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Enabling Implicit Time Integration for Compressible Flows by Partial Coloring: A Case Study of a Semi-matrix-free Preconditioning Technique

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Outline

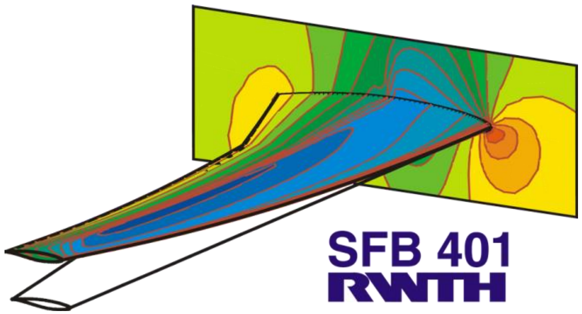
- Problem in Scientific Computing
- Combinatorial Model
- Heuristic Coloring Algorithm
- Experimental Results

QUADFLOW

Josef Ballmann
Mechanics

LFM

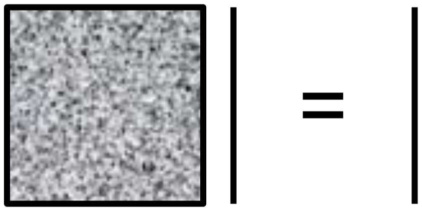
RWTH RHEINISCH-WESTFÄLISCHE TECHNISCHE HOCHSCHULE AACHEN

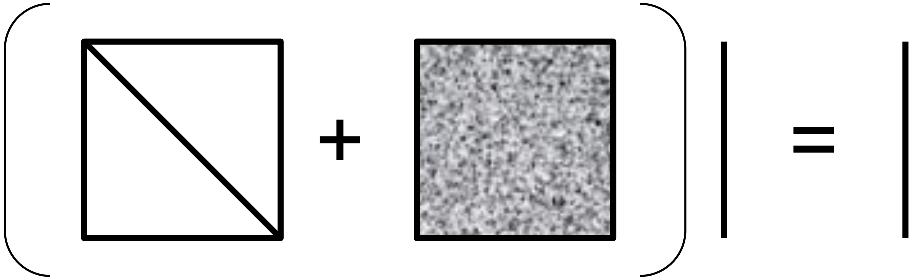


- Finite Volume
- Implicit Time Integration
- Unstructured Grids
- Adaptivity via Multiscale Analysis (Wolfgang Dahmen, Sigfried Müller, Mathematics, RWTH) igpm

Large Sparse Linear System

$$\left(\frac{|V|}{\Delta t} \mathbf{I} + \frac{\partial \mathbf{R}(\mathbf{u}^n)}{\partial \mathbf{u}^n} \right) \Delta \mathbf{u}^n = -\mathbf{R}(\mathbf{u}^n)$$





Automatic Differentiation (AD)

Given $\mathbf{x}_0 \in \mathbb{R}^n$, code to evaluate

$$f : \mathbb{R}^n \to \mathbb{R}^n$$

and $n \times p$ seed matrix S,

generate code to evaluate matrix-matrix product

$$\left.\frac{\partial f(\mathbf{x})}{\partial \mathbf{x}}\right|_{\mathbf{x}=\mathbf{x}_0} \cdot S$$

Relative runtime overhead: p

Preconditioning (PC)

Let $J(\mathbf{x}_0) := \left.\frac{\partial f(\mathbf{x})}{\partial \mathbf{x}}\right|_{\mathbf{x}=\mathbf{x}_0}$

Rather than $J\mathbf{y} = \mathbf{b}$

Solve $M^{-1}J\mathbf{y} = M^{-1}\mathbf{b}$

$$M \approx J$$

Missing Connections: AD and PC

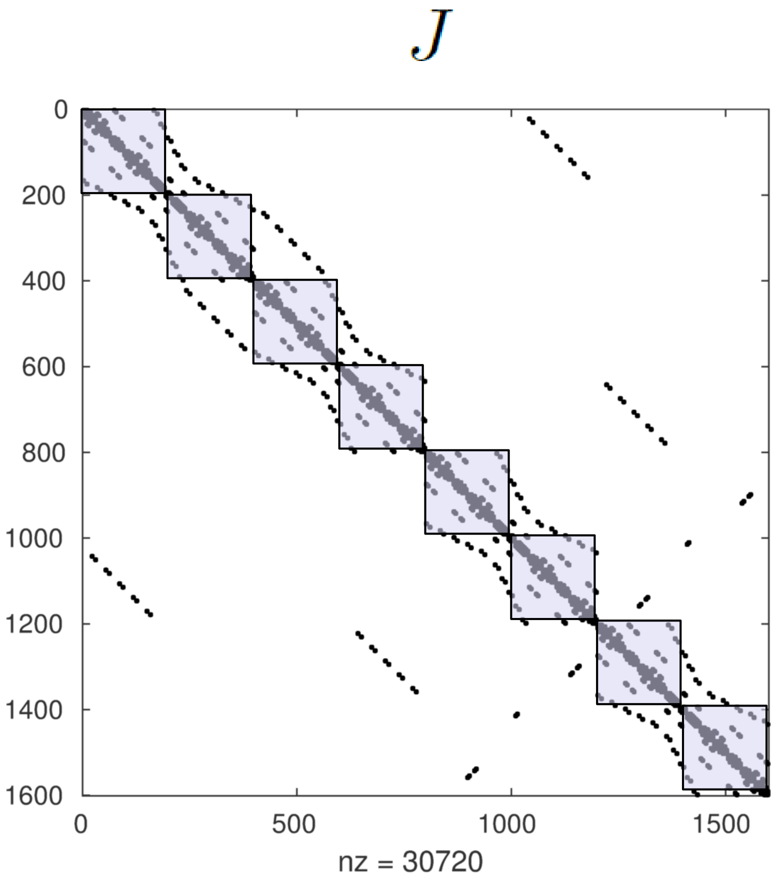
Automatic Differentiation:

