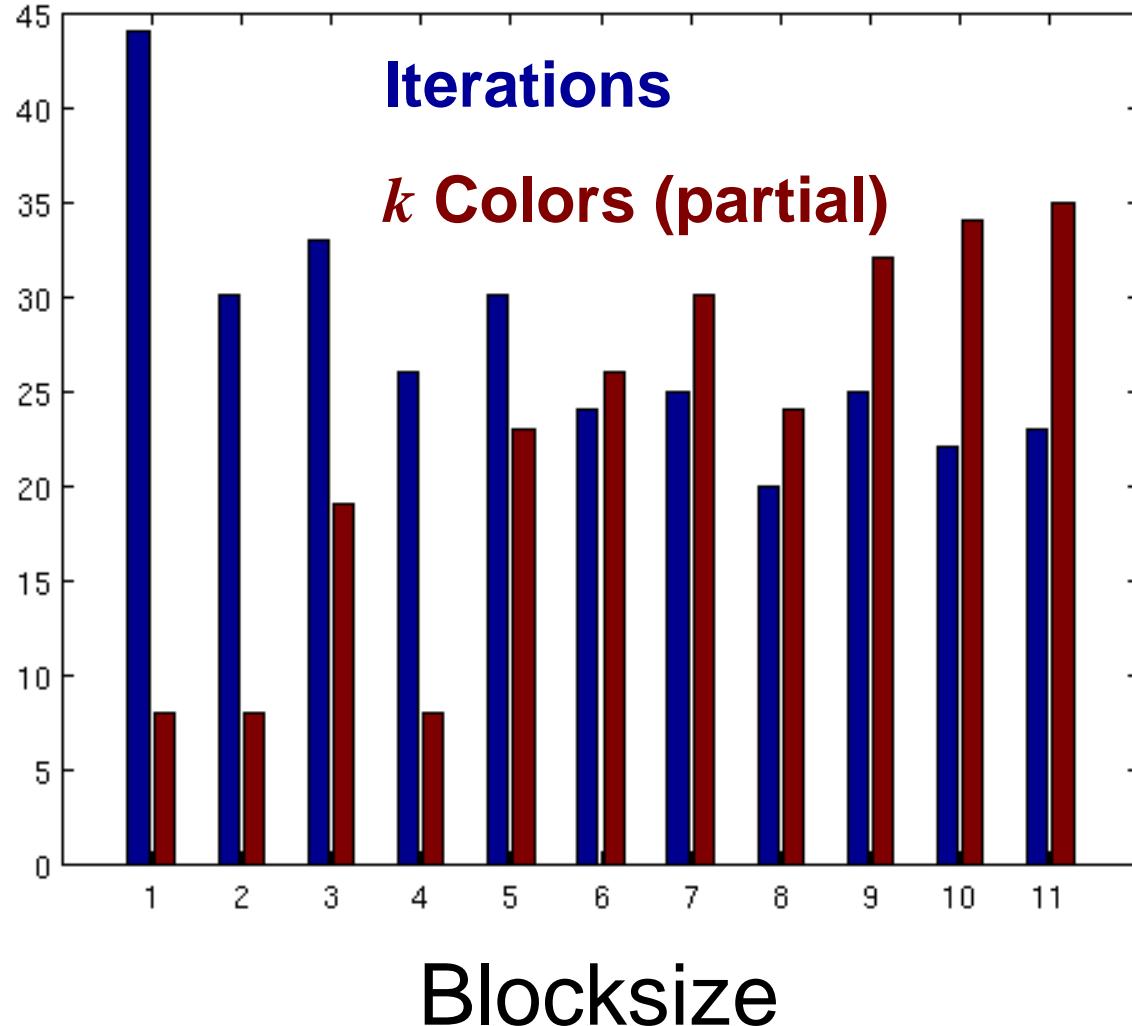
RHEINISCH-
WESTFÄLISCHE
TECHNISCHE
HOCHSCHULE
AACHEN

- Finite volume
- Implicit time integration
- Unstructured grid
- Adaptation via Multiscale analysis
(Wolfgang Dahmen, Siegfried Müller)



Institut für Geometrie und Praktische Mathematik **igpm**

Results for Blockdiagonal PC

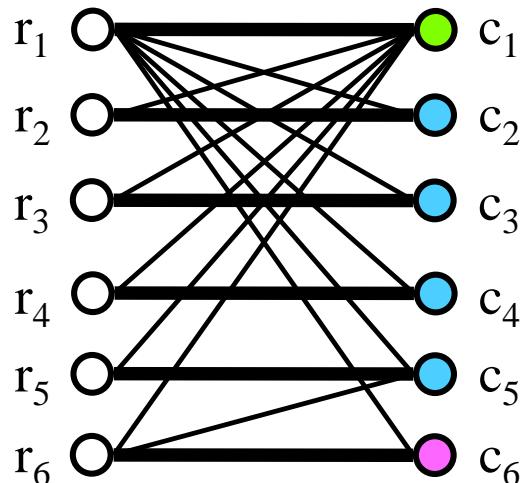


Without PC:
177 Iterations

Full:
 $k = 36$

- GMRES
- ILU(0)

Missing Connection: Coloring and ILU



```
for i = 1:n
    % All entries of A are entries of F with level = 0.
    index_nnz = find( A(i,:)==1 );
    level(i,index_nnz) = 0;
    F(i,index_nnz) = 1;
    % Update phase
    for k = 1:i-1 % node (i,k) with k < i
        if F(i,k)==1
            for j = k + find( F(k,k+1:n)==1 ) % node (k,j) with k < j
                lev = level(i,k) + level(k,j) + 1;
                if(lev <= el)
                    if F(i,j)==0
                        F(i,j) = 1;
                        level(i,j) = lev;
                    else
                        level(i,j) = min(level(i,j),lev);
                    end;
                end;
            end;
        end;
    end;
```

Symbolic ILU on bipartite graph

$$\begin{aligned} G(A) = (V_r, V_c, E) \quad & V_r = \{r_i \mid 1 \leq i \leq N\} \\ & V_c = \{c_i \mid 1 \leq i \leq N\} \\ & E = \{(r_i, c_j) \mid A(i, j) \neq 0\} \\ & \sigma : E \longrightarrow \mathbb{N} \\ & \sigma((r_i, c_j)) = \text{lev}(i, j) \end{aligned}$$

Path $(r_i, c_k, r_k, c_l, r_l, \dots, c_j)$ is called *fill path from r_i to c_j* , if for all indices m of inner nodes the inequality $m < \min(i, j)$ holds.

Sequence of Graphs for ILU(L)

$$G_\nu = (V_r, V_c, E_\nu), \quad \nu = 0, 1, \dots, N$$

$$\begin{aligned} G_0 = G(A) \quad & \forall (r_i, c_j) \in E_0 = E \\ & \sigma((r_i, c_j)) = 0 \end{aligned}$$

$$G_{\nu+1} = (V_r, V_c, E_{\nu+1})$$

$$\begin{aligned} E_{\nu+1} = E_\nu \cup \{ \exists \text{ Fill path } (r_i, c_k, r_k, c_j) \\ \text{ of length 3 in } G_\nu \text{ and} \\ t(k) := \text{lev}_\nu(i, k) + \text{lev}_\nu(k, j) + 1 \leq L \} \\ \sigma((r_i, c_j)) = \text{lev}_{\nu+1}(i, j) = \min_k (\text{lev}_\nu(i, j), t(k)) \end{aligned}$$

„Static“ Determination of Fill-in

Lemma:

$(r_i, c_j) \in E_N$ in G_N with $\text{lev}(i, j) = k$

\Leftrightarrow

\exists shortest fill path of length $2k + 1$
between r_i and c_j in G_0

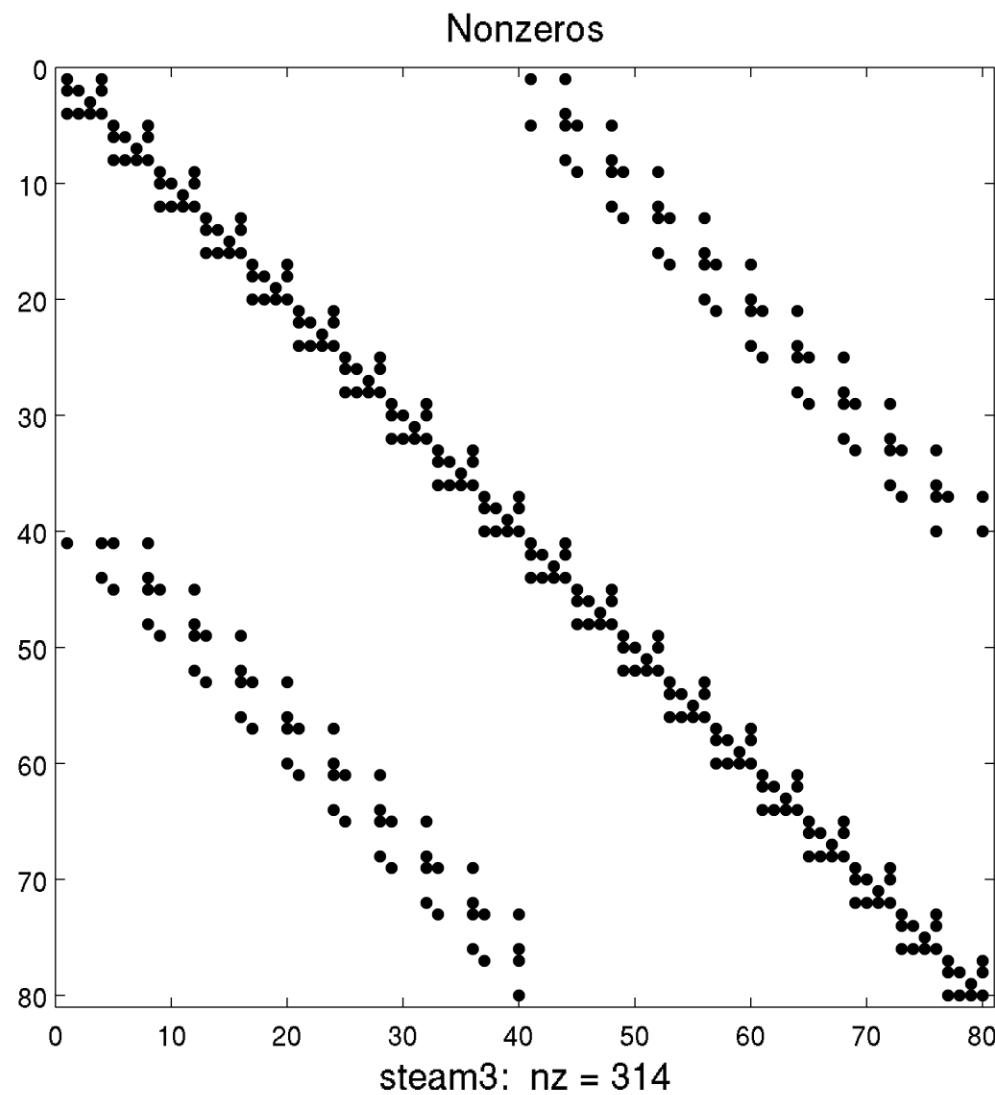
New Algorithm (PC + AD + Par)

- Compute $R_{\text{init}} = \rho(A)$
- Compute $R_{\text{init}} \dot{\cup} F = \text{SILU}(R_{\text{init}})$
- Color $\phi(R_{\text{init}}, A)$
- Compute $R_{\text{pot}} \subset A \setminus R_{\text{init}}$ such that
 $|\phi(R_{\text{init}}, A)| = |\phi(R_{\text{init}} \dot{\cup} R_{\text{pot}}, A)|$
- Compute $R_{\text{add}} \subseteq R_{\text{pot}}$ such that
 $\text{SILU}(R_{\text{init}}) \cup R_{\text{add}} = \text{SILU}(R_{\text{init}} \dot{\cup} R_{\text{add}})$
- Compute $[L, U] = \text{NILU}(R_{\text{init}} \dot{\cup} R_{\text{add}})$

steam3

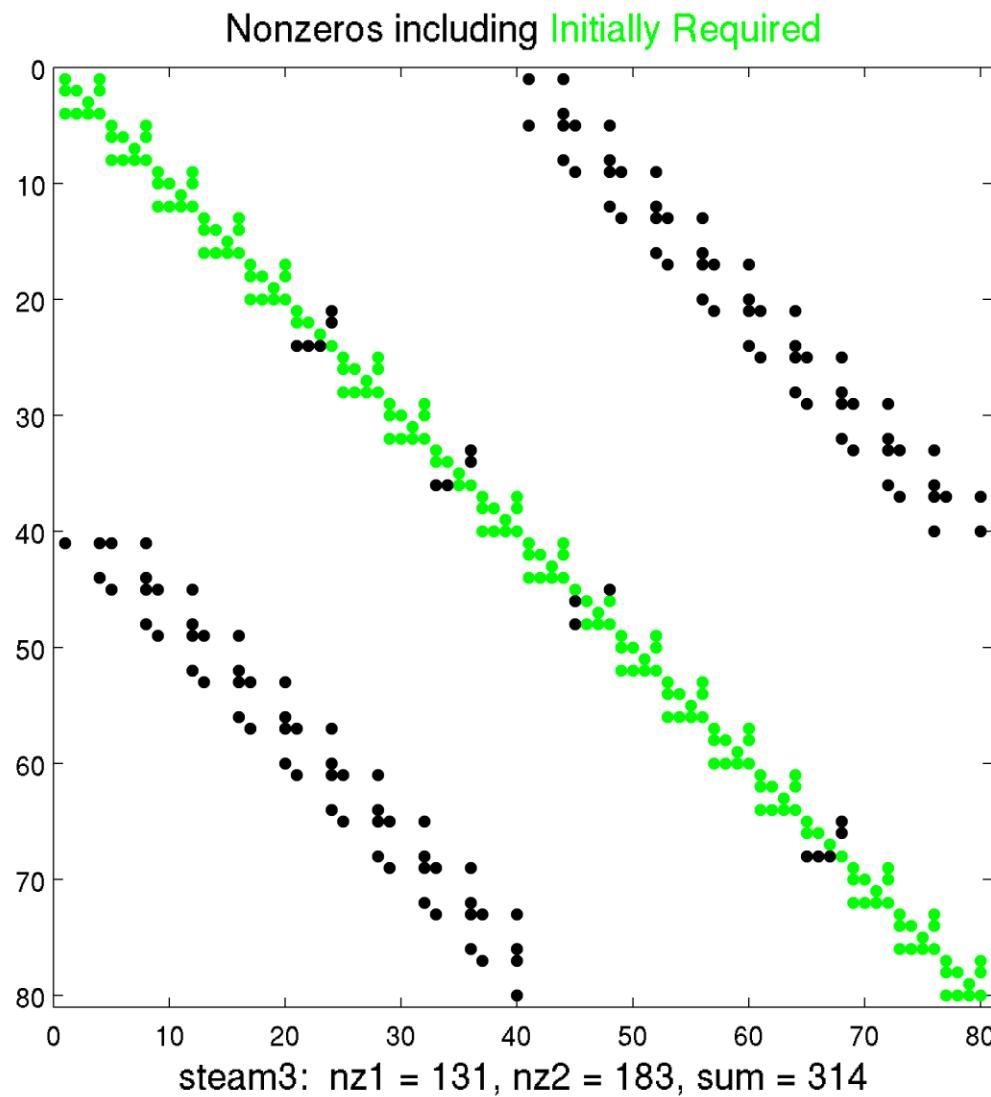
- Visualization of idea
- Small example without Fill-in

