

# Solving sequences of linear systems by preconditioned iterative methods

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joint work with

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Supported by the project “Information Society”  
of the Academy of Sciences of the Czech Republic under No. 1ET400300415

CSC'05, June 21–23, 2005.

Toulouse, France, EU



# Outline

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1. Motivation
2. Our goal: Reuse of matrix **approximations / preconditioners**
3. Reuse of structural information (**preconditioner patterns**)
4. Reuse of structural + numerical information (**preconditioners**)
5. Conclusions
6. Advertisement



# 1. Motivation / Newton's method

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## 1. Solving systems of nonlinear equations

$$F(x) = 0$$



Sequences of linear systems of the form

$$J(x_k)\Delta x = -F(x_k), \quad J(x_k) \approx F'(x_k)$$

solved until for some  $k, k = 1, 2, \dots$

$$\|F(x_k)\| < tol$$

$J(x_k)$  may change at points influenced by nonlinearities



# 1. Motivation / Nonlinear convection-diffusion

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## 2. Solving nonlinear convection-diffusion problems

$$-\Delta u + u \nabla u = f$$



E.g., from the upwind discretization in 2D, with  $u \geq 0$  we get for grid internal nodes  $(i, j)$

$$u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1} - 4u_{ij} + hu_{ij}(2u_{ij} - u_{i-1,j} - u_{i,j-1}) = h^2 f_{ij}$$

It is a matrix with five diagonals

Entries in its three diagonals may change in subsequent linear systems







# 1. Motivation / Parabolic equation

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## 3. Solving equations with a parabolic term

$$\frac{\partial u}{\partial t} - \Delta u = f$$



E.g., 2D problem with  $2^{nd}$  order centered differences in space and backward Euler time discretization for grid internal nodes  $(i, j)$  and time step  $t + 1$

$$h^2(u_{ij}^{t+1} - u_{ij}^t) + \tau(u_{i+1,j}^{t+1} + u_{i-1,j}^{t+1} + u_{i,j+1}^{t+1} + u_{i,j-1}^{t+1} - 4u_{ij}^{t+1}) = h^2\tau f_{ij}^{t+1}$$

Again, we get a matrix with five diagonals

Diagonal entries may change with time steps



## 2. Our goal / Reuse of approximations: I.

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Reuse of approximations of matrices in sequences of linear systems

Solving sequences of systems of linear equations

$$A^0 x = b^0, A^1 x = b^1, \dots$$

by **preconditioned iterative methods** with preconditioners

$$M^0, M^1, \dots$$

**Goal:** computing  $M^{i+k}$  from  $A^{i+k}$  for some  $k \geq 1$ ,  
and possibly reuse additional information from  $M^i$  and  $A^i$ .





## 2. Our goal / Reuse of approximations: II.

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Two basic strategies for the information reuse



## 2. Our goal / Reuse of approximations: II.

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Two basic strategies for the information reuse

### 1. Reuse of matrix patterns

- Using pattern of  $M^i$ .
- Using pattern of  $\hat{A}_i$  ( $A_i$ , or a part of  $A_i$ ).



## 2. Our goal / Reuse of approximations: II.

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### Two basic strategies for the information reuse

#### 1. Reuse of matrix patterns

- Using pattern of  $M^i$ .
- Using pattern of  $\hat{A}_i$  ( $A_i$ , or a part of  $A_i$ ).

#### 2. Reuse of both patterns and values

- Using entries of  $M^i$ .
- Using entries of  $\hat{A}_i$  ( $A_i$ , or a part of  $A_i$ ).



## 2. Our goal / Related work: I.

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### Some related work

- Preconditioners from quasi-Newton updates (Morales, Nocedal, 2000)
- **Freezing** approximate **Jacobians** over a couple of subsequent systems (MNK: Shamanskii, 1967; Brent, 1973).
- **Freezing** the **preconditioner** over a couple of subsequent systems (MFNK: Knoll, McHugh, 1998).
- Some simple preconditioners (e.g., Jacobi, ILU(0) for PDEs) may be readily available even in parallel and/or matrix-free environment
- Preconditioners from a related matrix, operator (e.g., based on orthogonal grid, Truchas code, LANL, 2003; cf. Knoll, Keyes, 2004) **a lot of approaches**)
- Solving systems in adaptive filtering by incomplete factorizations + iterative refinement (Comon, Trystram, 1987)
- Approximate diagonal updates (Benzi, Bertaccini, 2003; Bertaccini, 2004)



## 2. Our goal / Related work: II.

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### Some related work (continued)

- **World** of updates of Krylov subspaces (e.g., Morgan 1995-2002); Baglama, Calvetti, Golub, Reichel, 1999; Carpentieri et. al., 2003; de Sturler, 1996; Erhel, Burrage, Pohl, 1996; Duff, Giraud, Langou, Martin, 2005; Giraud et. al. 2004–2005; Parks et al. 2004)
- Dense updates of decompositions (Bartels, Golub, Saunders, 1970; Gill, Golub, Murray, Saunders, 1974)
- Sparse updates of decompositions (Hager, Davis, 1999–2004).