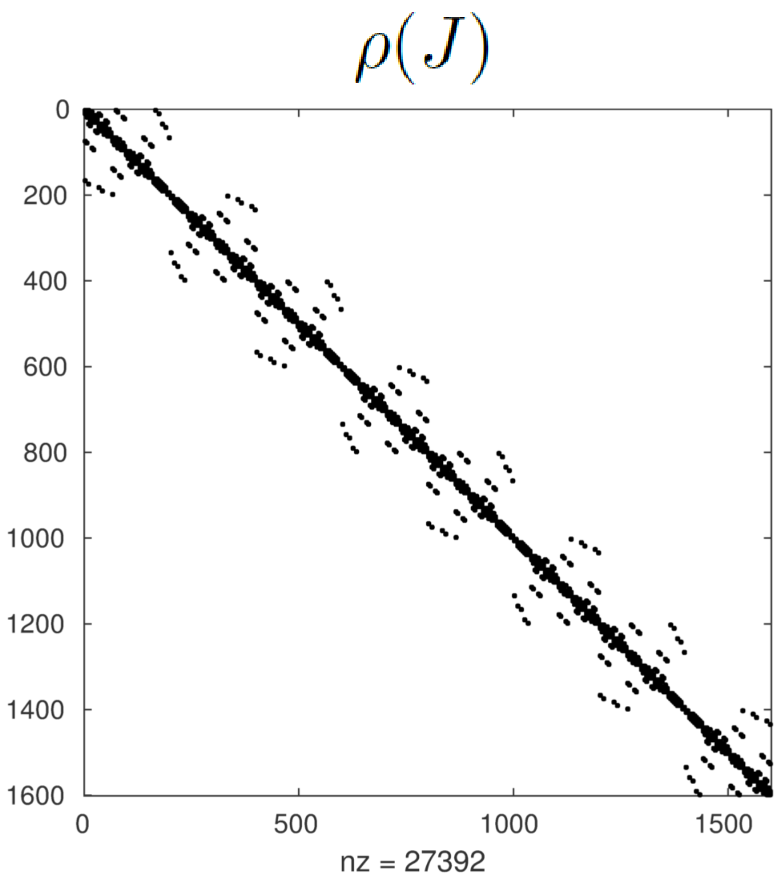
- Access to complete row/column
- Access to groups of complete rows/columns

Preconditioning:

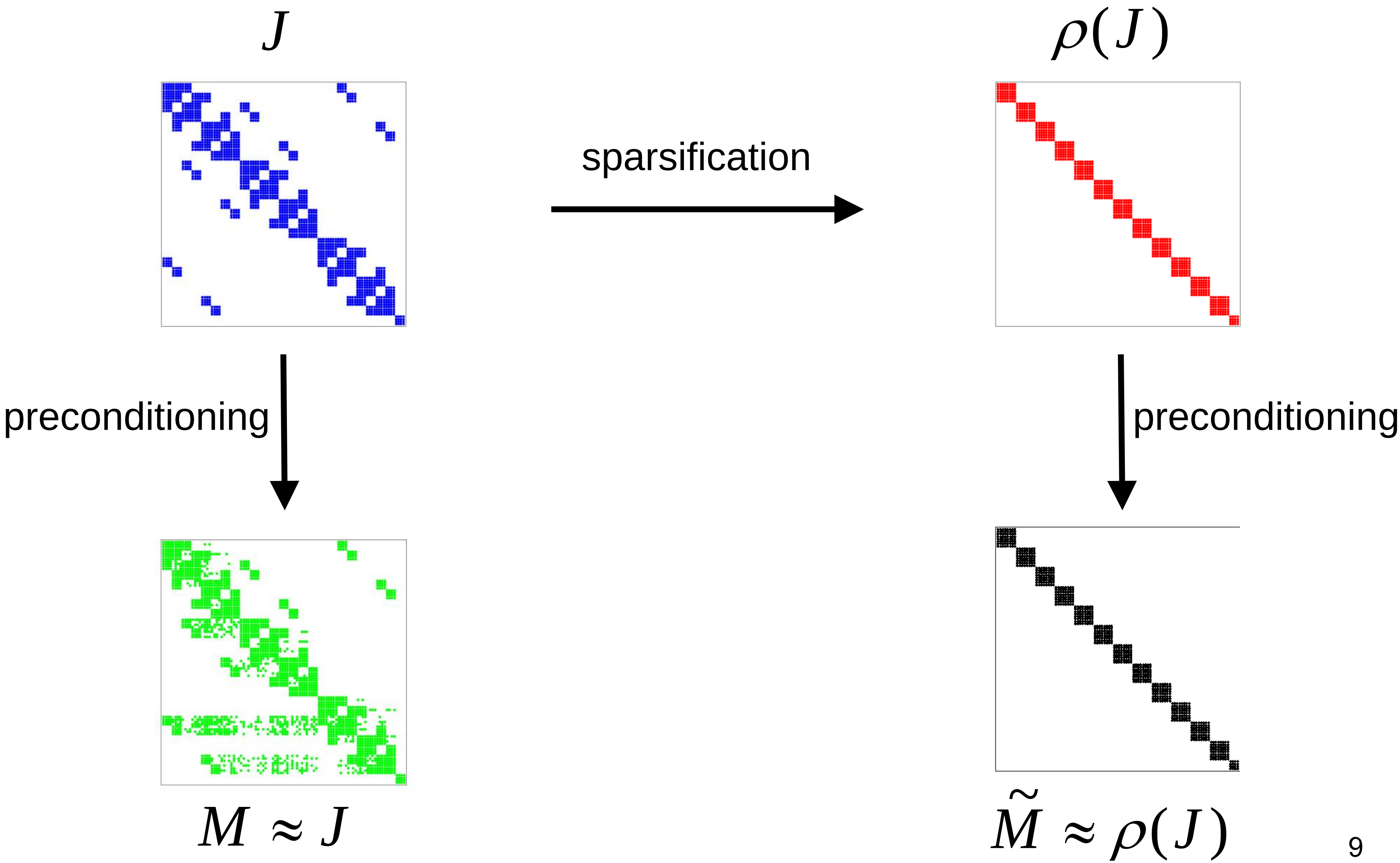
- Access to individual elements
- Access to chunks of rows/columns