steam3



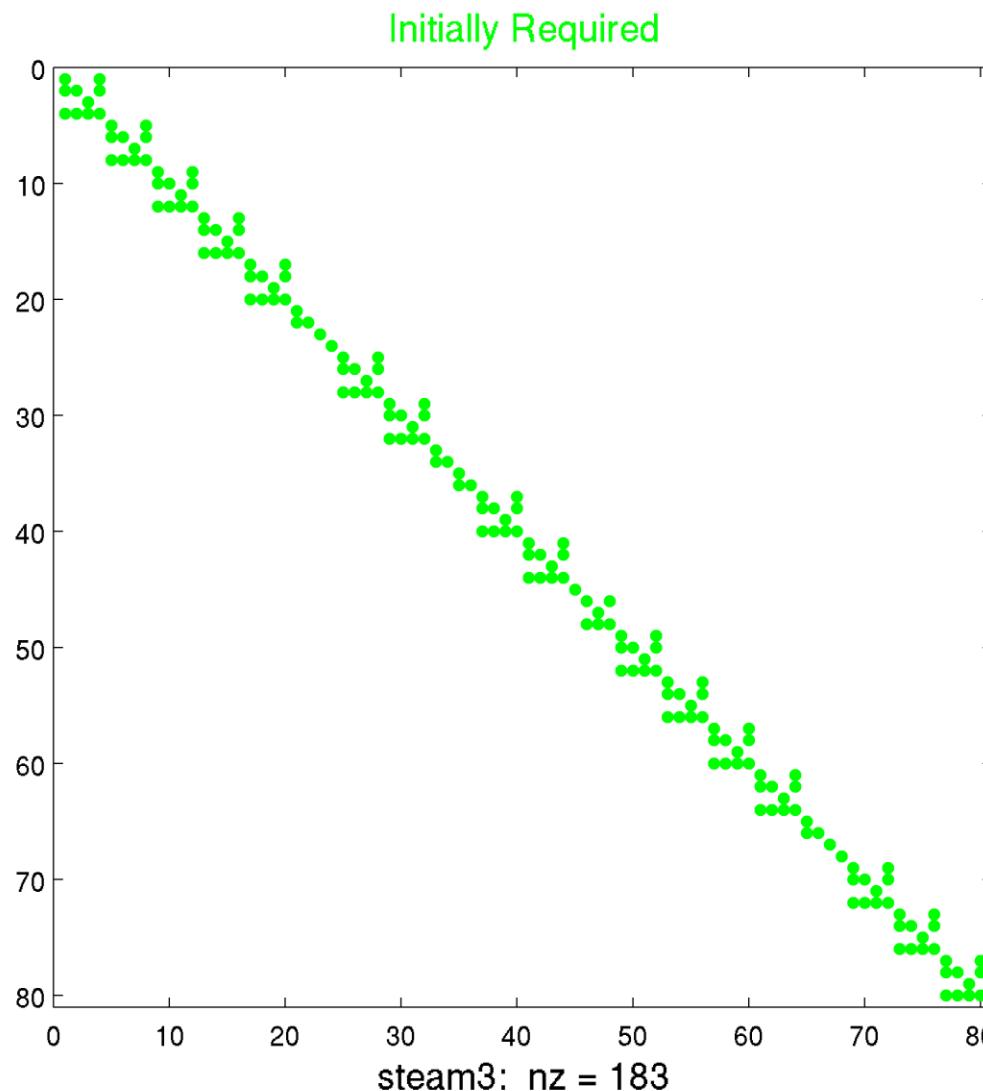
A

steam3

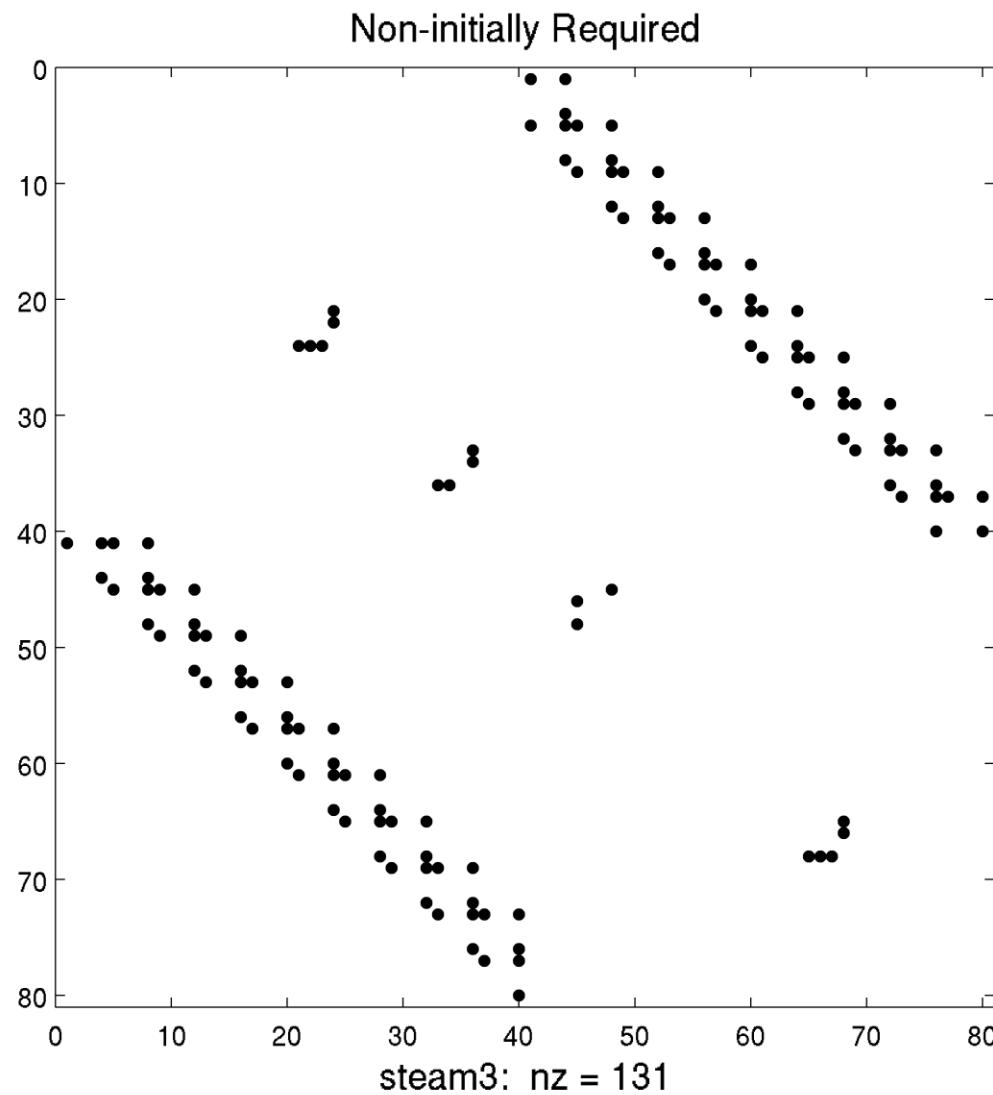


R_{init}

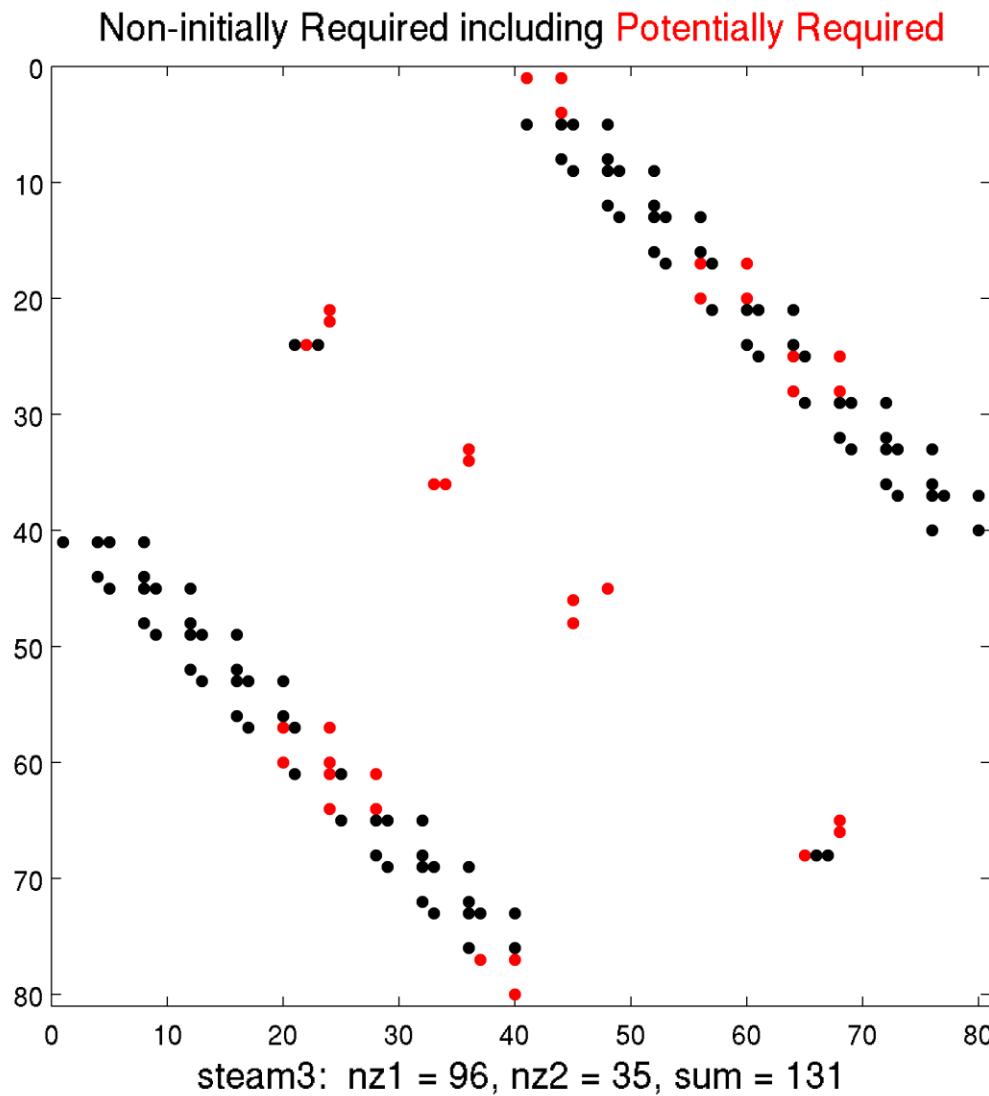
steam3

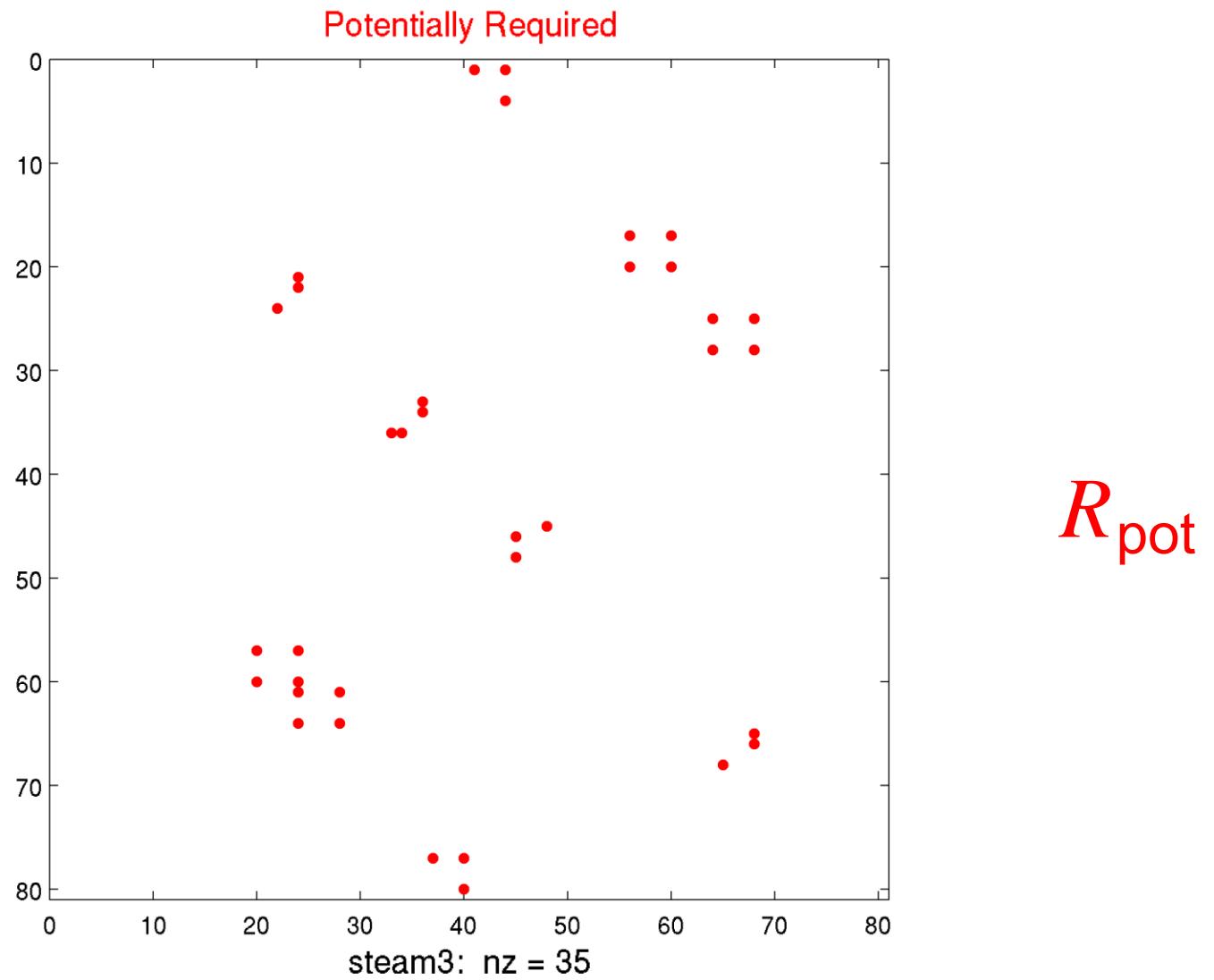


steam3

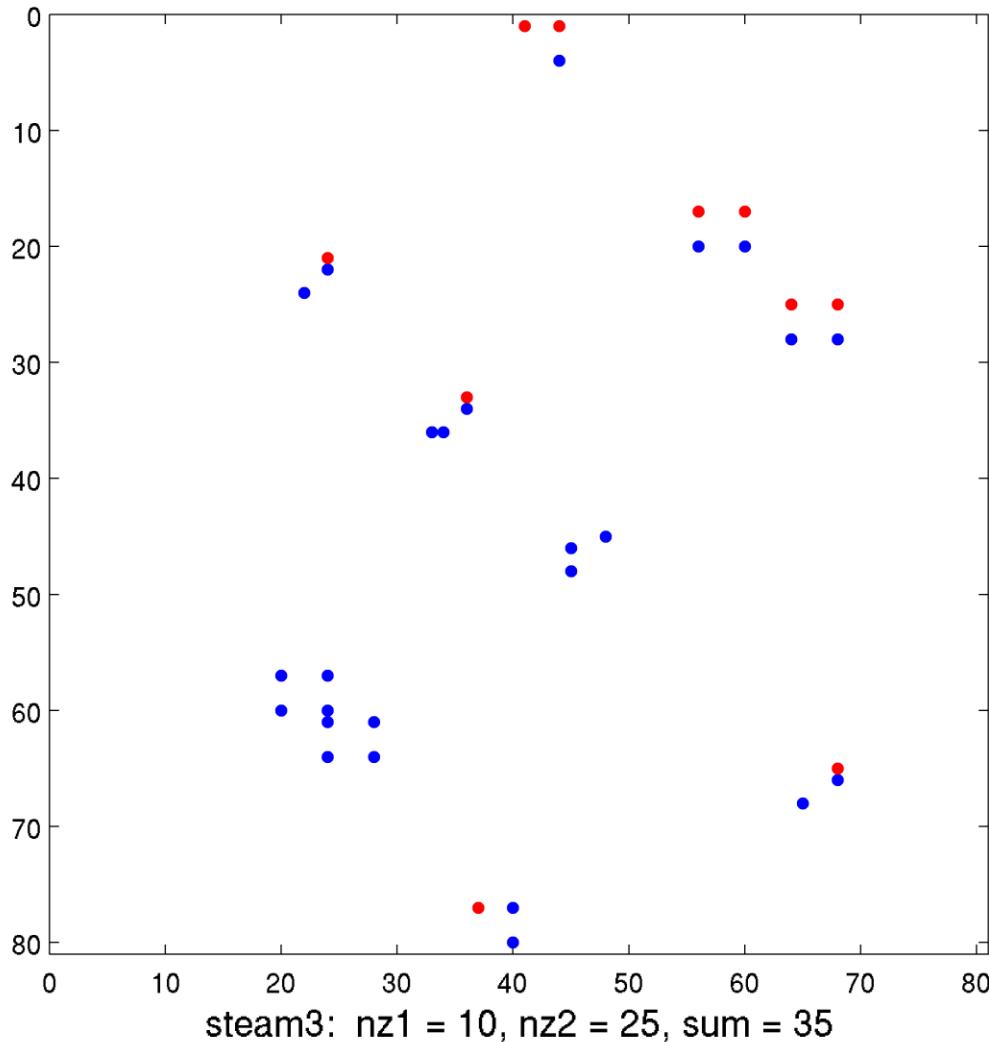

$$A \setminus R_{\text{init}}$$

steam3

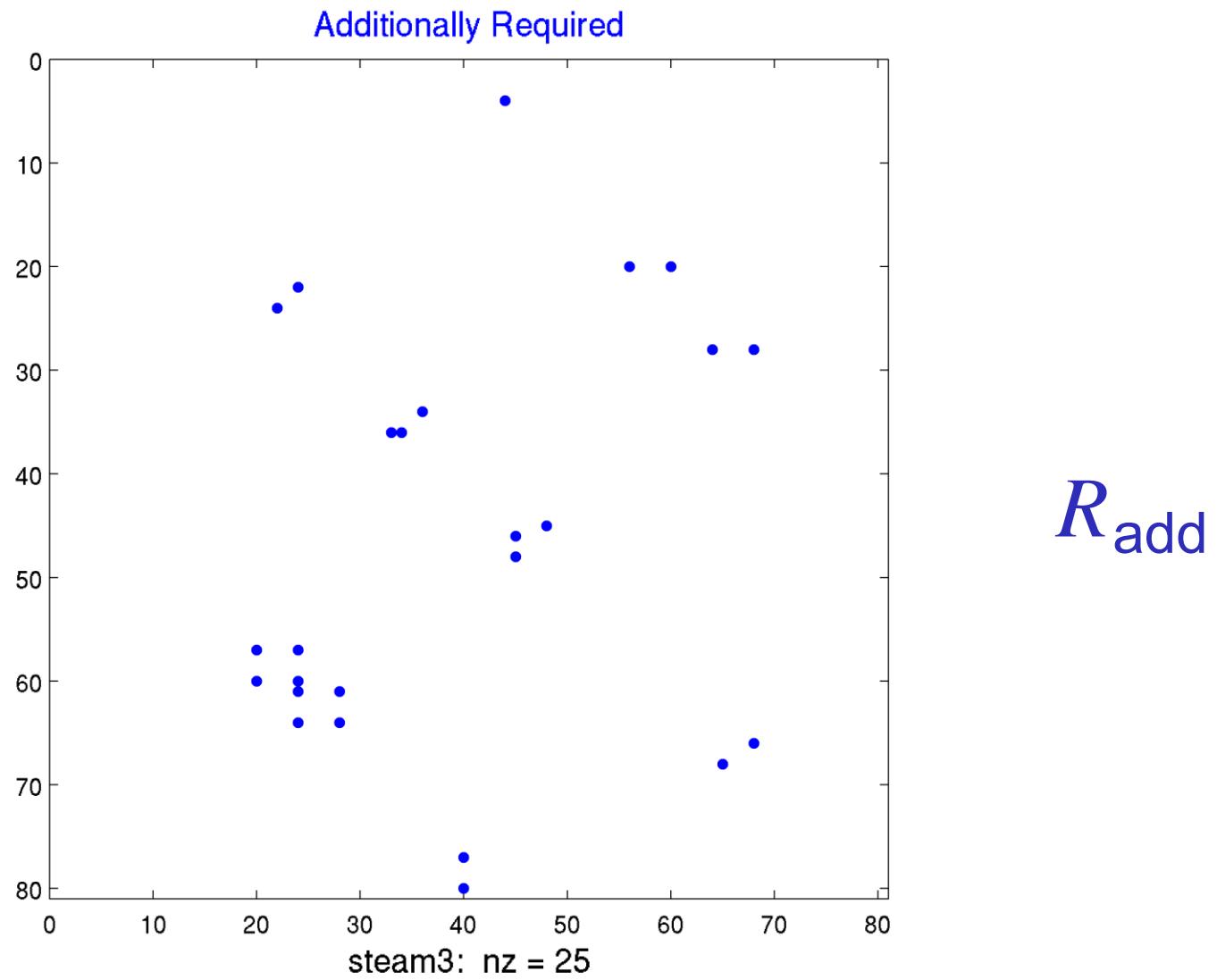




Potentially Required including Additionally Required



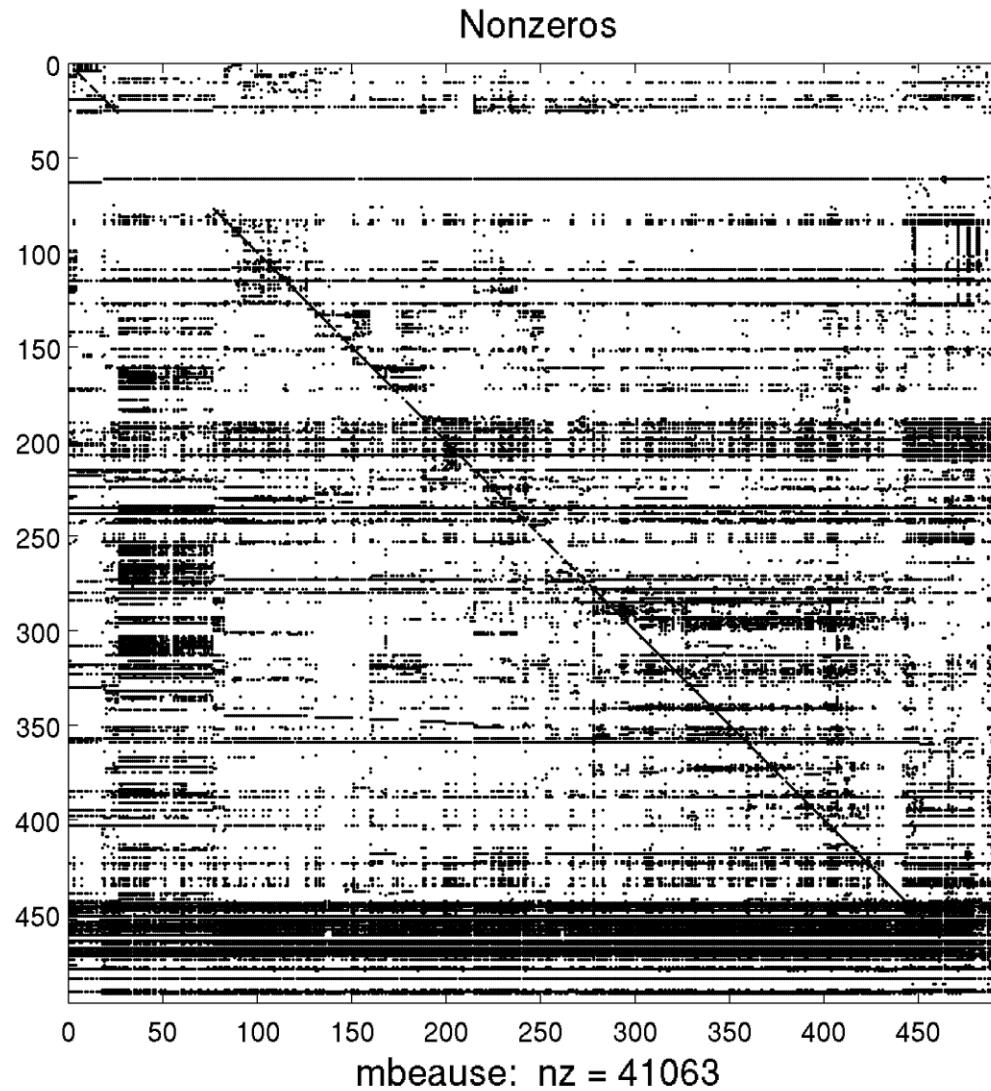
R_{add}



mbeause

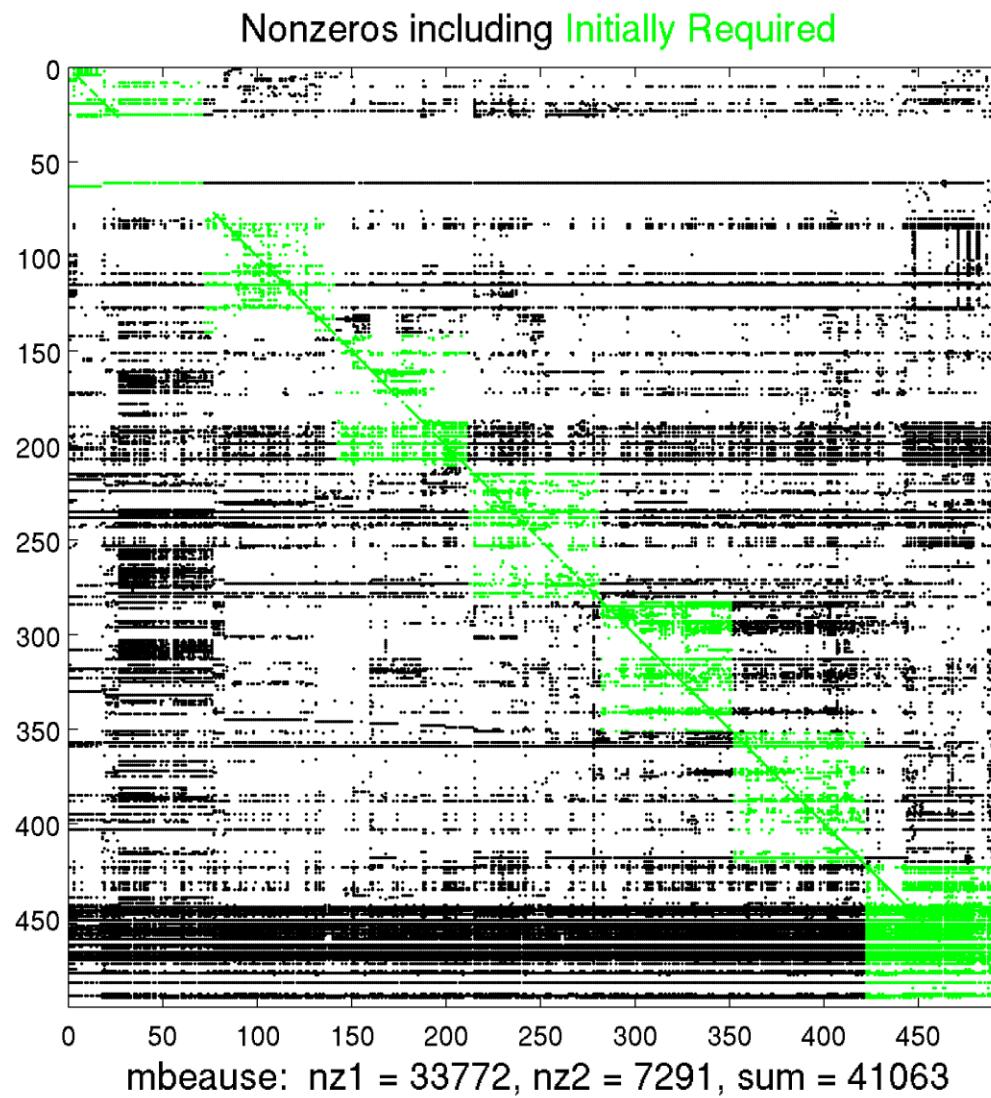
- Visualization of idea
- Larger example with Fill-in