## 2. Our goal / Related work: III.

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### Some related work (continued)

- Use of cheap **matrix estimations** based on graph coloring techniques in matrix free-environment if we know the matrix structure. This is a **classical field**; a (very restricted) selection of references: Curtis, Powell; Reid, 1974; Coleman, Moré, 1983; Coleman, Moré, 1984; Coleman, Verma, 1998;

### The procedure

- \* Estimate the matrix  $A_i$  by a few matvecs
- \* Get the preconditioner  $M_i$  directly from  $A_i$
- extensions to SPD (Hessian) approximations; extensions to use both  $A$  and  $A^T$  in automatic differentiation; more sophisticated estimation of resulting entries (substitution methods)
- to get only a **part of the matrix** which changes in the outer iterations: **partial graph coloring**, Gebremedhin, Manne, Pothen, 2004.



## 2. Our goal: An example

The 2D nonlinear convection-diffusion problem (Kelley, 1995); 5-point finite differences; uniform grid  $70 \times 70$ ; first 8 systems; ILUT(0.1,5)

$$\Delta u - Ru\nabla u = 2000x(1-x)y(1-y), \quad R = 500$$

A-matrix	M-matrix	CG - its
$A^1$	$M^1$	25
$A^2$	$M^1$	98
$A^3$	$M^1$	90
$A^4$	$M^1$	135
$A^5$	$M^1$	179
$A^6$	$M^1$	229
$A^7$	$M^1$	275
$A^8$	$M^1$	345
$A^{1-8}$	$M^{1-8}$	$25 \pm 10$

Freezing the preconditioner may not be enough



## 3. Reuse of matrix patterns

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What do we gain if we use a sparsified pattern for preconditioner computation?

1. **Traditionally:** Sparsified pattern  $\rightarrow$  cheaper preconditioner computation
2. **Proposal 1:** Sparsified pattern + matrix-free environment  $\rightarrow$  cheaper but approximate matrix estimation via matvecs (Cullum, T., 2004)
3. **Proposal 2:** Freezing the matrix pattern in a matrix-free environment: use of the sparsified pattern of a different matrix from a sequence.
4. **Proposal 3:** Freezing the preconditioner pattern (from a different preconditioner)





## 3. Reuse of matrix patterns: II.

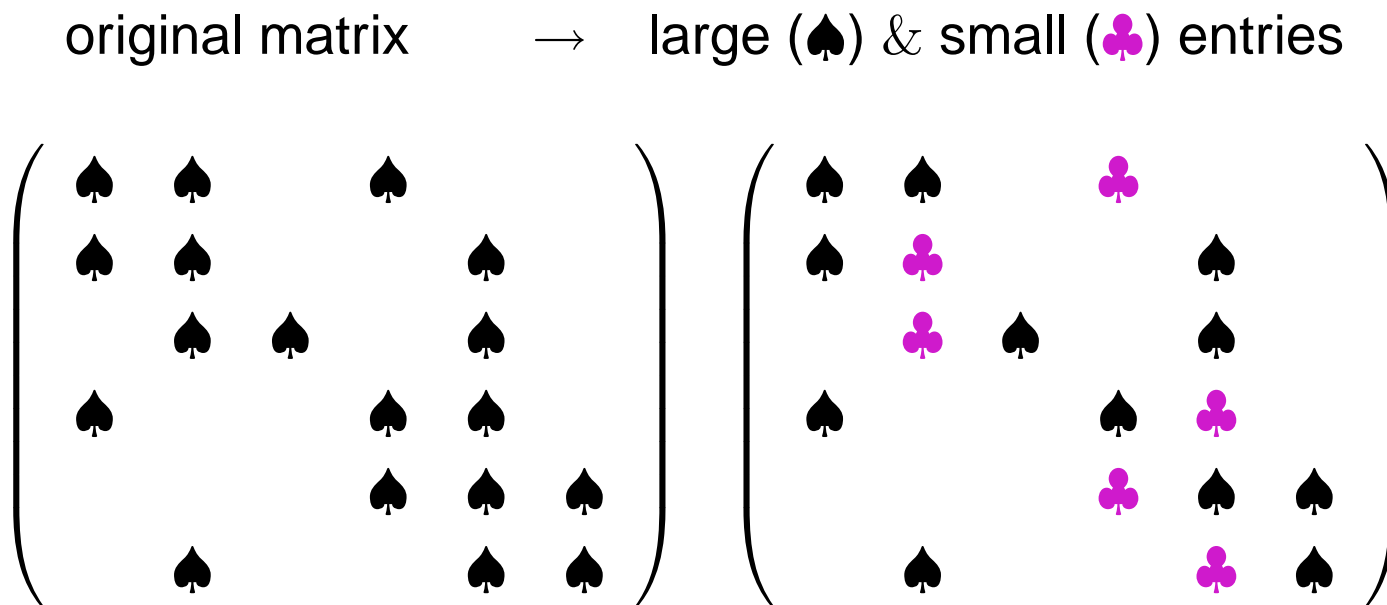
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**Traditionally:** Sparsified pattern leads to **cheaper preconditioner computation.**