Sparsification



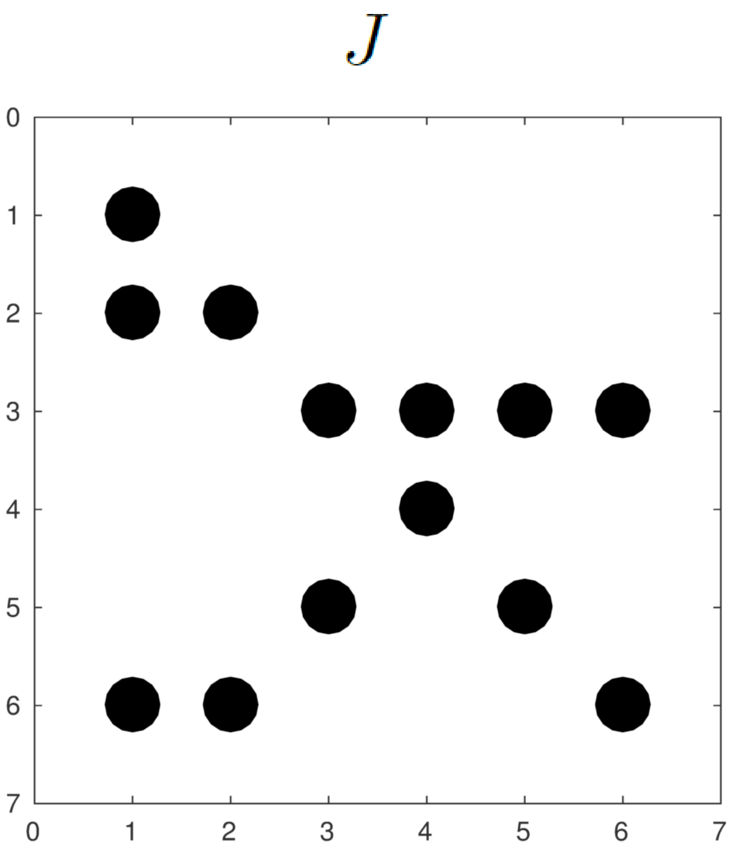


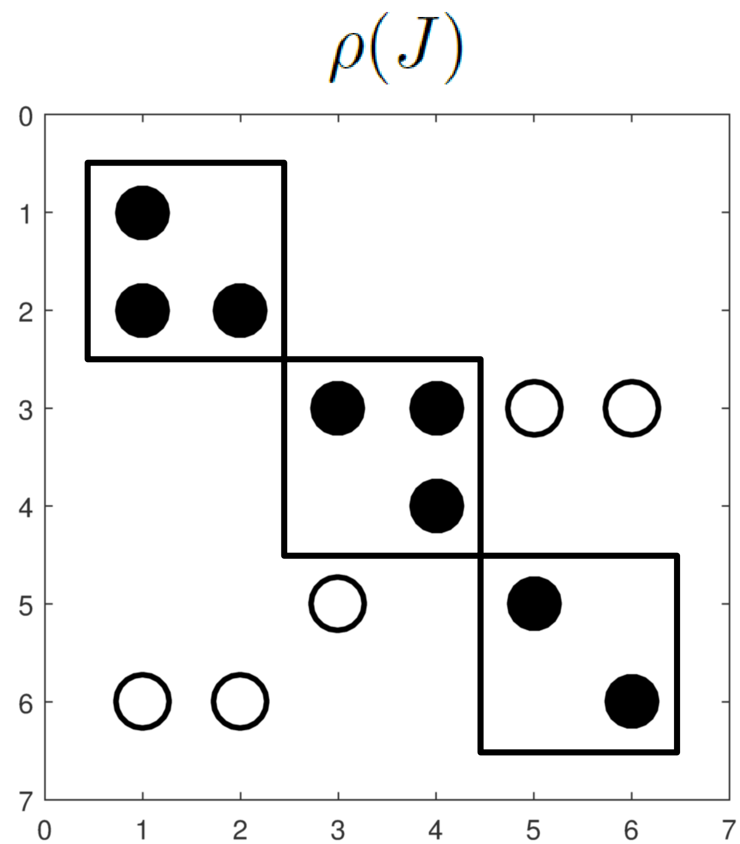
Main Idea

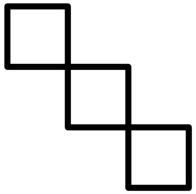


J
$\rho(J)$
sparsification
preconditioning
preconditioning
$M \approx J$
$\tilde{M} \approx \rho(J)$

Full vs Partial





$\rho(J)$ 

Scientific Computing Problem

Problem $\textsc{Block Seed}$:

Let J be a sparse $n \times n$ Jacobian matrix with known nonzero pattern and let $\rho(J)$ denote its sparsification using $k \times k$ blocks on the diagonal of J.
Find binary $n \times p$ seed matrix S with minimal number of columns p such that all nonzeros of $\rho(J)$ also appear in $J \cdot S$.