mbeause

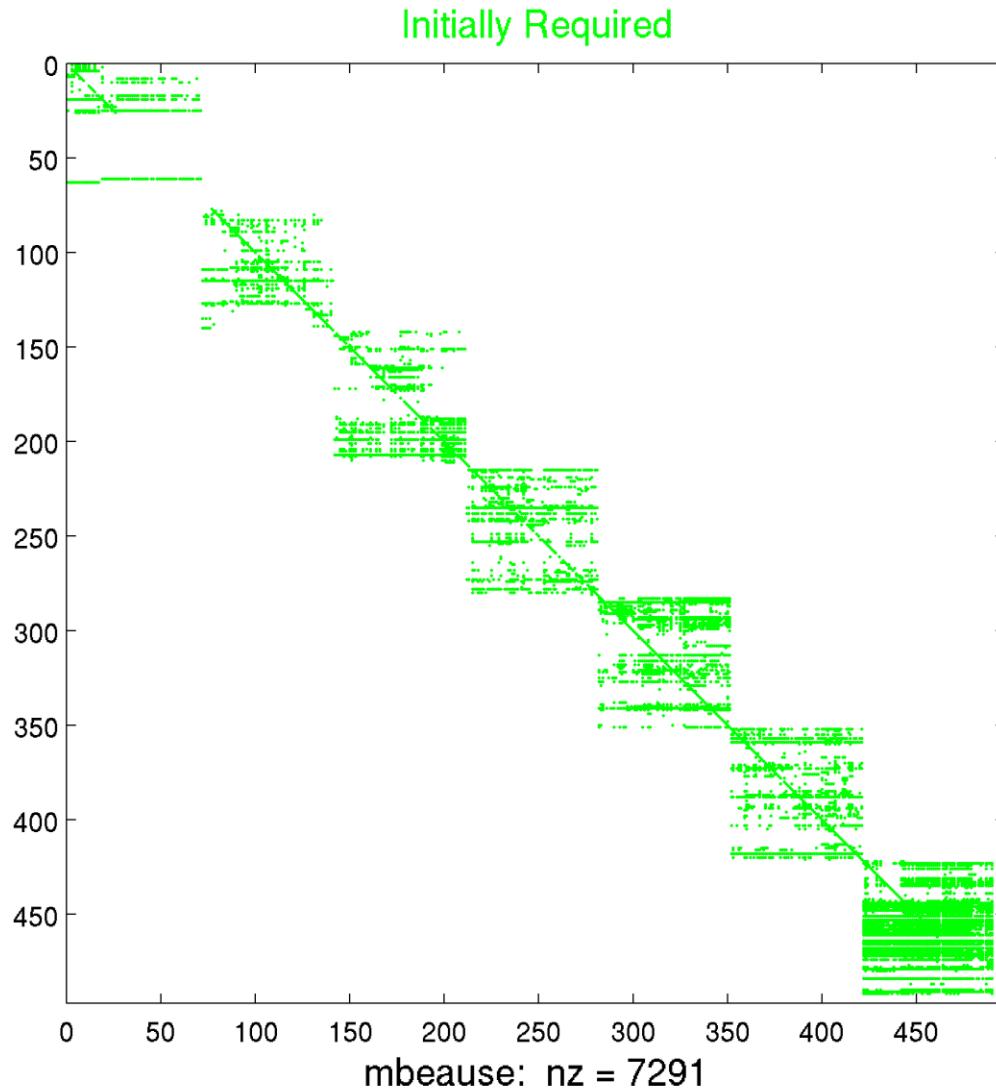


A

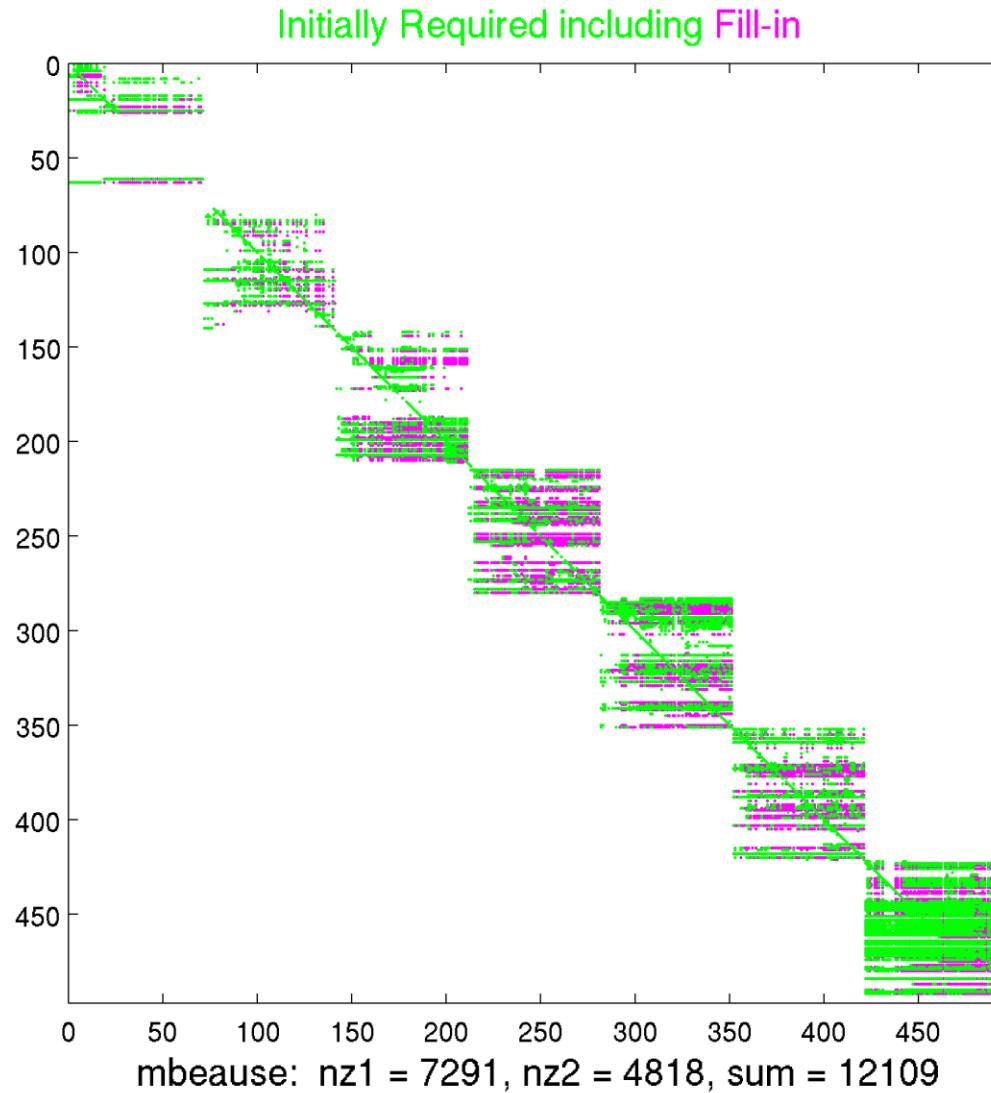
mbeause



mbeause

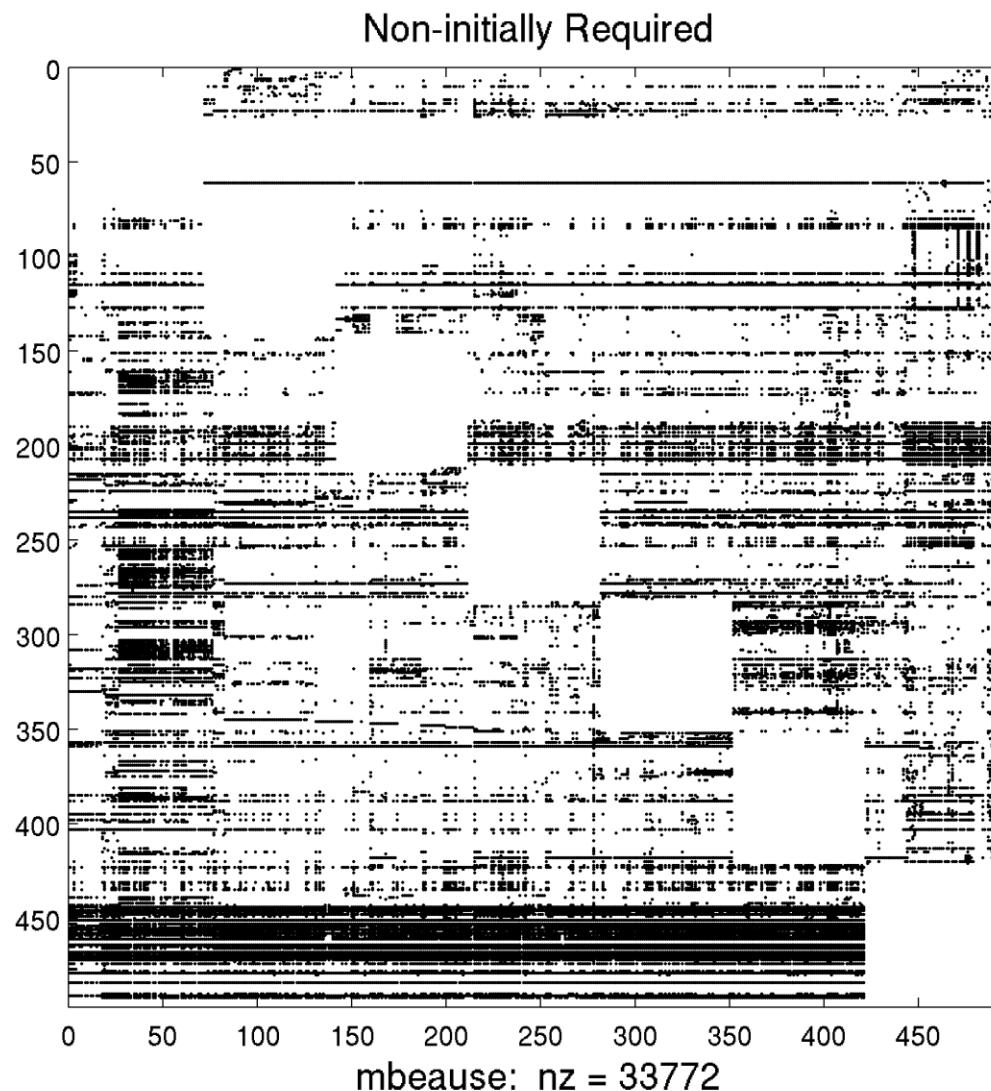


mbeause



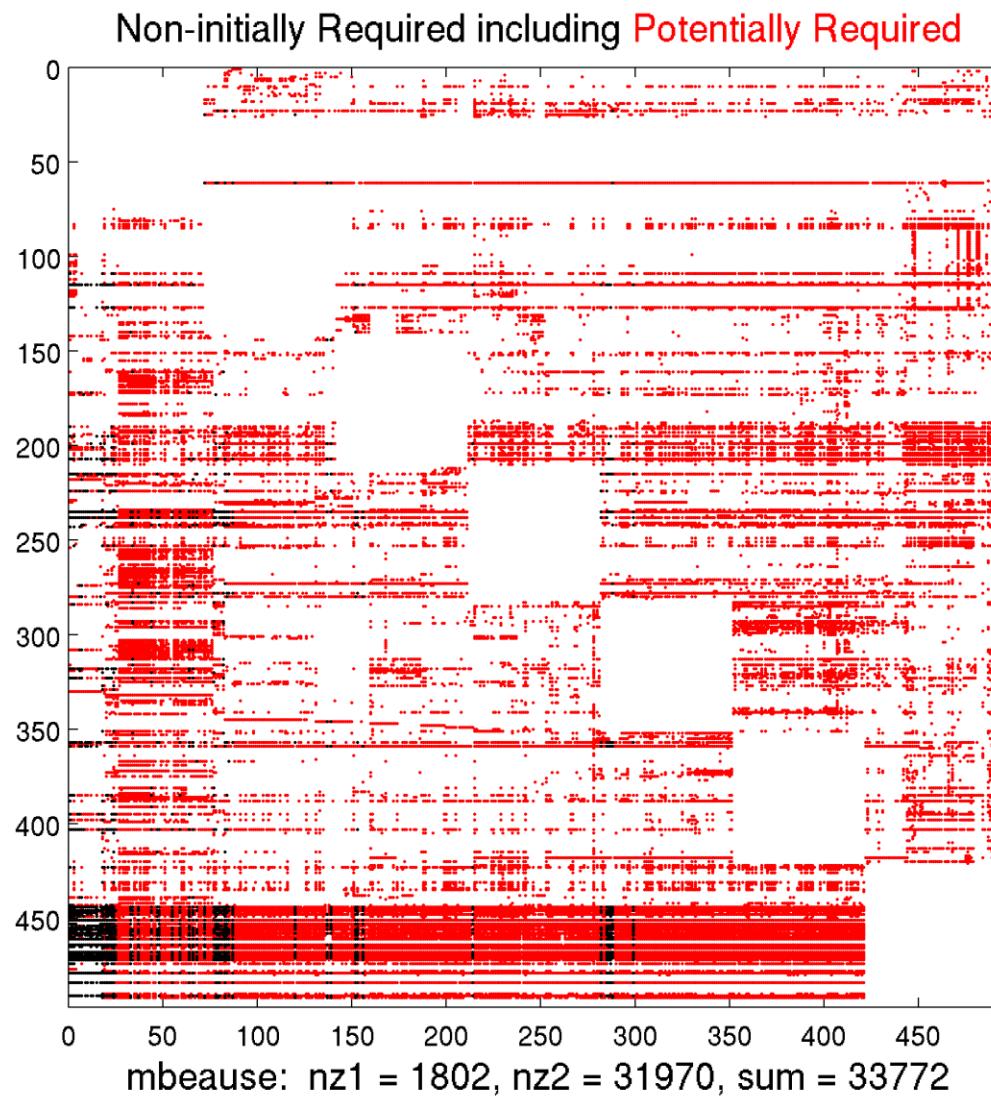
F

mbeause

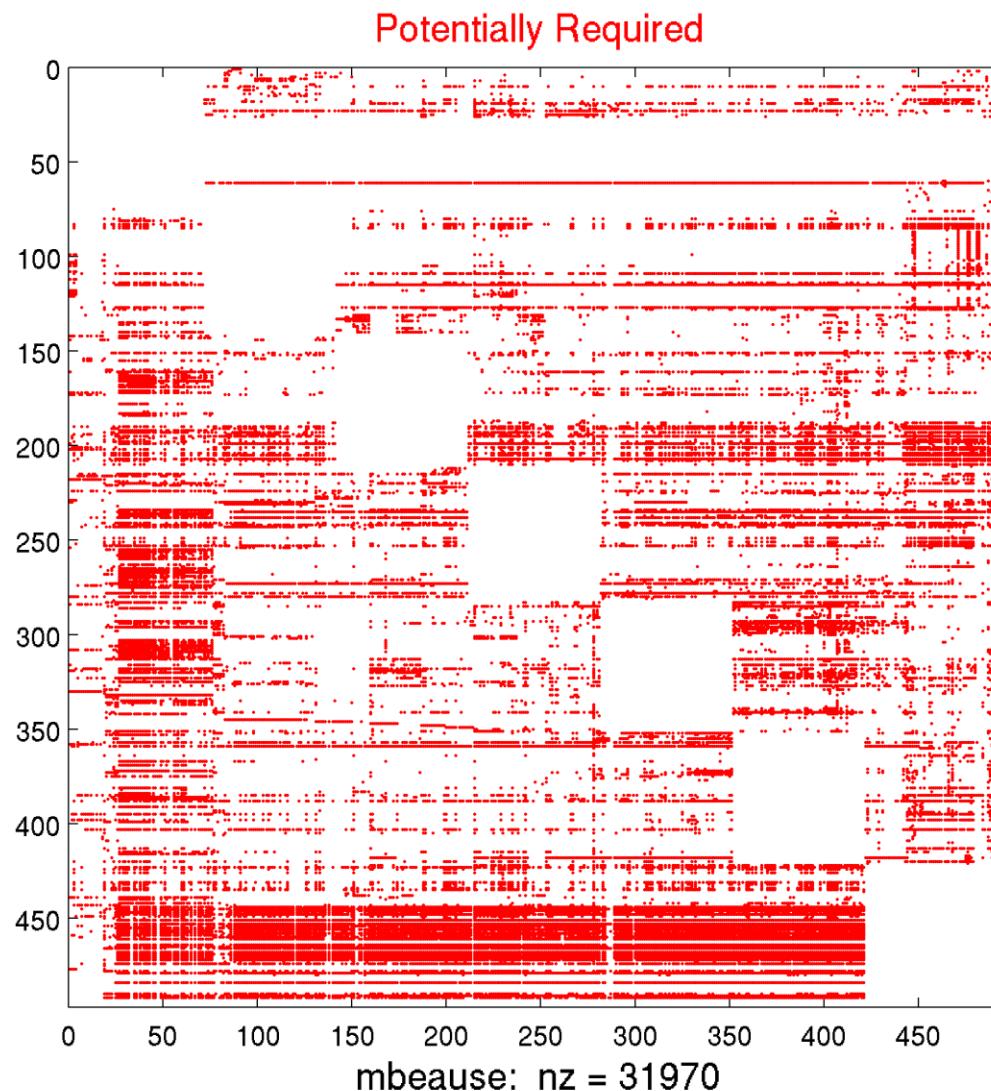


$A \setminus R_{\text{init}}$

mbeause

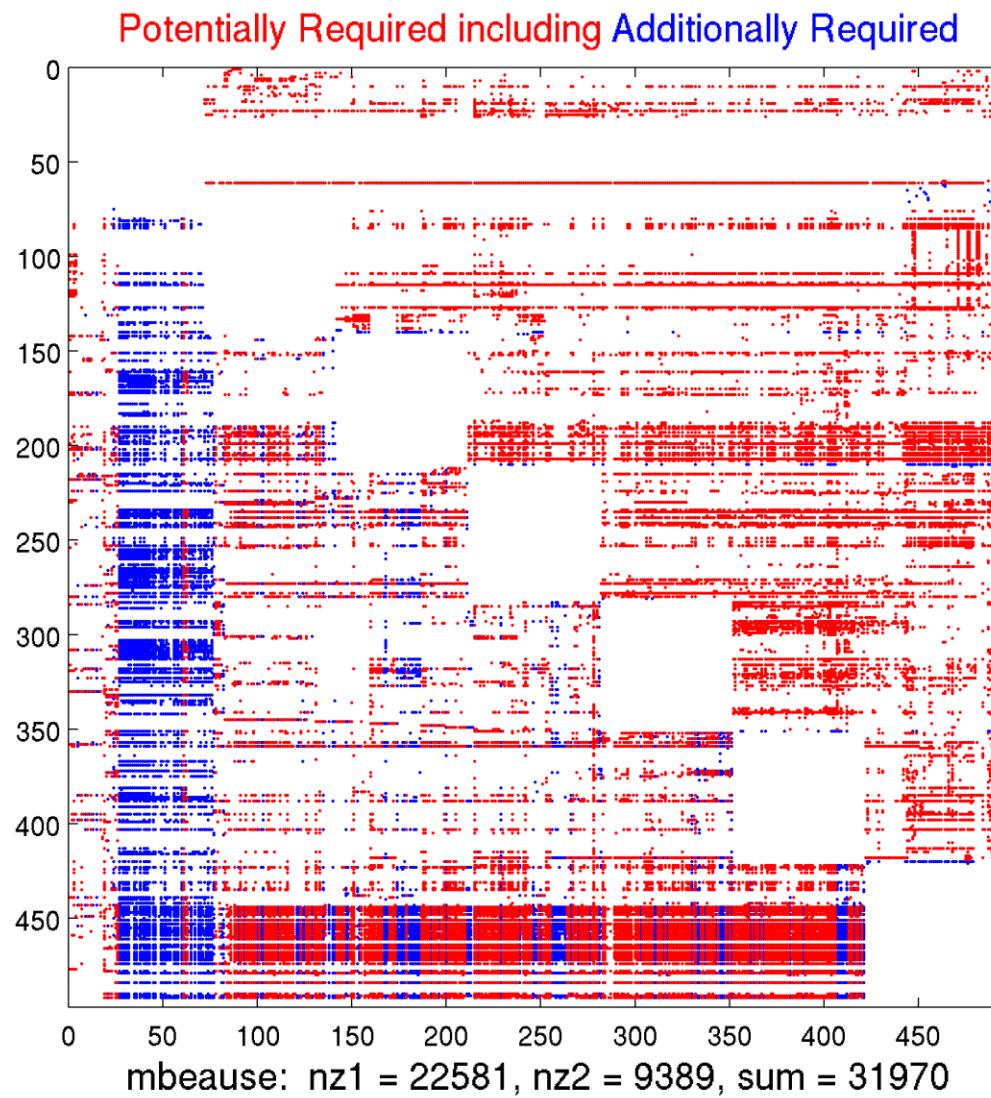


mbeause

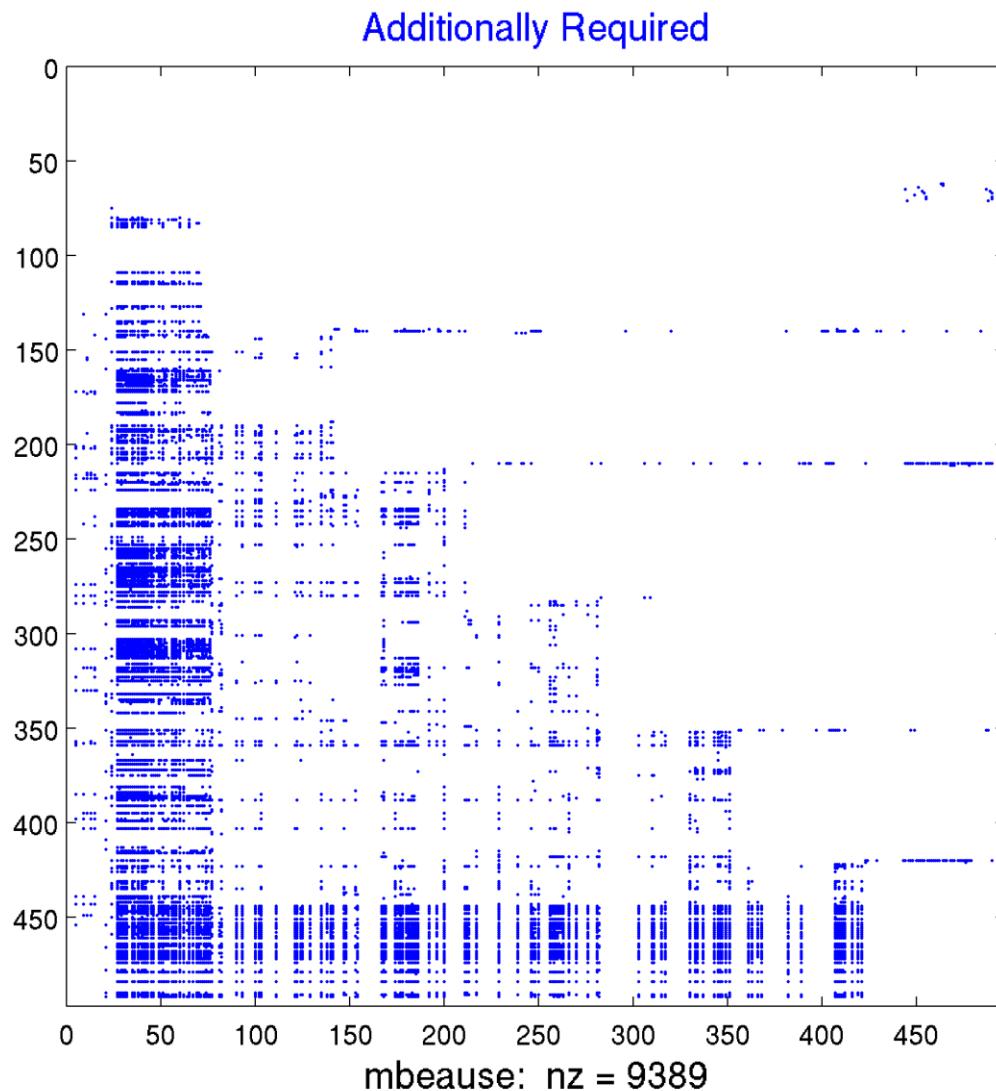


R_{pot}

mbeause

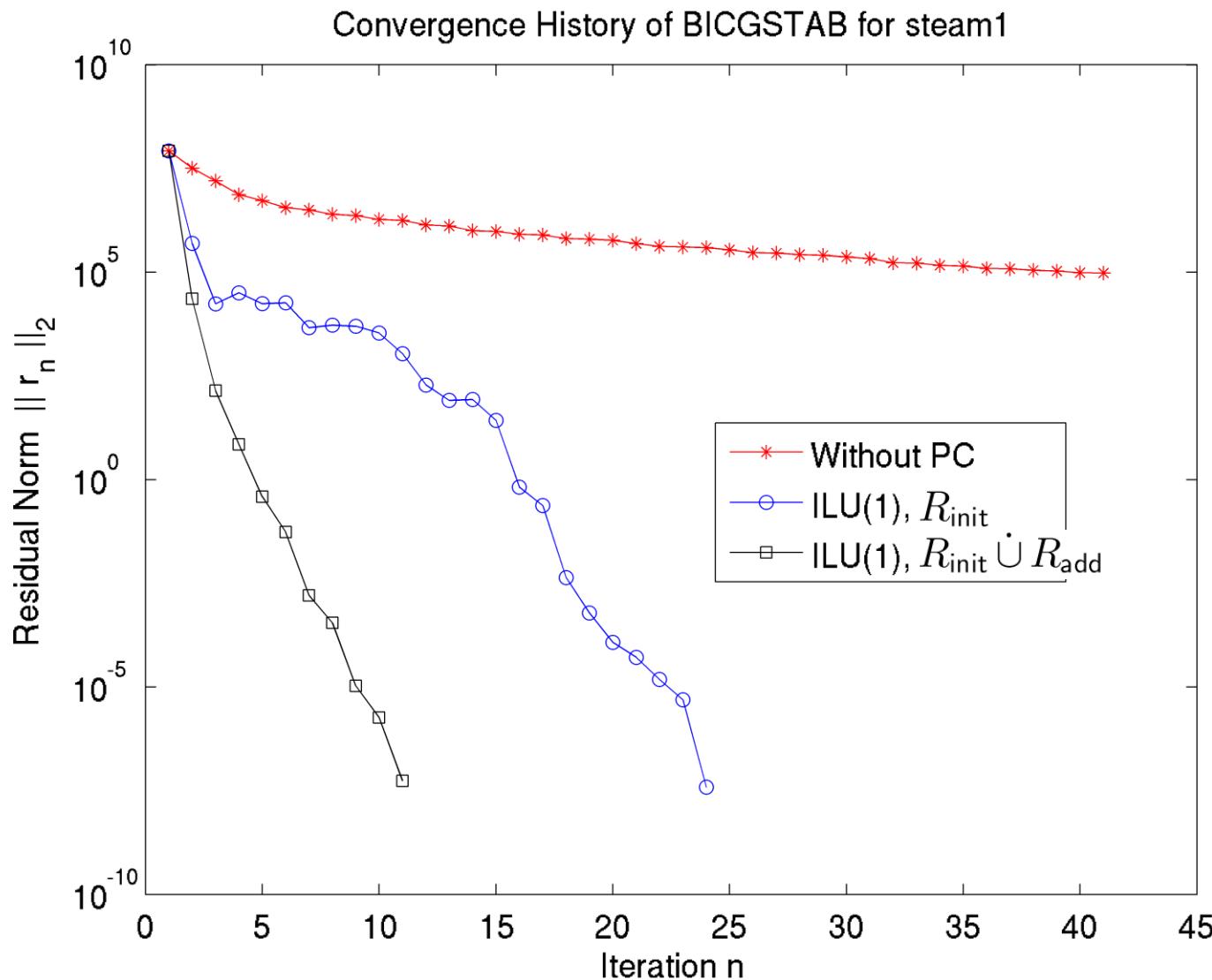


mbeause



R_{add}

steam1



Full:
 $k = 25$

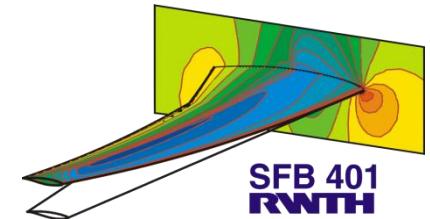
Partial:
 $k = 6$

Summary

- Graphs are suitable in scientific computing
- Preconditioning in connection with automatic differentiation is a new field
- Do not consider fields separately
- Use synergetic effects from different fields
- Interest in collaboration (ADiMat, ...)?