### 3. Reuse of matrix patterns: II.

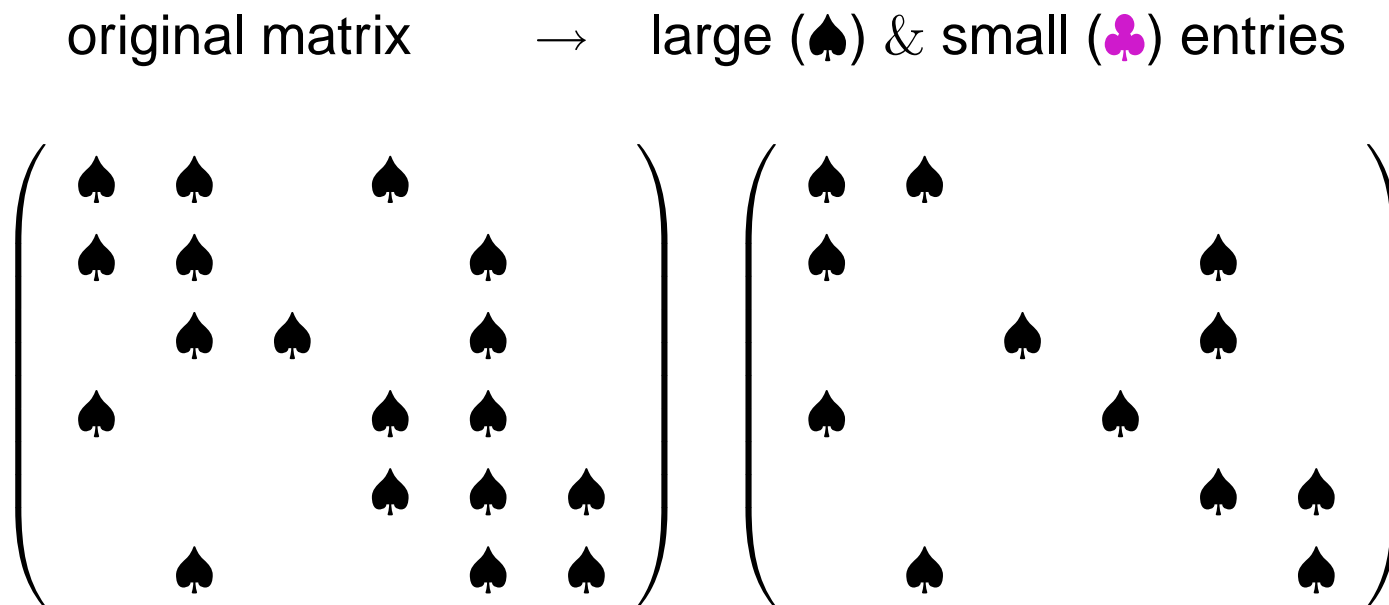
Traditionally: Sparsified pattern leads to cheaper preconditioner computation.





### 3. Reuse of matrix patterns: II.

Traditionally: Sparsified pattern leads to cheaper preconditioner computation.