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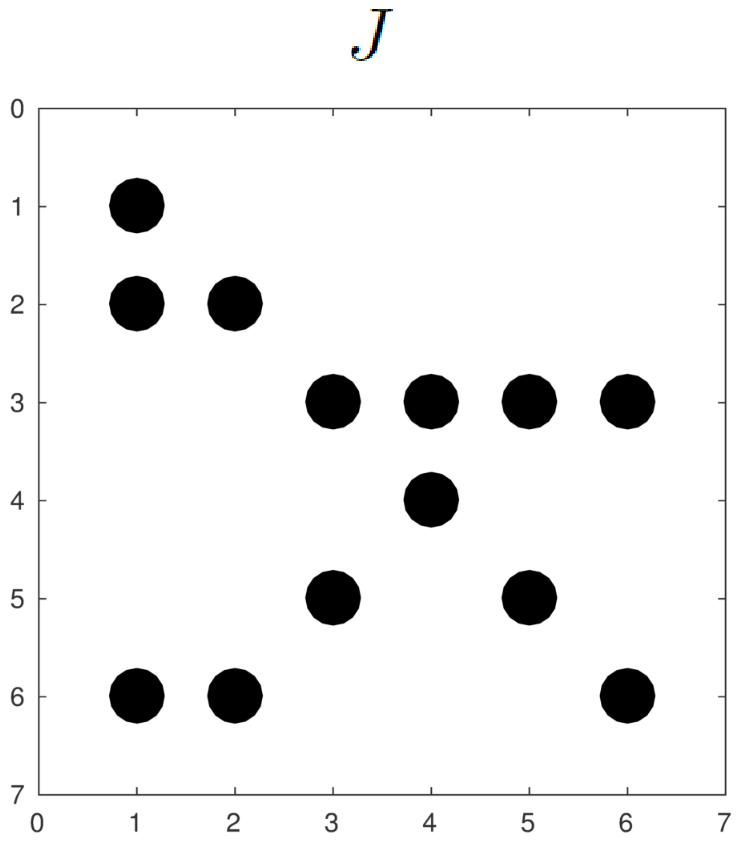
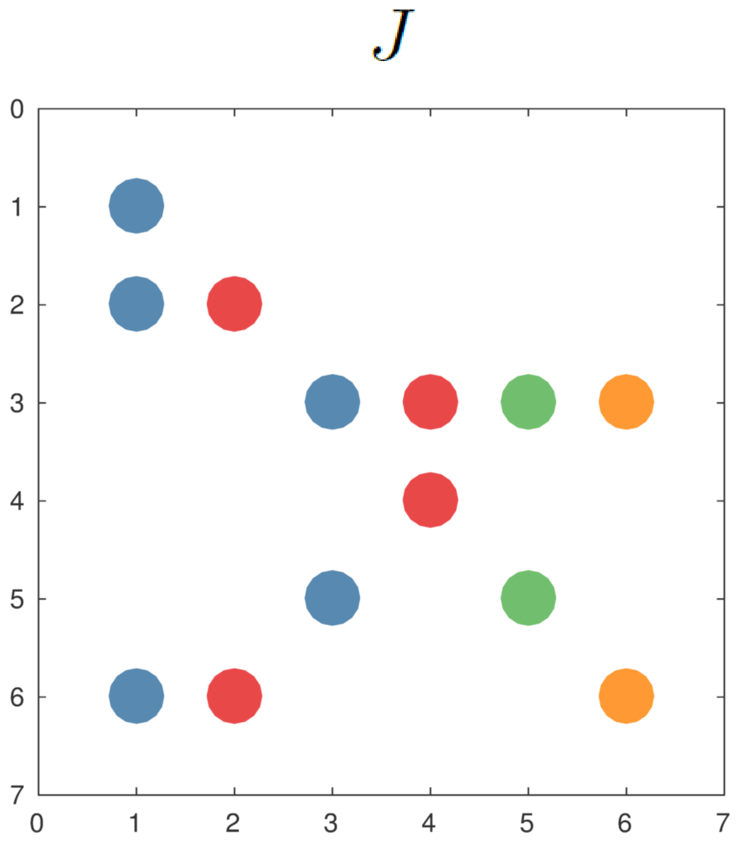
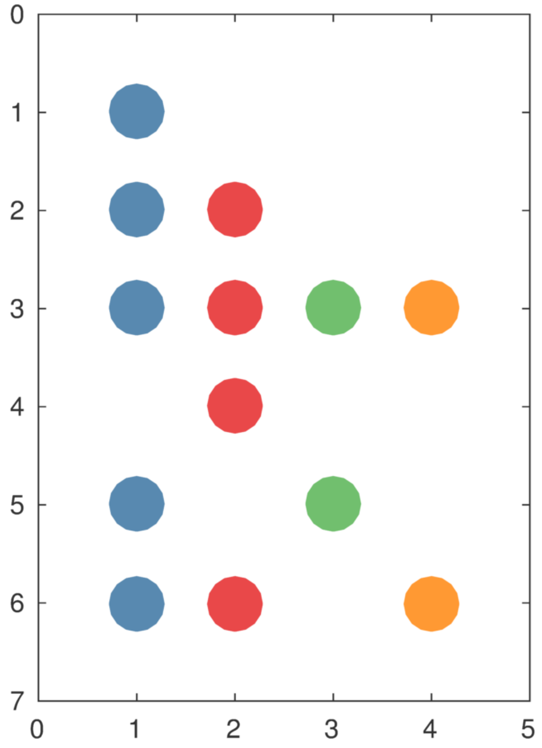
Full Coloring