Thank you for your attention!

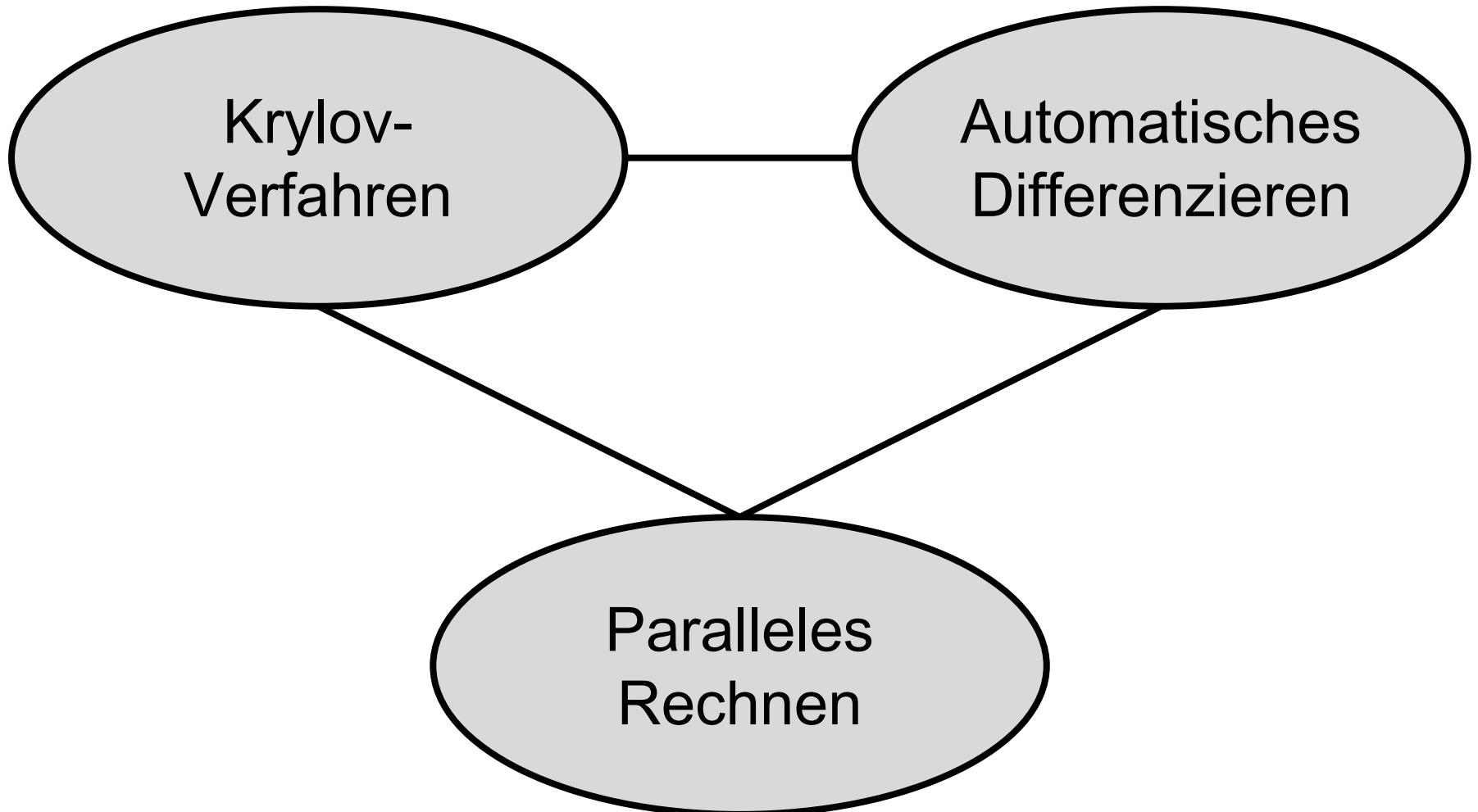
- SFB 401: Strömungsbeeinflussung und Strömungs-Struktur-Wechselwirkung an Tragflügeln
- SFB 540: Modellgestützte experimentelle Analyse kinetischer Phänomene in mehrphasigen fluiden Reaktionssystemen
- Graduiertenkolleg 775: Hierarchie und Symmetrie in mathematischen Modellen
- SPP 1253: Optimierung mit partiellen Differentialgleichungen
- Exzellenz: Graduiertenschule AICES
- BMBF: Verbundprojekt MeProRisk



Future Work

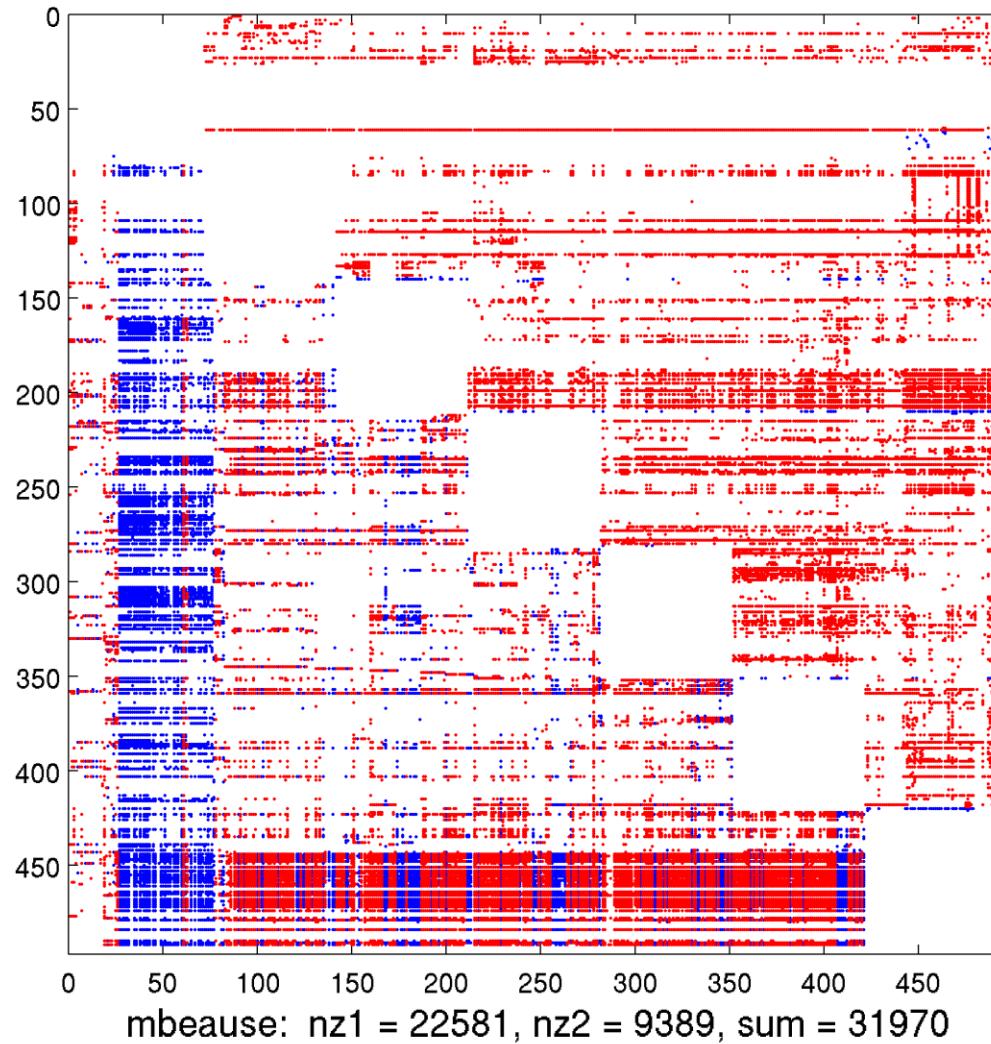
- Choice of $R_{\text{add}} \subseteq R_{\text{pot}}$
 - ◆ More aggressive strategies
 - ◆ Parallelism in $M\mathbf{y} = \mathbf{z}$
- Einfluss der Parameter Level und Blockgröße
- Vorkonditionierung so, dass ganz R_{pot} verwendet wird
- Färbung und R_{add} kombiniert betrachten
- Algorithmen zur Färbung
- Mehr Erfahrungen mit realen Anwendungen

Teilgebiete



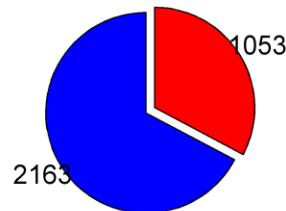
mbeause

Potentially Required including Additionally Required

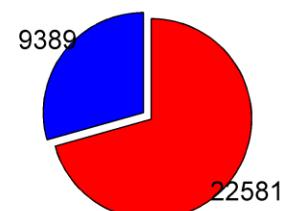


Aufteilung von R_{pot}

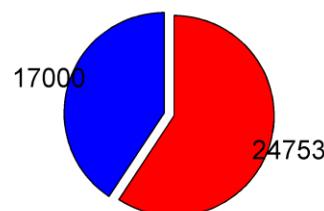
gemat11



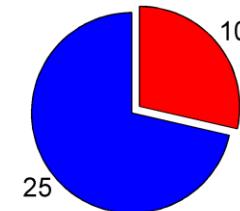
mbeause



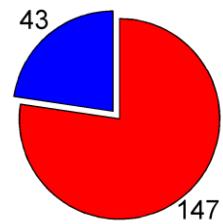
orani678



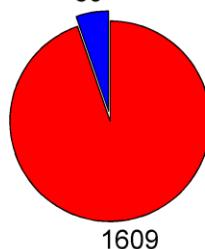
steam3



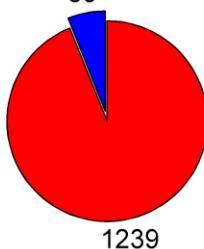
steam1



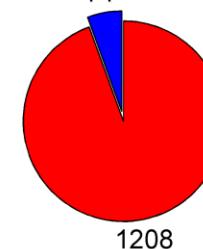
hor_131



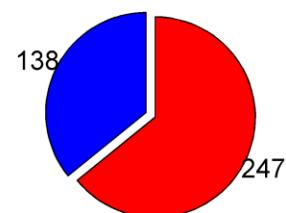
orsirr_1



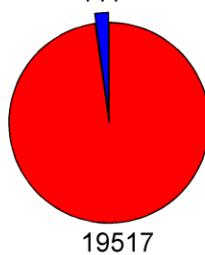
orsirr_2



steam2



cavity16



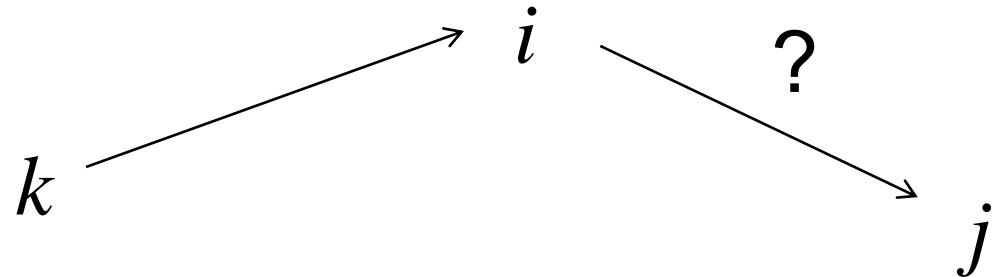
Additionally Required
Not Additionally Req.

Schnelle Strategie

(i)

zur Auswahl von $R_{\text{add}} \subseteq R_{\text{pot}}$

Betrachte Fill-in an Position (i,j) :



Fall 1: $i < j$

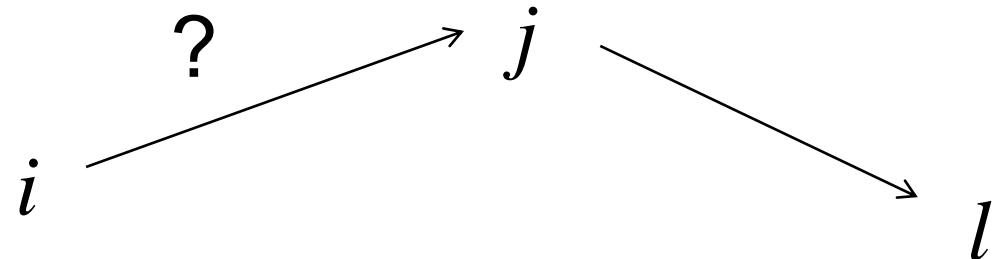
Falls es Vorgänger k von i gibt mit $k > i$,
dann Fill-in, also nicht einschließen in R_{add}

Schnelle Strategie

(ii)

zur Auswahl von $R_{\text{add}} \subseteq R_{\text{pot}}$

Betrachte Fill-in an Position (i,j) :



Fall 2: $i > j$:

Falls es Nachfolger l von j gibt mit $j > l$,
dann Fill-in, also nicht einschließen in R_{add}

Sketch of proof

- Let p_{rsb} be the smallest number of colors for a RSB.
- Let p_{rd2} be the smallest number of colors for a RD2.

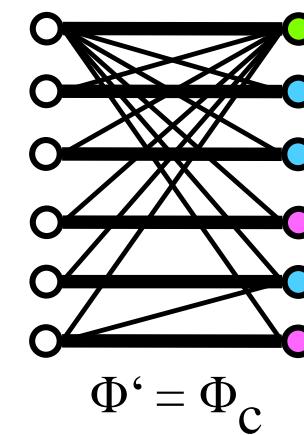
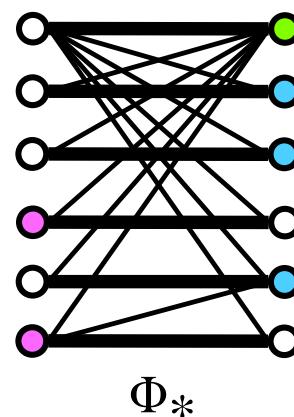
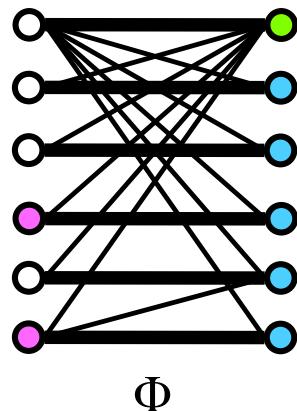
To prove $p_{rsb} = p_{rd2}$ show the following:

- Lemma 1: $p_{rsb} \geq p_{rd2}$
- Lemma 2: $p_{rd2} \geq p_{rsb}$

Lemma 1: $p_{rsb} \geq p_{rd2}$

We transform an RSB Φ with the fewest number of colors into an RD2 coloring Φ_c where the number of colors is not larger.

1. The mapping Φ will be transformed into an RSB Φ_* , where exactly one of both incident vertices of each edge in E_D is colored with nonzero.
2. The coloring Φ_* is transformed into an RSB Φ' , where all vertices $r_i \in V_r$ are colored with $\Phi'(r_i) = 0$.
3. The mapping Φ' is also an RD2 coloring.



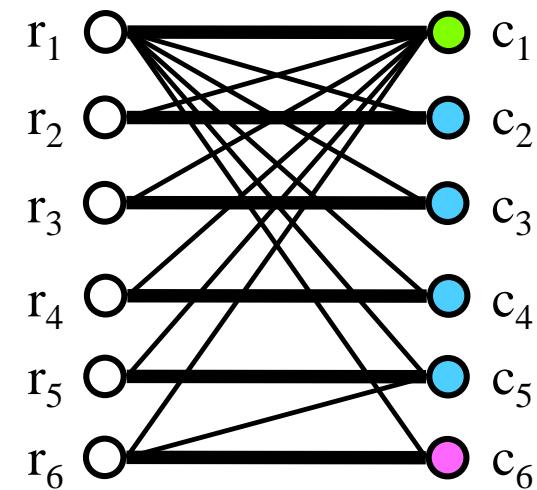
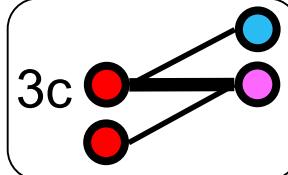
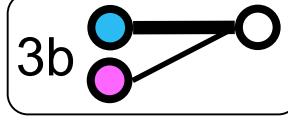
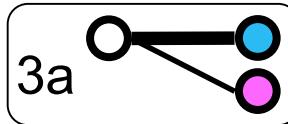
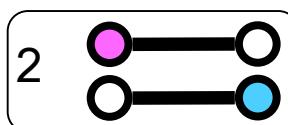
Lemma 2: $p_{rd2} \geq p_{rsb}$

A given RD2 coloring with the fewest number of colors is also an RSB.

RD2



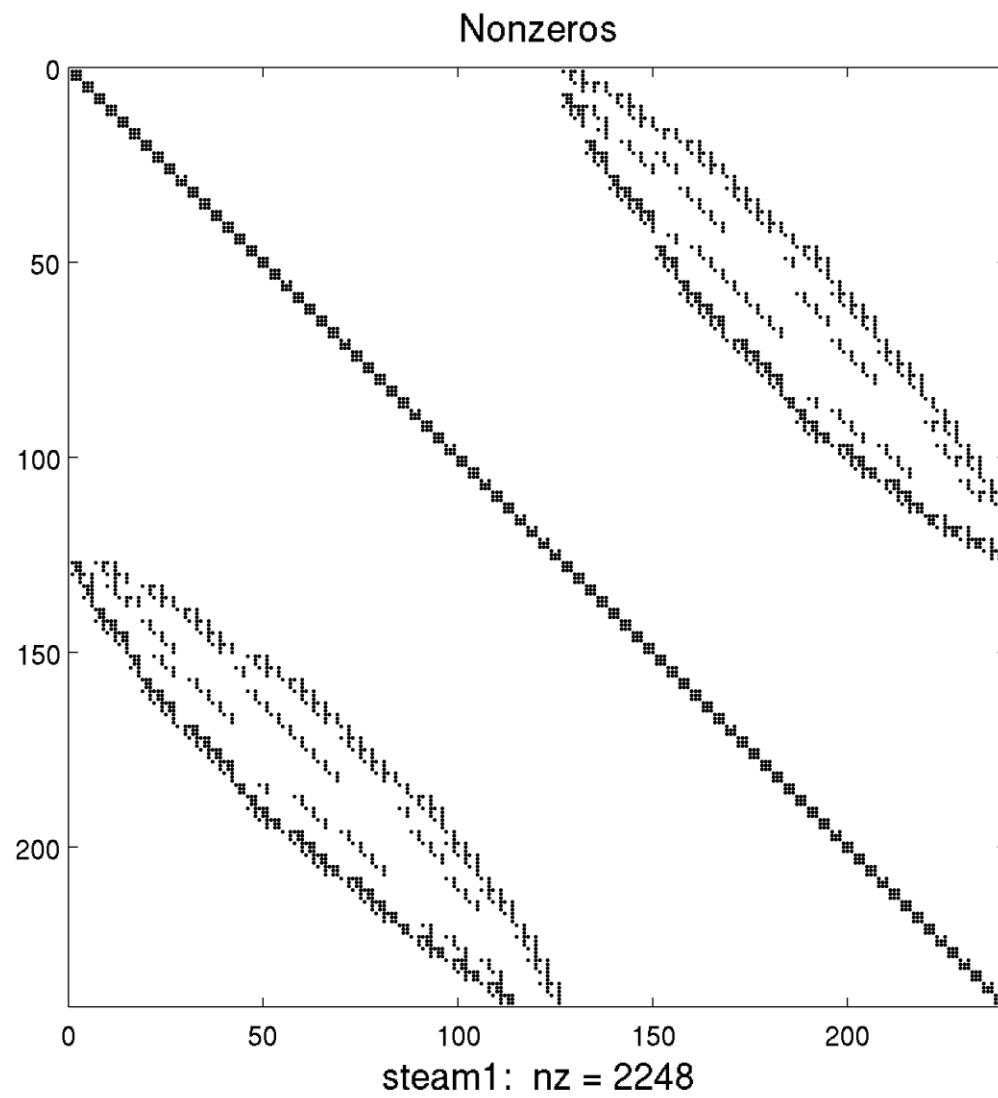
RSB



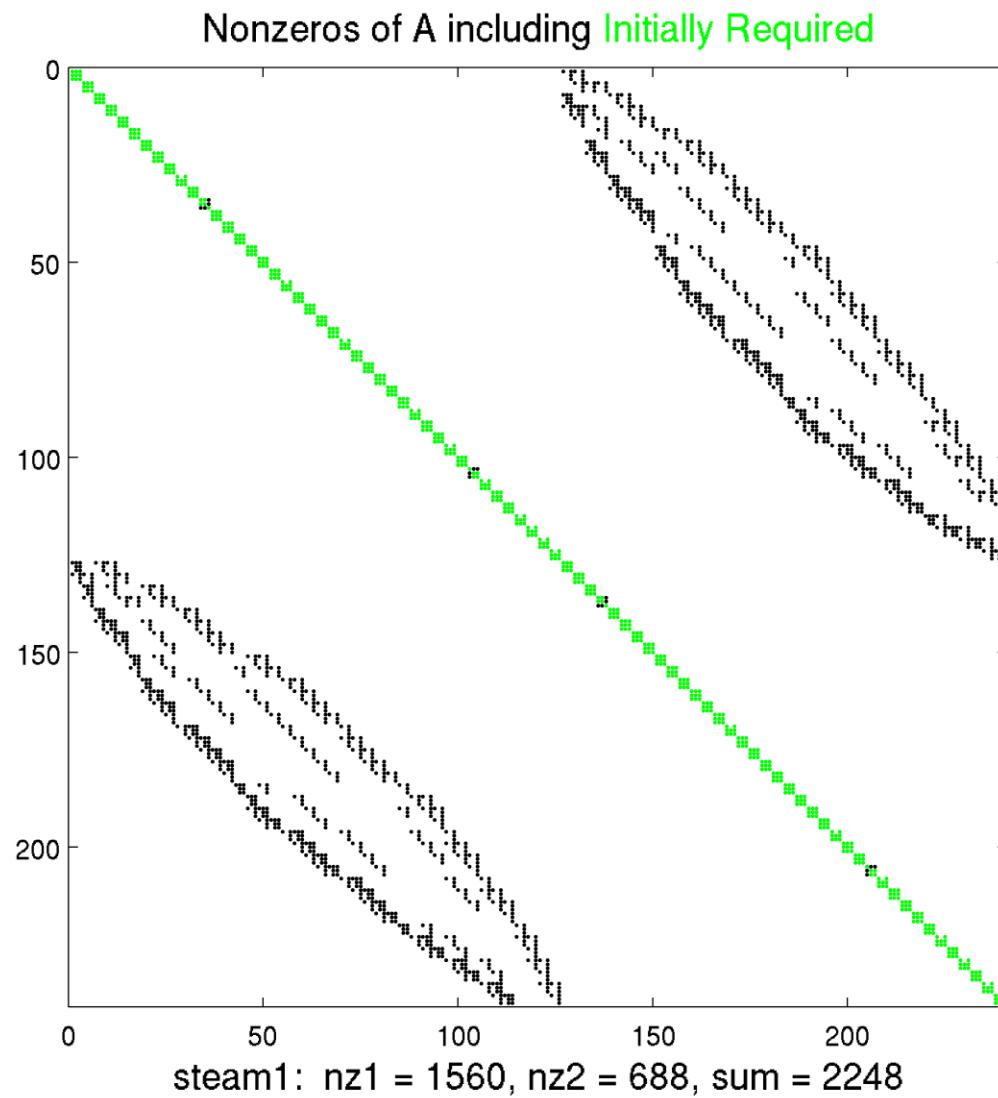
Steam1

- Visualisierung der Idee (Phänomene schlechter erkennbar)
- Allerdings ohne Fill-in