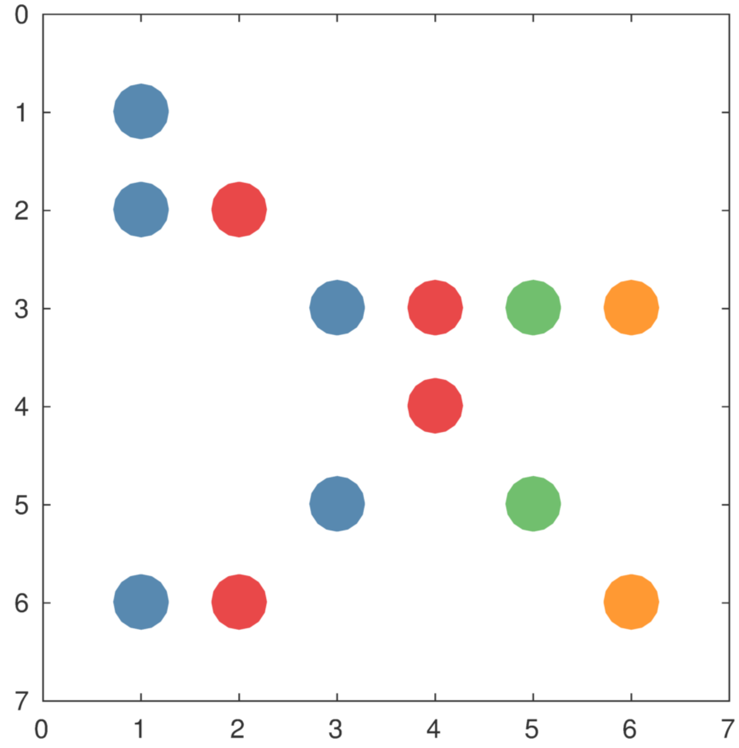


Full Coloring

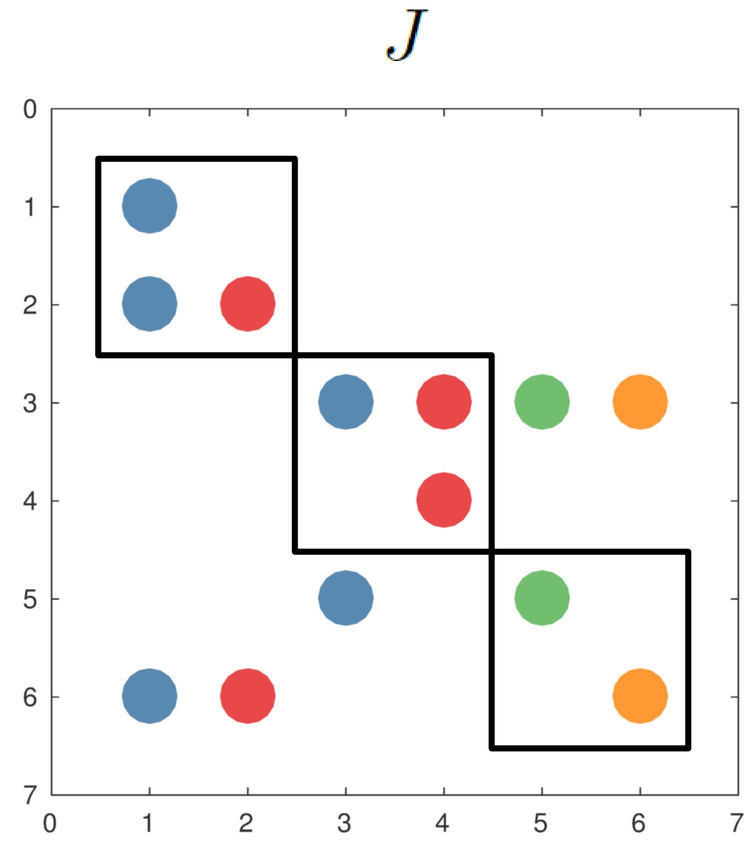
$J \cdot S$



J

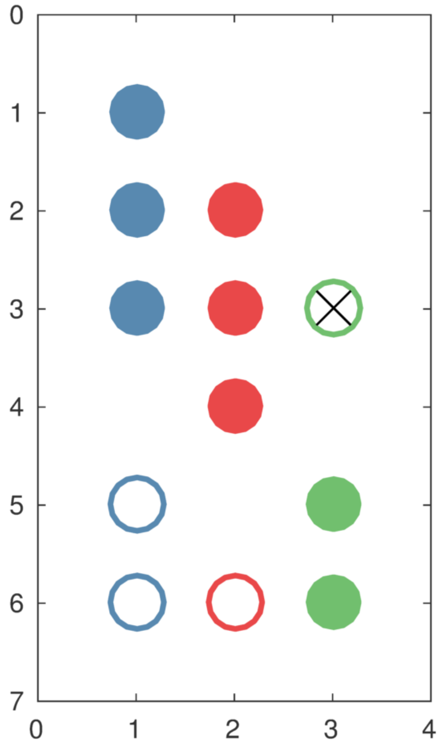


Partial Coloring

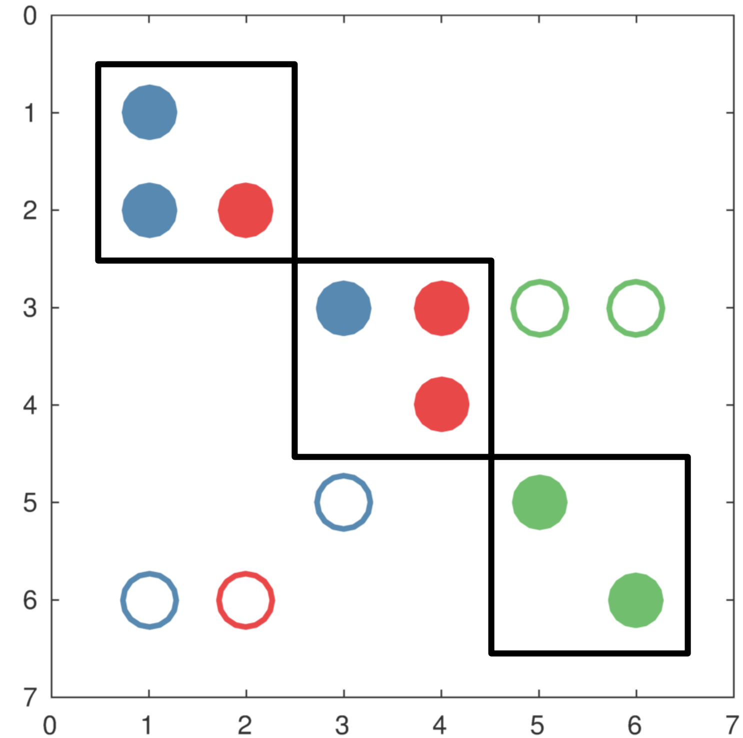


Partial Coloring

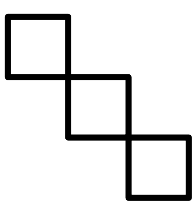
$J \cdot S$



$\rho(J)$



$\rho(J)$



Definition: ρ-Orthogonality

$J(:,i)$ structurally ρ-orthogonal to $J(:,j)$

$$:\overset{\text{def}}{=}$$

There is no row position ℓ in which $J(\ell,i)$ and $J(\ell,j)$ are nonzeros and at least one of them belongs to $\rho(J)$.

Definition: ρ-Column Intersection Graph

$G_\rho = (V, E_\rho)$ associated with a pair of $n \times n$ Jacobian matrices J and $\rho(J)$, where

- $V = \{v_1, v_2, \ldots, v_n\}$ v_i represents $J(:, i)$
- $(v_i, v_j) \in E_\rho$ iff $J(:, i)$ and $J(:, j)$ are not structurally ρ-orthogonal.

Combinatorial Problem

Problem $\textsc{Minimum Block Coloring}$:

Find a coloring of the ρ-column intersection graph G_ρ with a minimal number of colors.

Equivalent to problem $\textsc{Block Seed}$.

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Greedy Partial Coloring Heuristic

$n_c \leftarrow 1$, colors $\leftarrow [\,]$
$H_J(:,1) \leftarrow [0,0,\ldots,0]^T$
$H_{\rho(J)}(:,1) \leftarrow [0,0,\ldots,0]^T$
for $i = 1 : n$ **do**
    for $j = 1 : n_c$ **do**
        condA $\leftarrow$ any$(H_J(:,j) + \rho(J)(:,i) > 1)$
        condB $\leftarrow$ any$(H_{\rho(J)}(:,j) + J(:,i) > 1)$
        if $\neg$condA and $\neg$condB **then**
            % Assign color j to column i of J
            $H_J(:,j) \leftarrow H_J(:,j) + J(:,i)$
            $H_J(H_J > 1) \leftarrow 1$
            $H_{\rho(J)}(:,j) \leftarrow H_{\rho(J)}(:,j) + \rho(J)(:,i)$
            $H_{\rho(J)}(H_{\rho(J)} > 1) \leftarrow 1$
            colors $\leftarrow$ [colors $\;\; j$]
            $n_c \leftarrow \max(n_c, j+1)$
            Exit from loop over j and goto next i
$p = \max(\text{colors})$
return p, colors