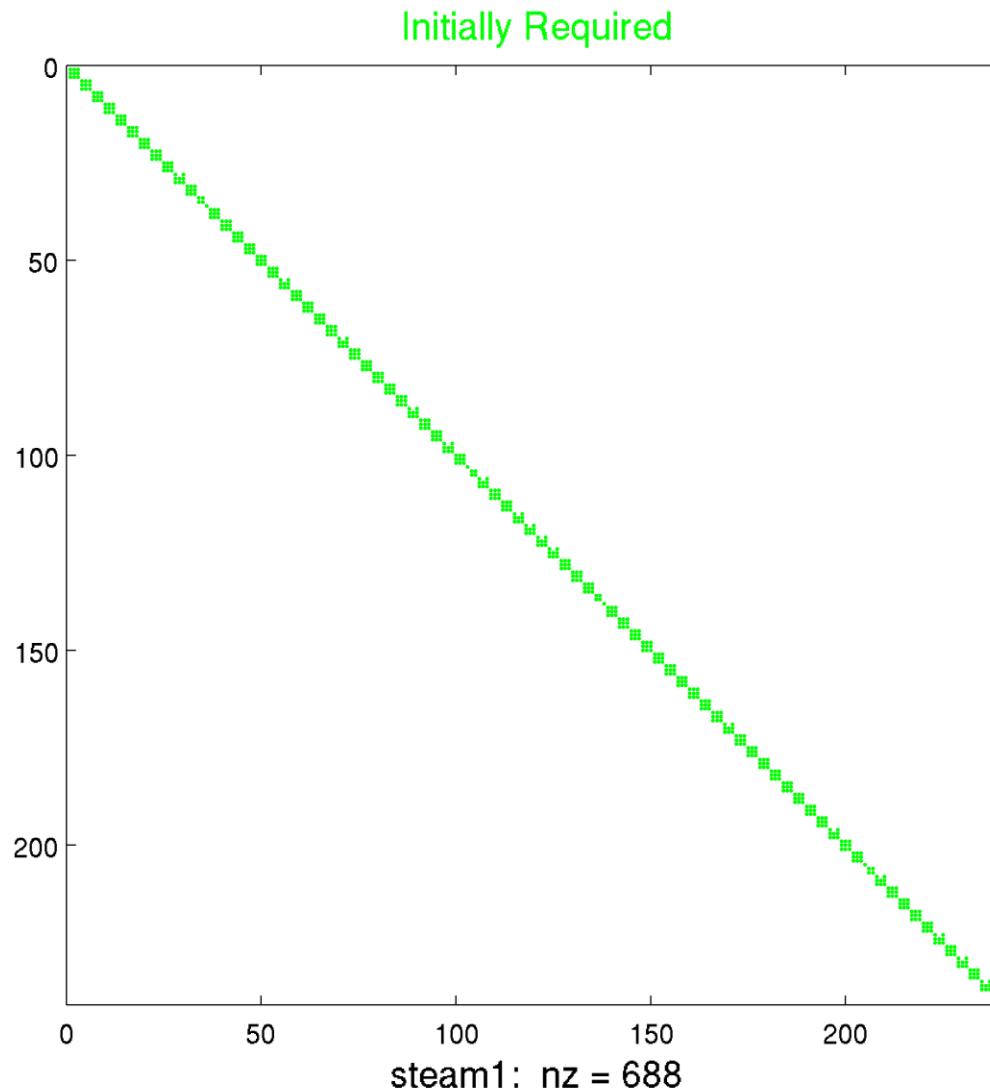
steam1



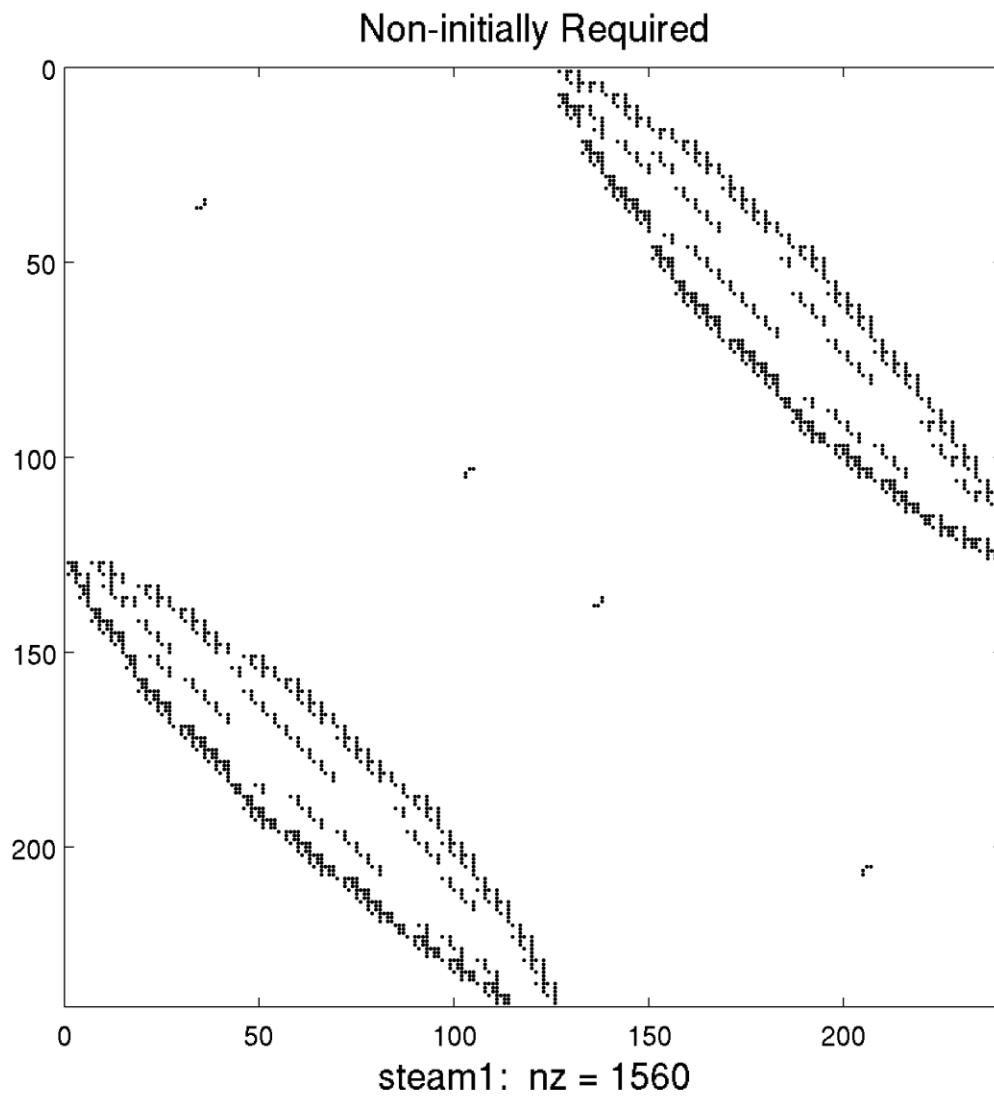
steam1



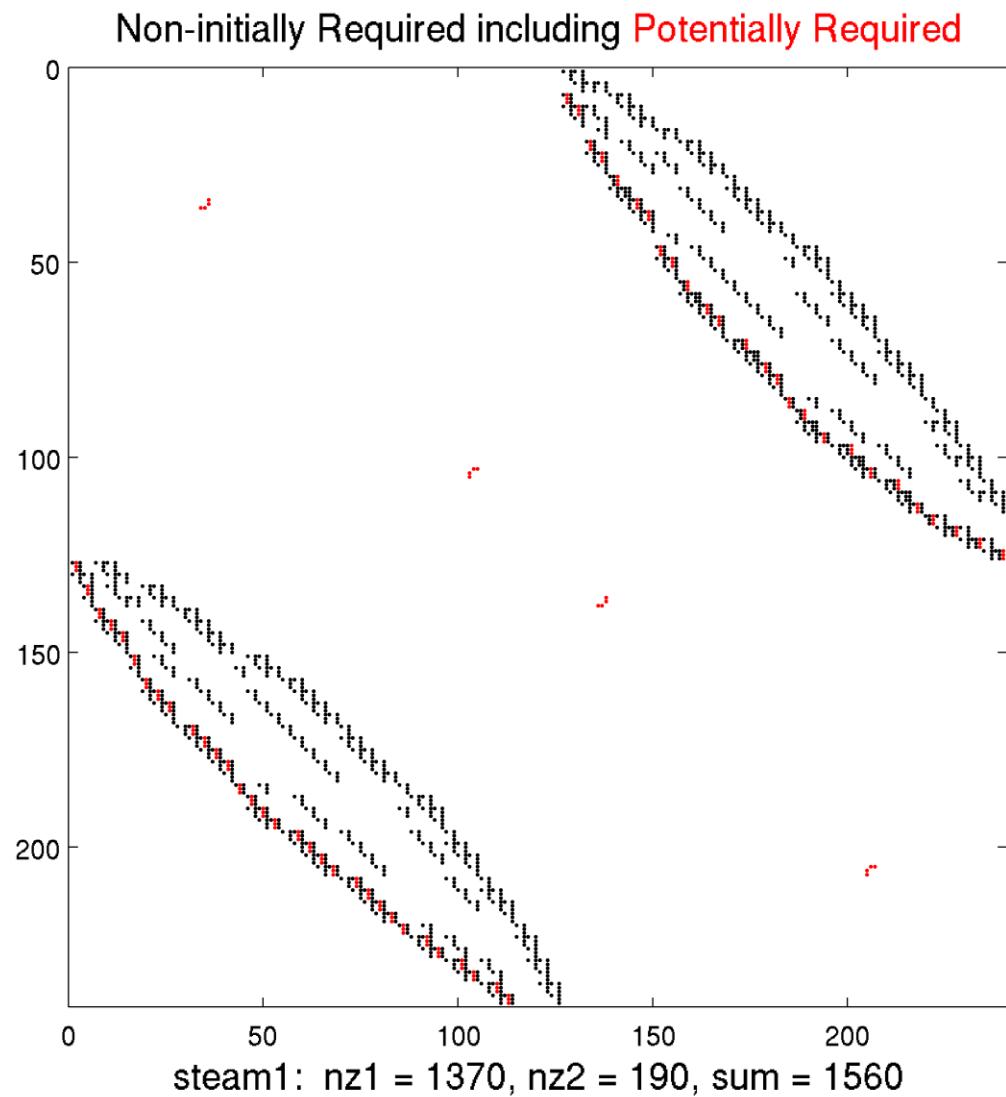
steam1



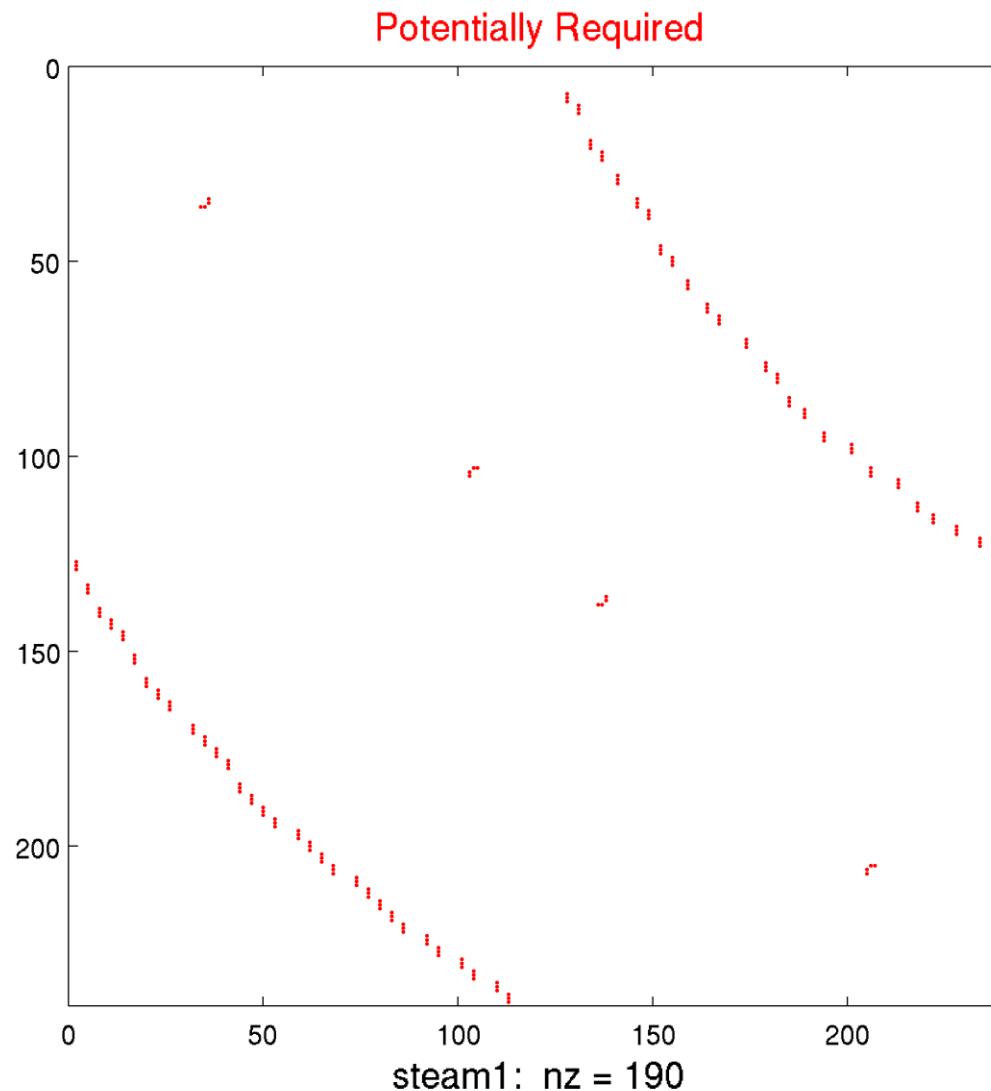
steam1



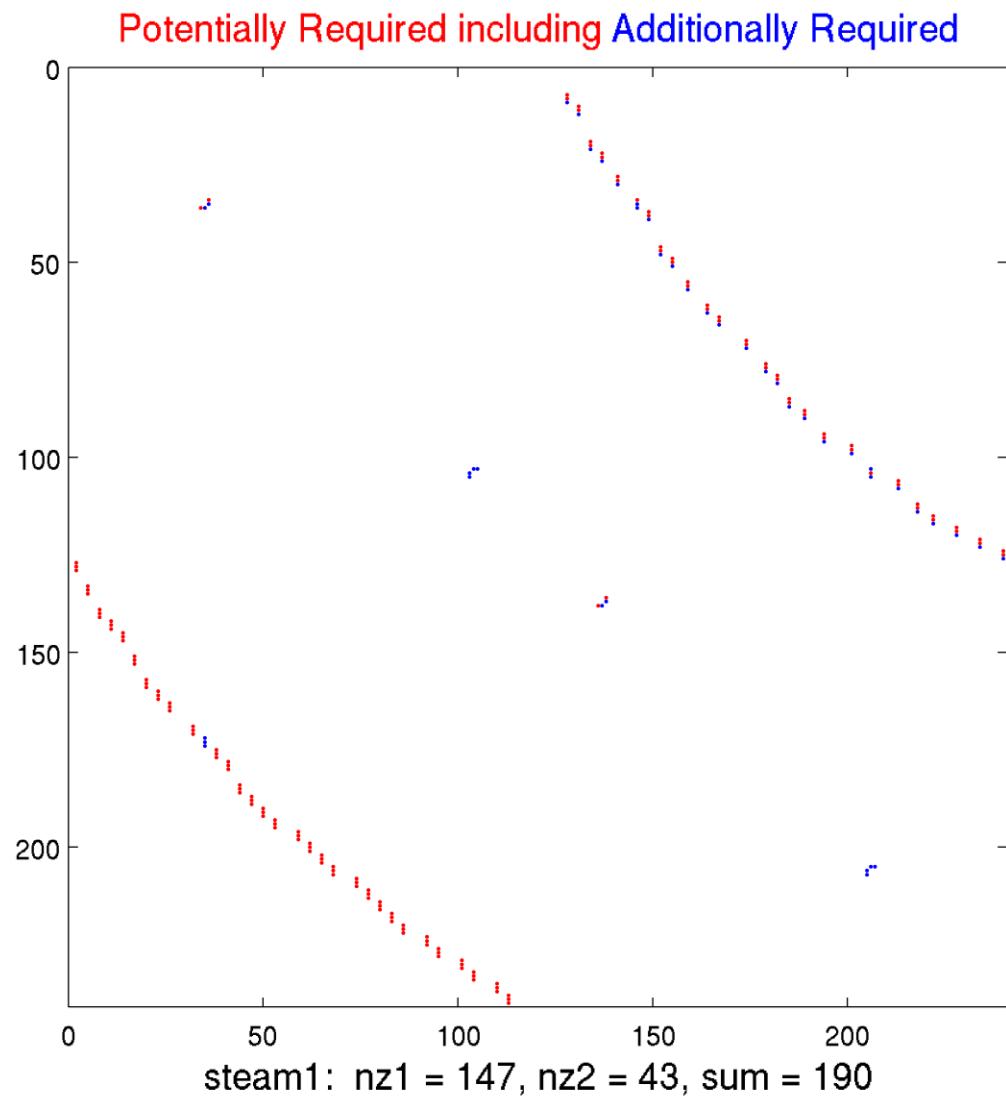
steam1



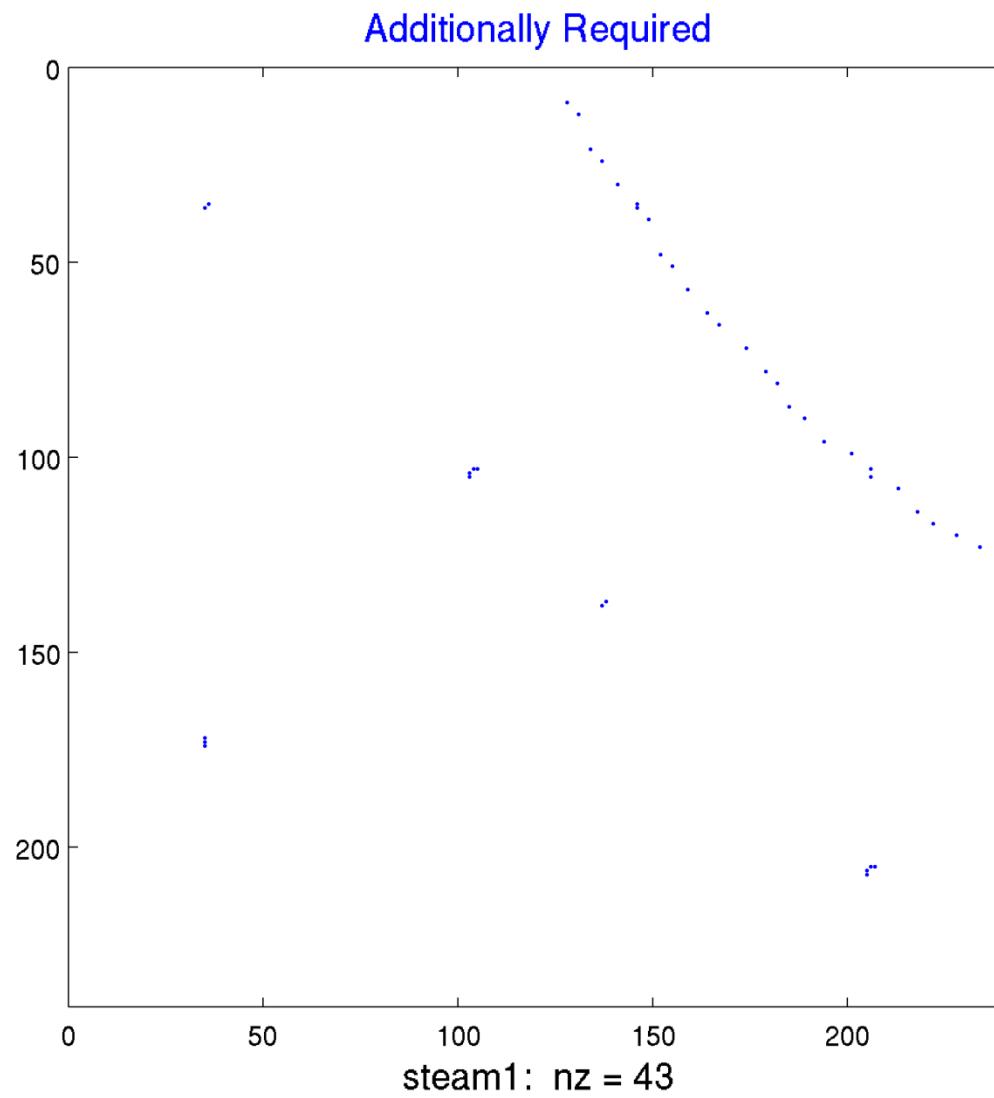
steam1



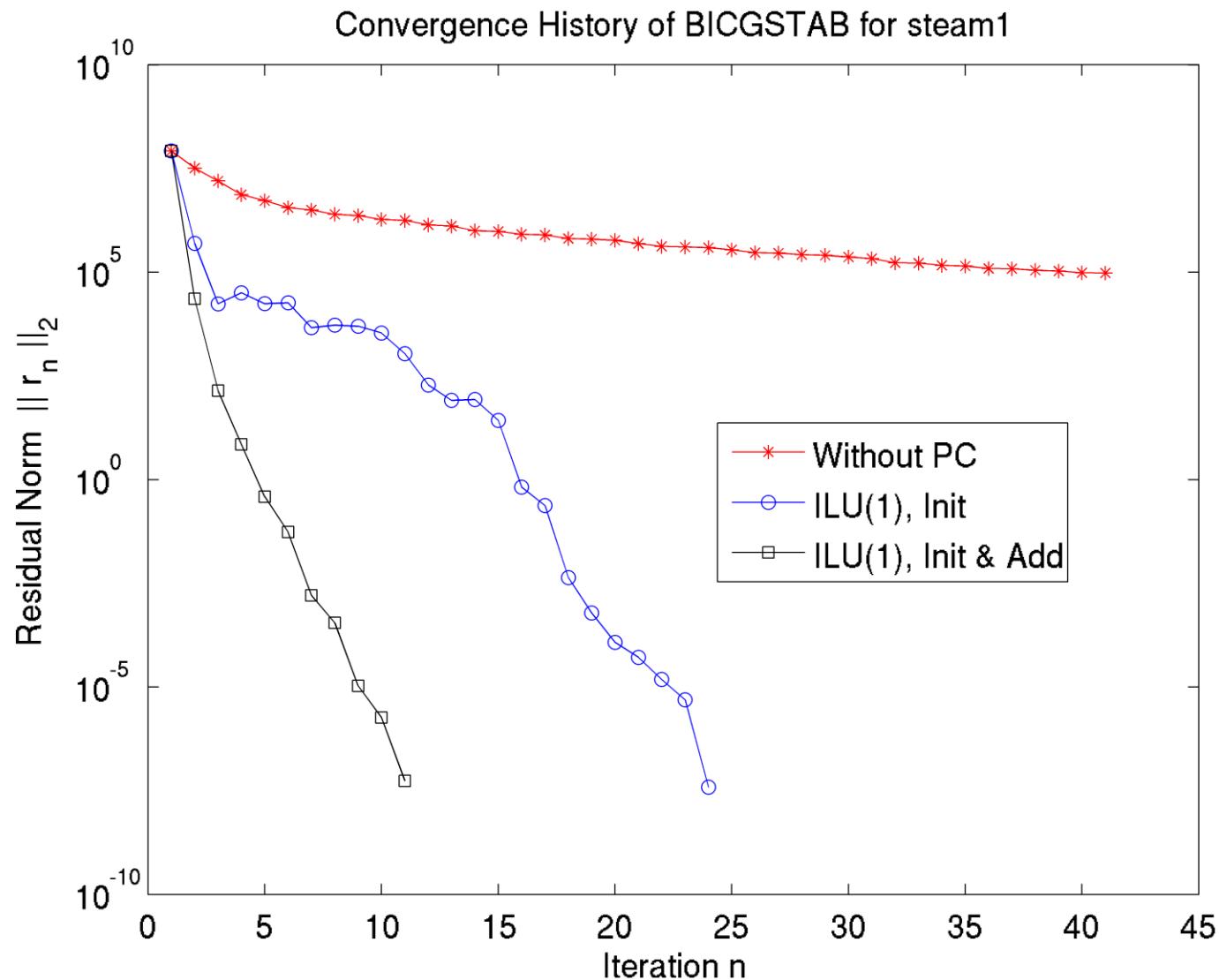
steam1



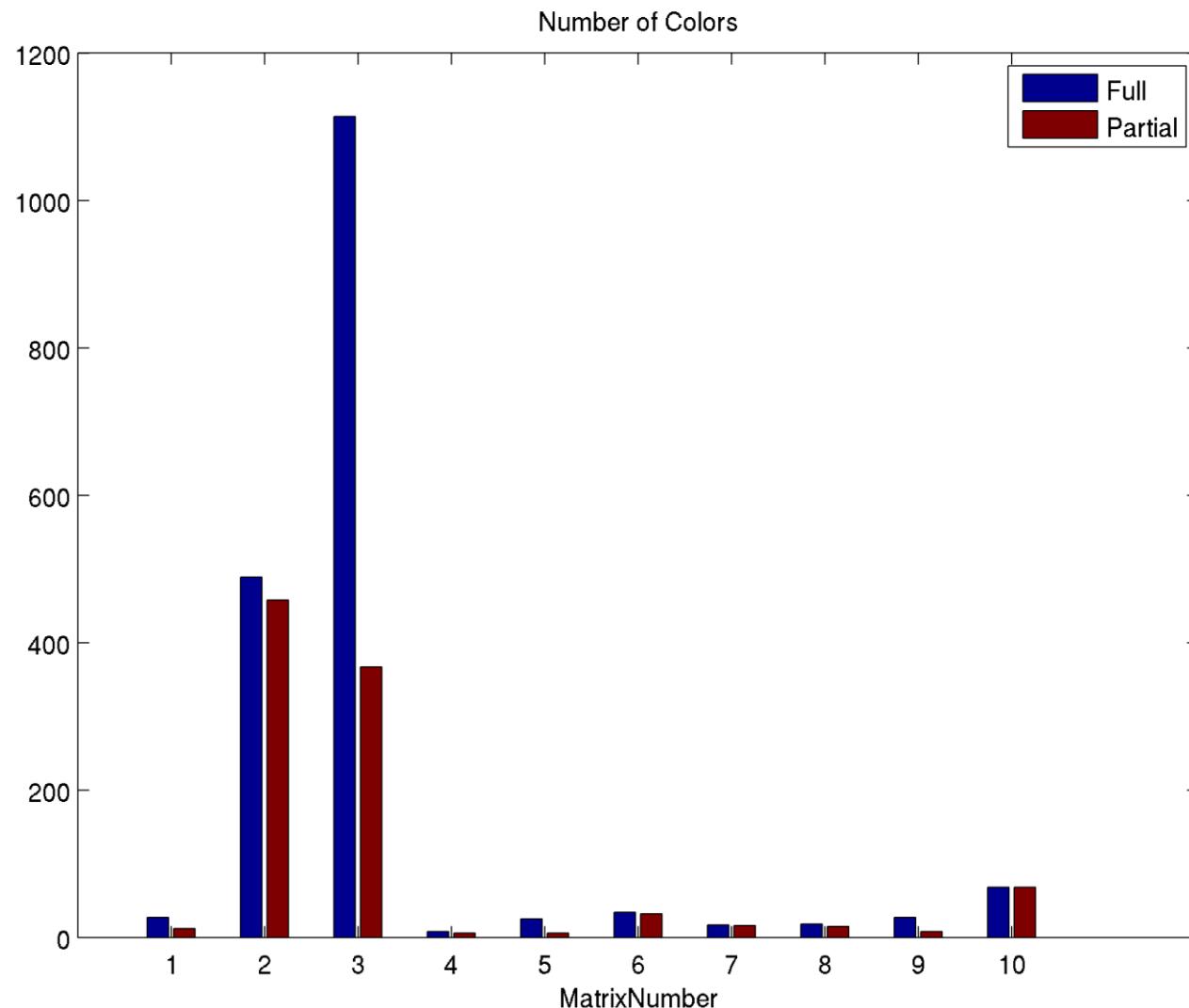
steam1



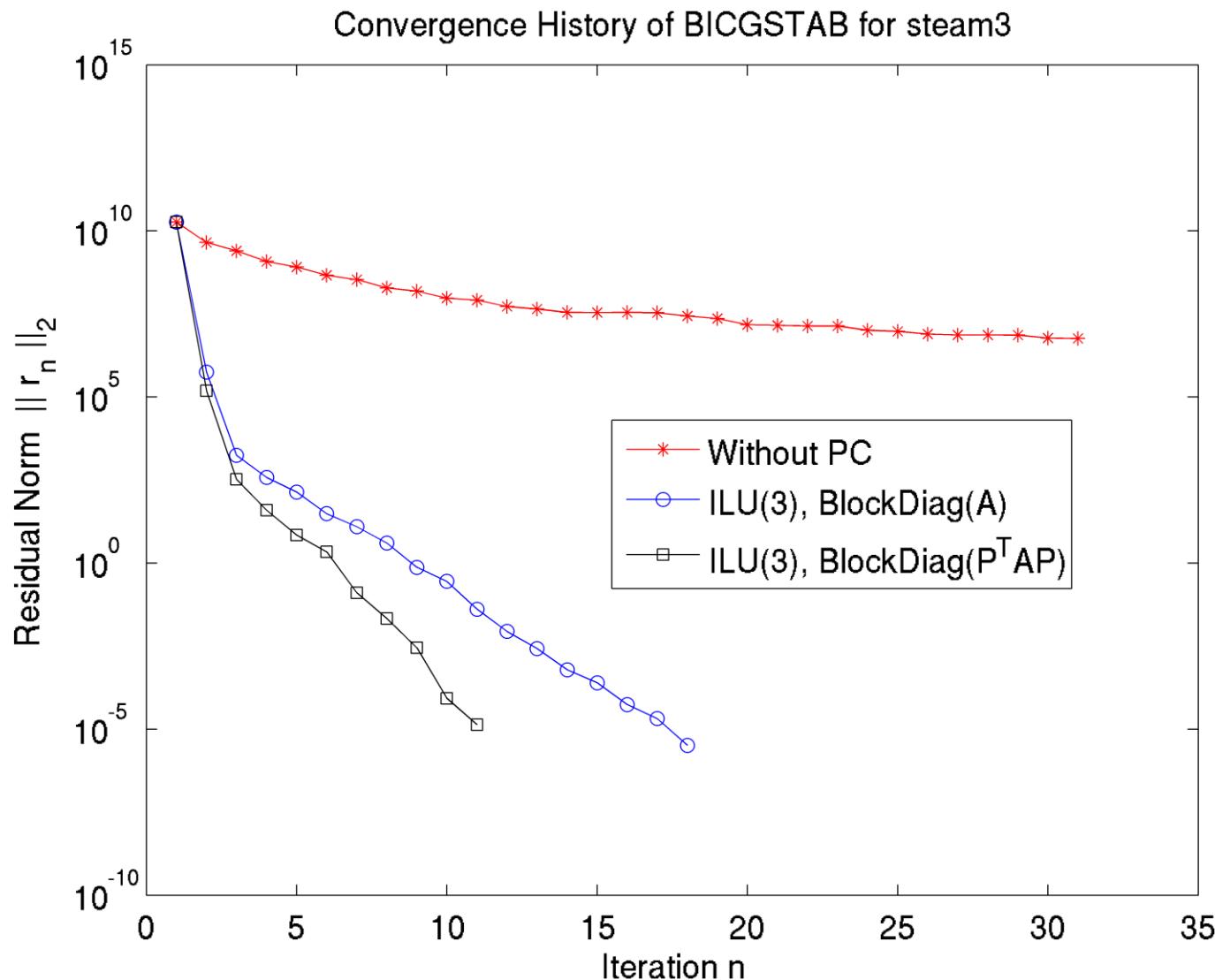
steam1



Vergleich Farbanzahlen



steam3

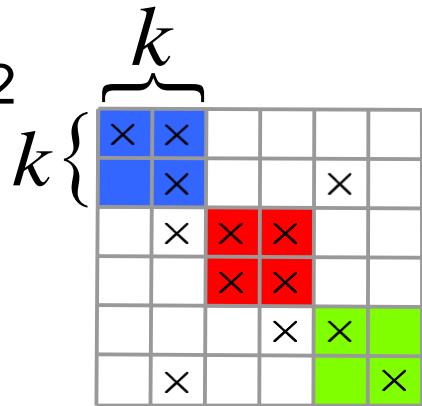


Block Size Identifying Problem

$\max_k \frac{\text{#req. elements}(k)}{\text{#colors}(k)^2}$

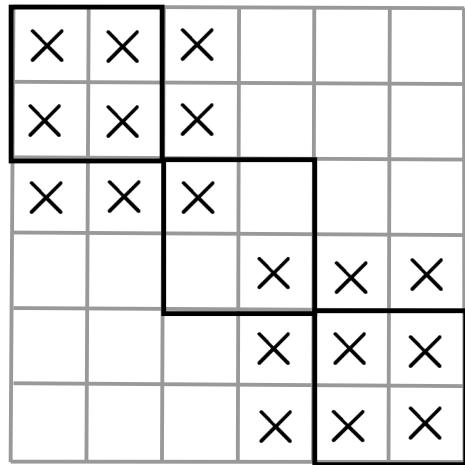
s.t. $\text{#colors}(k) < c$

$\text{#required elements}(k) < r$



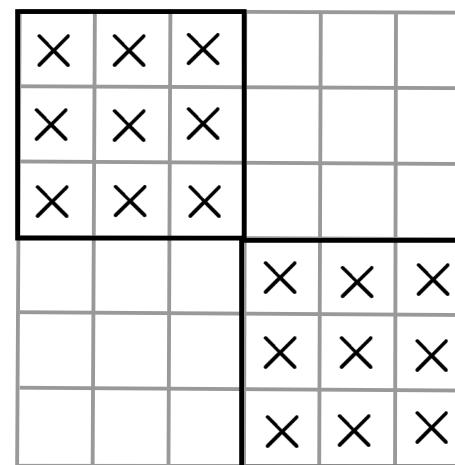
- Find block size k such that ratio of number of required elements and number of colors (squared) is maximized