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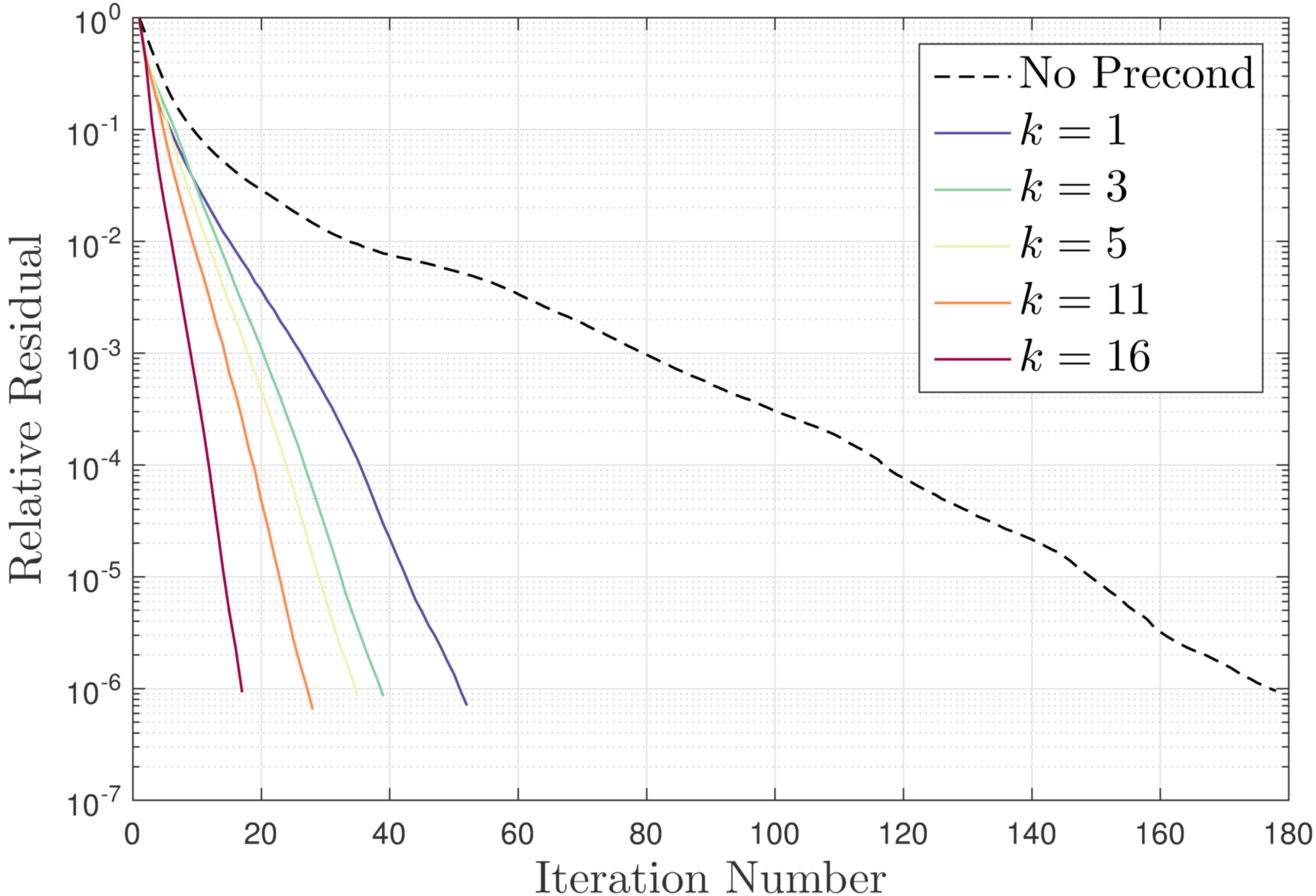