Block Size?



$k=2$:

- #req. elements(k)=10
- #colors(k)=3



$k=3$:

- #req. elements(k)=18
- #colors(k)=3

QUADFLOW

Matrix J	dim	k	#nonzeros		#colors		#iterations	
			J	\tilde{J}	J	\tilde{J}	w/o pc	w/ pc
Quadflow	1.600	4	30.720	6.400	36	8	177	26

University of Florida Sparse Matrix Collection

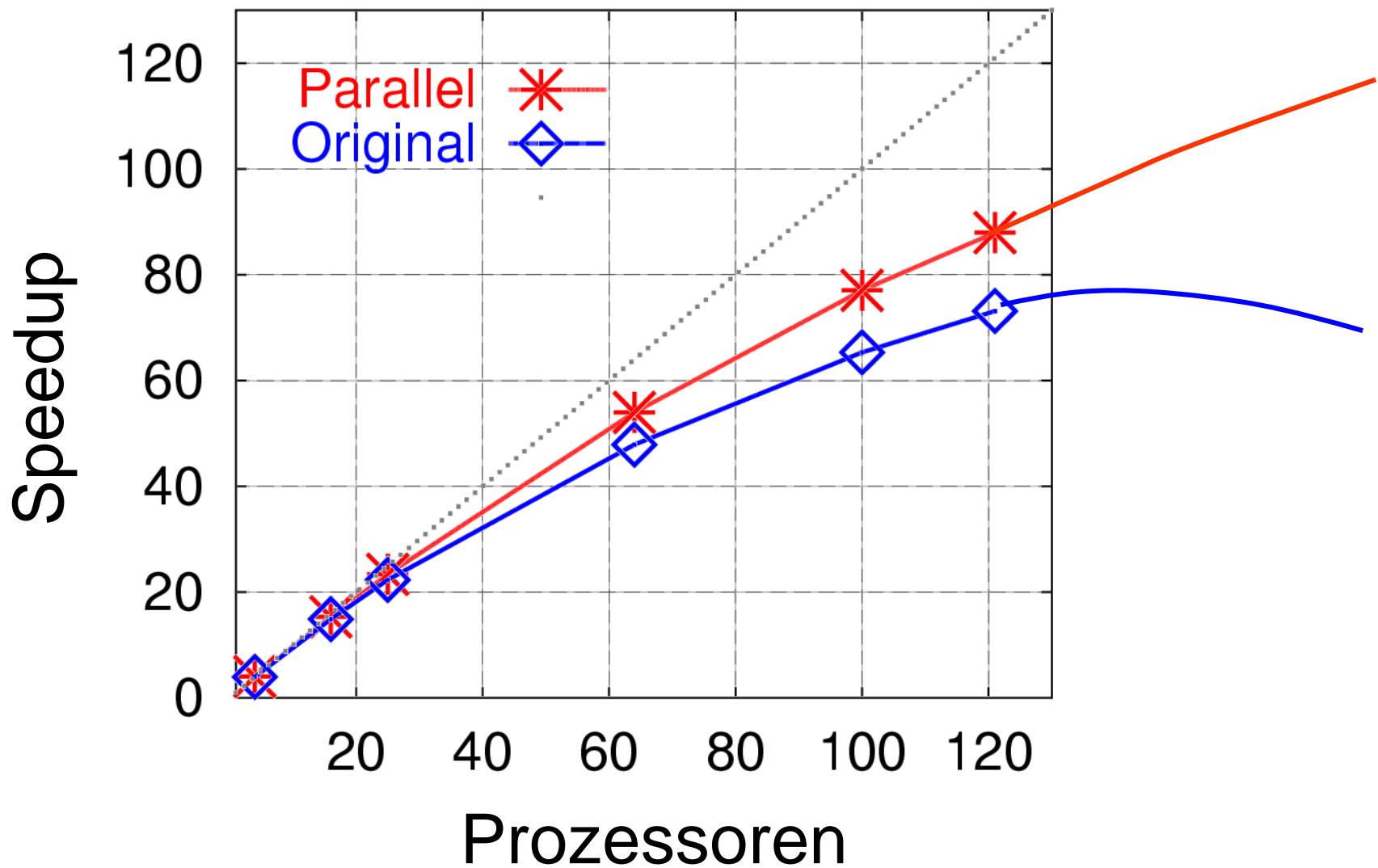
Matrix J	dim	k	#nonzeros		#colors		#iterations	
			J	\tilde{J}	J	\tilde{J}	w/o pc	w/ pc
685_bus	685	1	3.249	685	14	6	213	10
bcsstk10	1.086	5	22.070	2.810	27	12	536	1
fs_541_1	541	1	4.282	541	15	7	9	5
sherman2	1.080	6	23.094	4.950	55	12	364	1

```

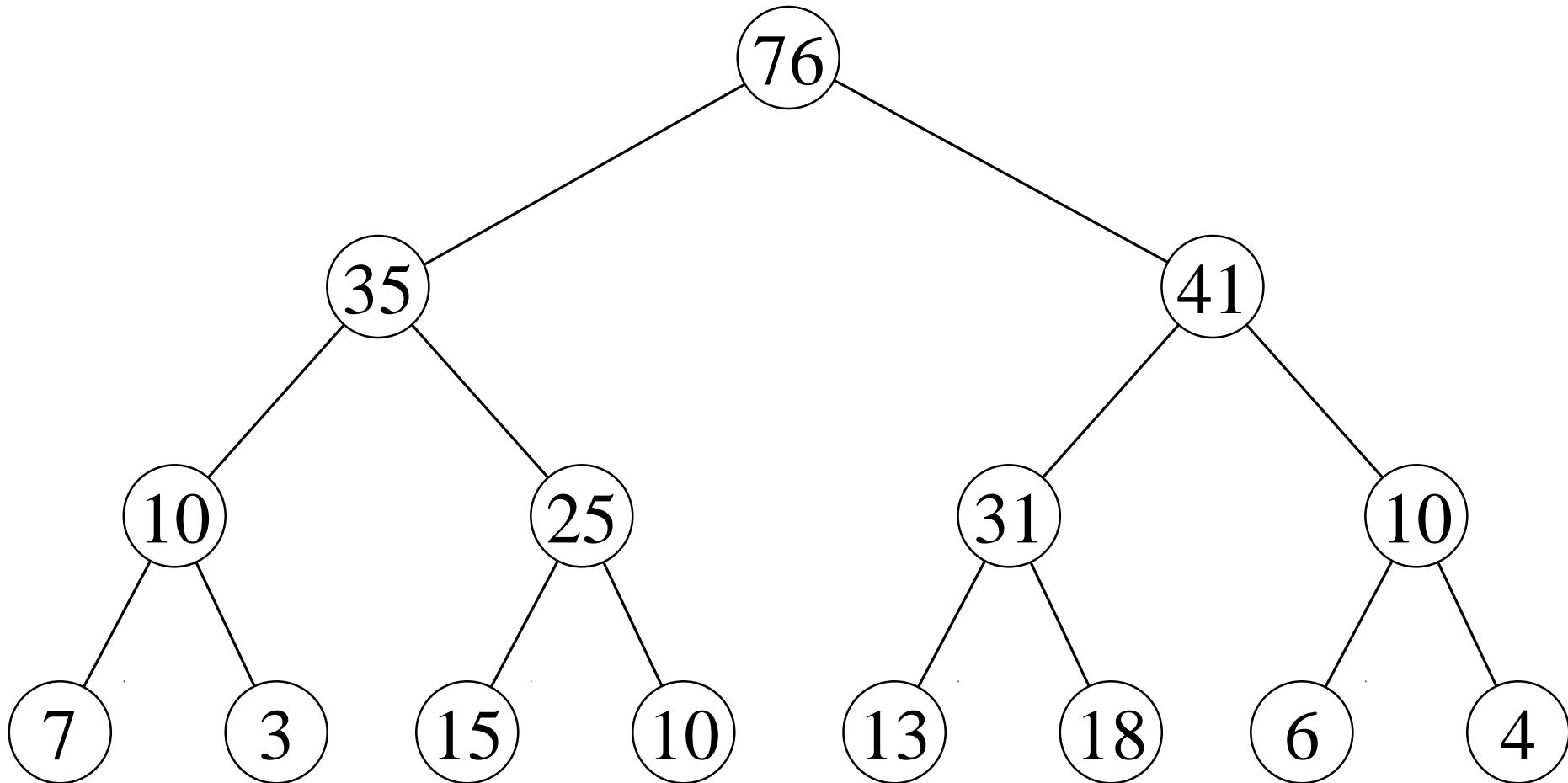
for i = 1:n
    % All entries of A are entries of F with level = 0.
    index_nnz = find( A(i,:)==1 );
    level(i,index_nnz) = 0;
    F(i,index_nnz) = 1;
    % Update phase
    for k = 1:i-1 % node (i,k) with k<i
        if F(i,k)==1
            for j = k + find( F(k,k+1:n)==1 ) % node (k,j) with k<j