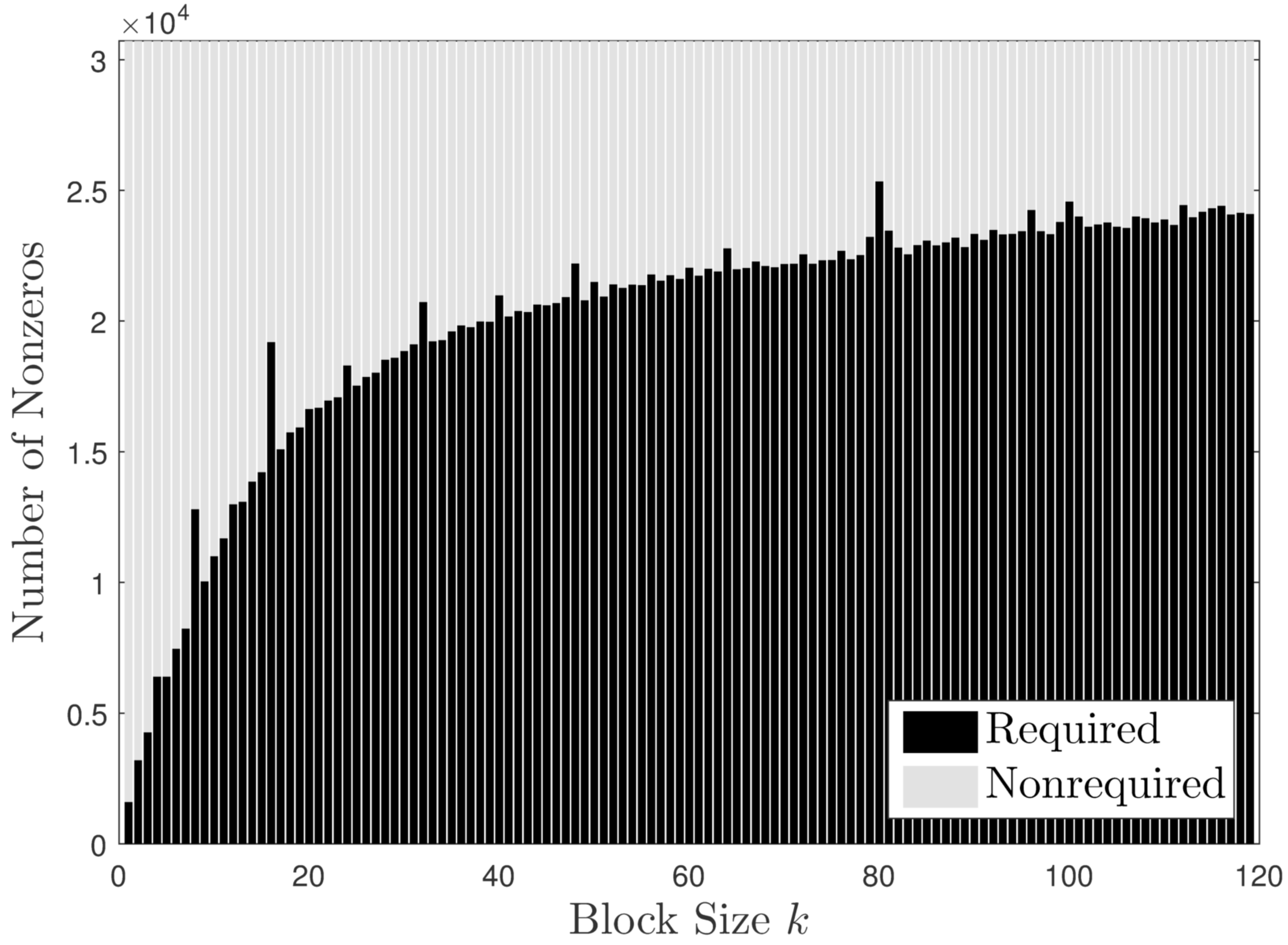
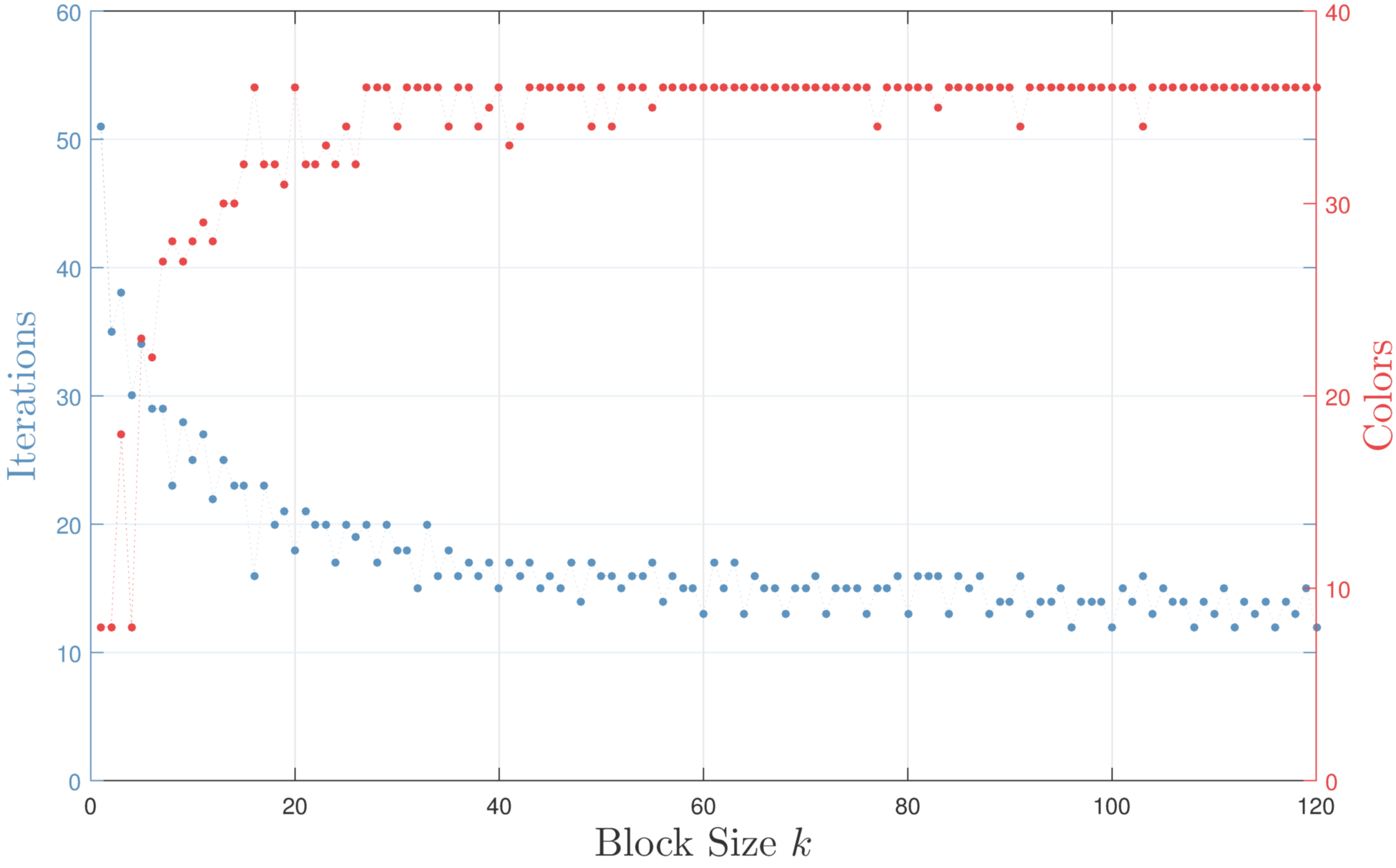
Convergence Behavior with GMRES, ILU(0)



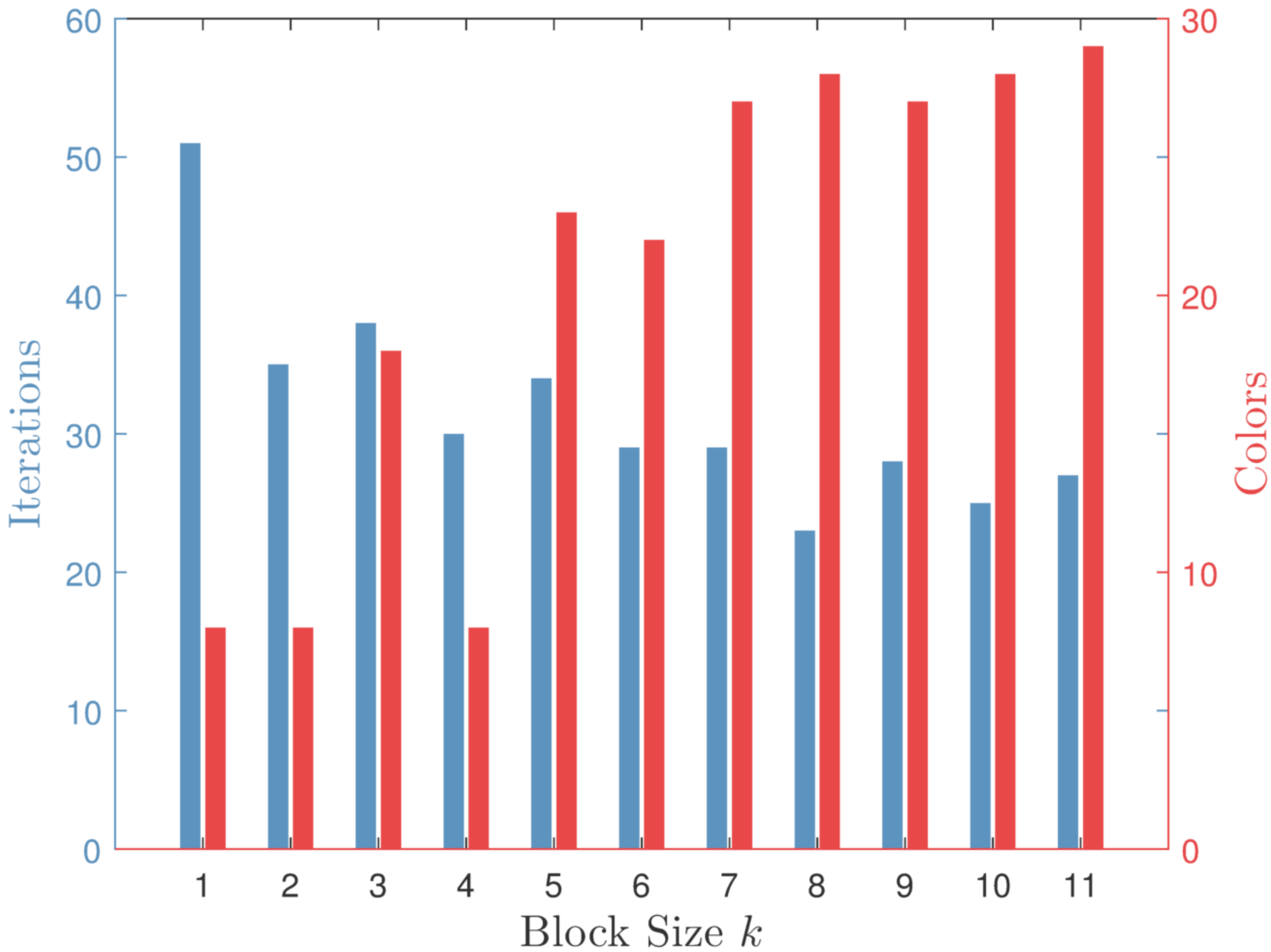
Number of Nonzeros



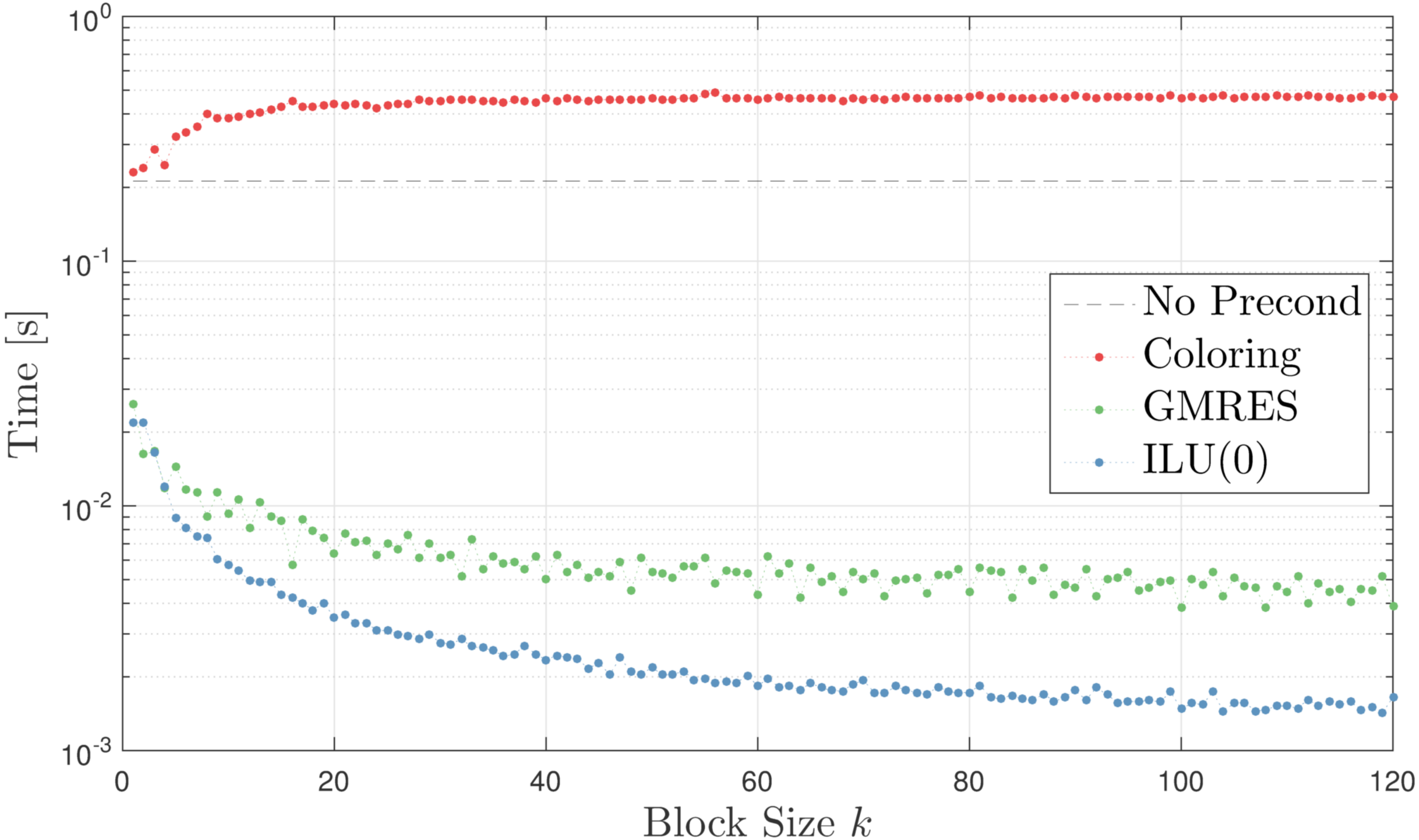
Iterations and Colors



Zoom into Previous Figure



Execution Times



Concluding Remarks

- Formulation of a combinatorial problem arising from preconditioning using automatic differentiation
- Graph model encoding this situation as a partial coloring problem
- Design of heuristic partial coloring algorithm
- Application to case study from CFD

Major References

- QUADFLOW: Bramkamp, Lamby, and Müller. An adaptive multiscale finite volume solver for unsteady and steady state ow computations. *Journal of Computational Physics*, 197(2):460-490, 2004.
- Sparsity: Gebremedhin, Manne, and Pothen. What color is your Jacobian? Graph coloring for computing derivatives. *SIAM Review*, 47(4):629-705, 2005
- Sparsification: Cullum and Tuma. Matrix-free preconditioning using partial matrix estimation. *BIT Numerical Mathematics*, 46(4):711-729, 2006.