                lev = level(i,k) + level(k,j) + 1;
                if(lev <= el)
                    if F(i,j)==0
                        F(i,j) = 1;
                        level(i,j) = lev;
                    else
                        level(i,j) = min(level(i,j),lev);
                    end;
                end
            end;
        end;
    end
end

```

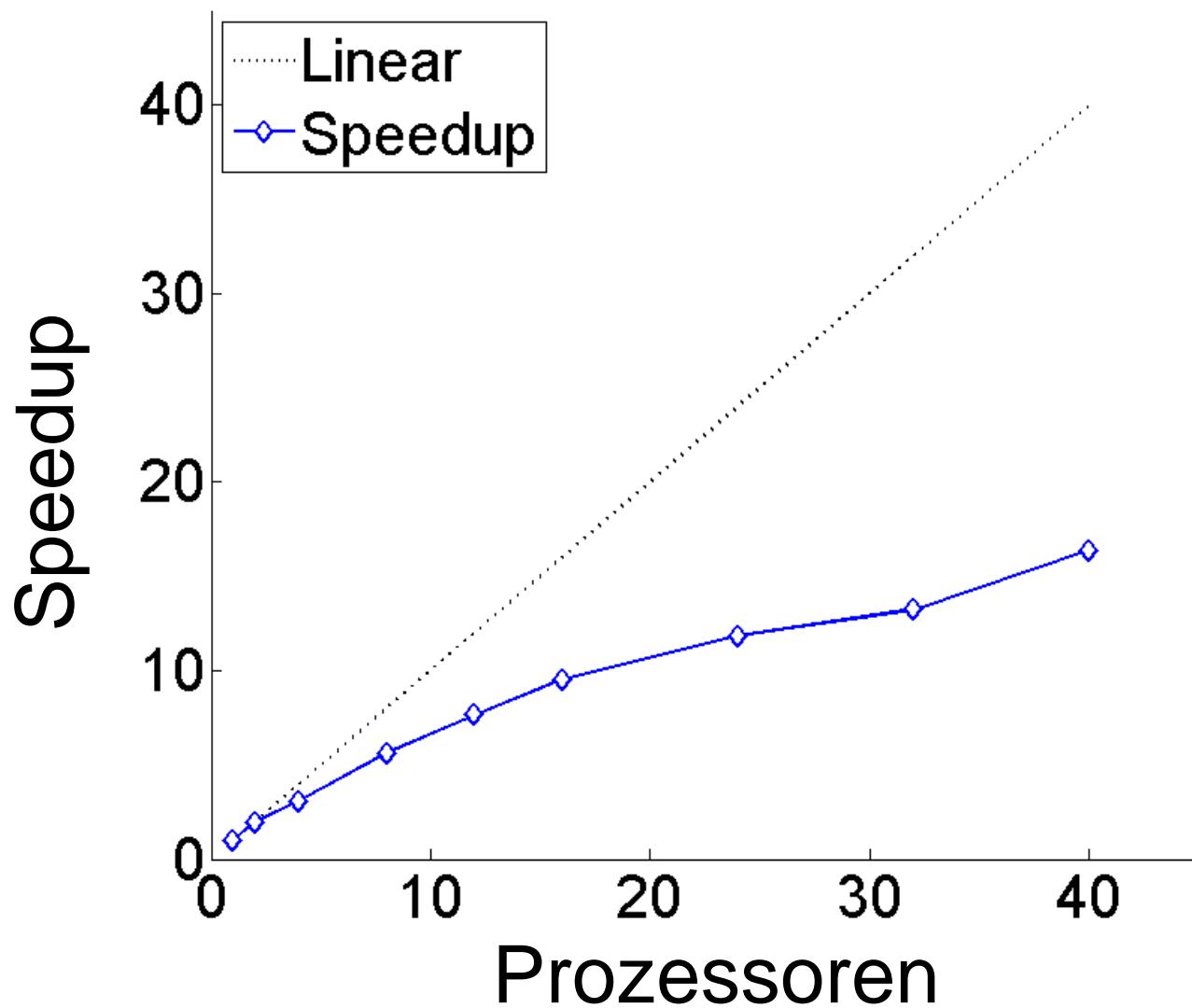

Neue parallele Varianten von QMR



Rekursives Doppeln



Zweiphasen-Problem



Zweiphasen-Strömung

$$\rho(\varphi) \left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} \right) = -\nabla p + \rho(\varphi) \mathbf{g} + \nabla \cdot (\mu(\varphi) \mathbf{D}(\mathbf{u})) + f_\Gamma$$
$$\nabla \cdot \mathbf{u} = 0$$

$$\frac{\partial \varphi}{\partial t} + \mathbf{u} \cdot \nabla \varphi = 0$$

Reparametrisierung:

$$\|\nabla \varphi\|_2 = 1$$