## 3. Reuse of matrix patterns: Proposal 1

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Proposal 1: Sparsified pattern + matrix-free environment → **cheaper** but **approximate** matrix estimation via matvecs (Cullum, T., 2004)



## 3. Reuse of matrix patterns: Proposal 1

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Proposal 1: Sparsified pattern + matrix-free environment → **cheaper** but **approximate** matrix estimation via matvecs (Cullum, T., 2004)

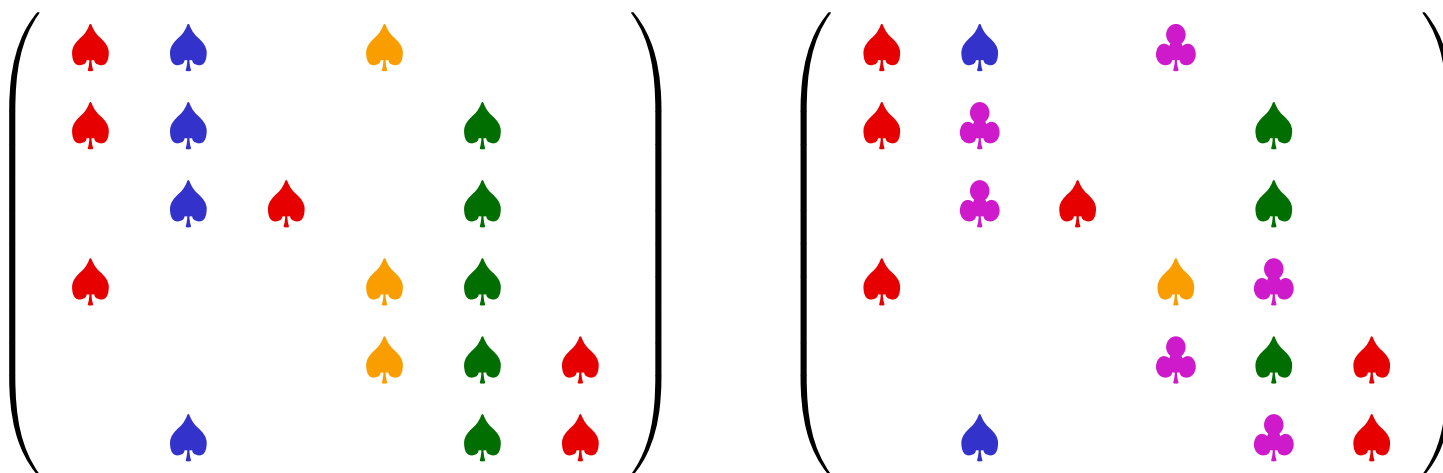
First, a gentle introduction into matrix estimation





### 3. Reuse of matrix patterns: Proposal 1

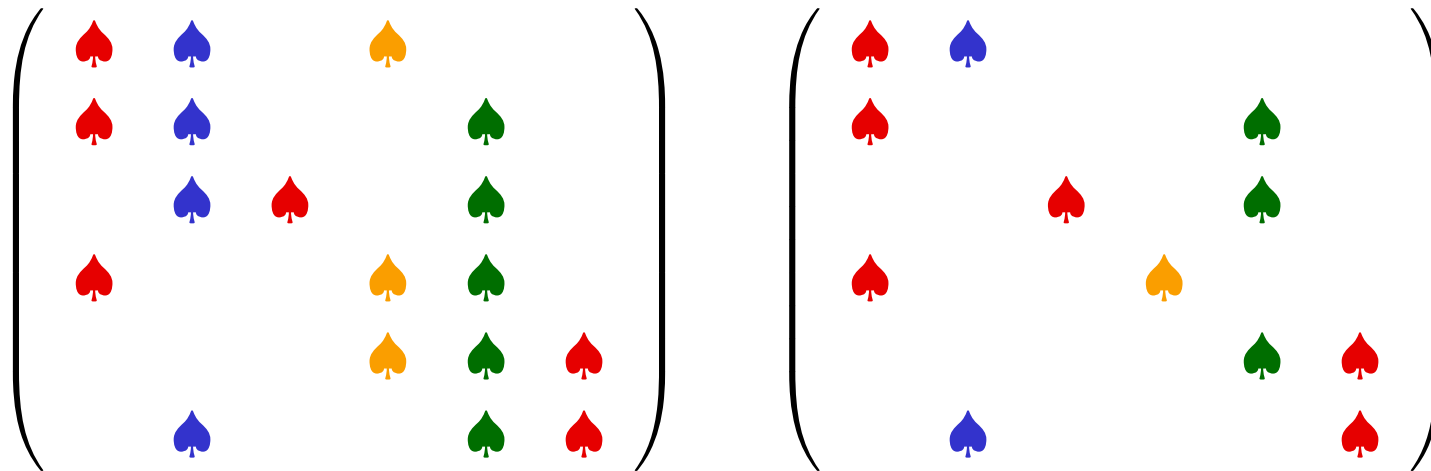
four matvecs needed → large (coloured ♠) & small (♣) entries





### 3. Reuse of matrix patterns: Proposal 1

large (coloured ♠) & small (♣) entries  $\rightarrow$  only two matvecs needed

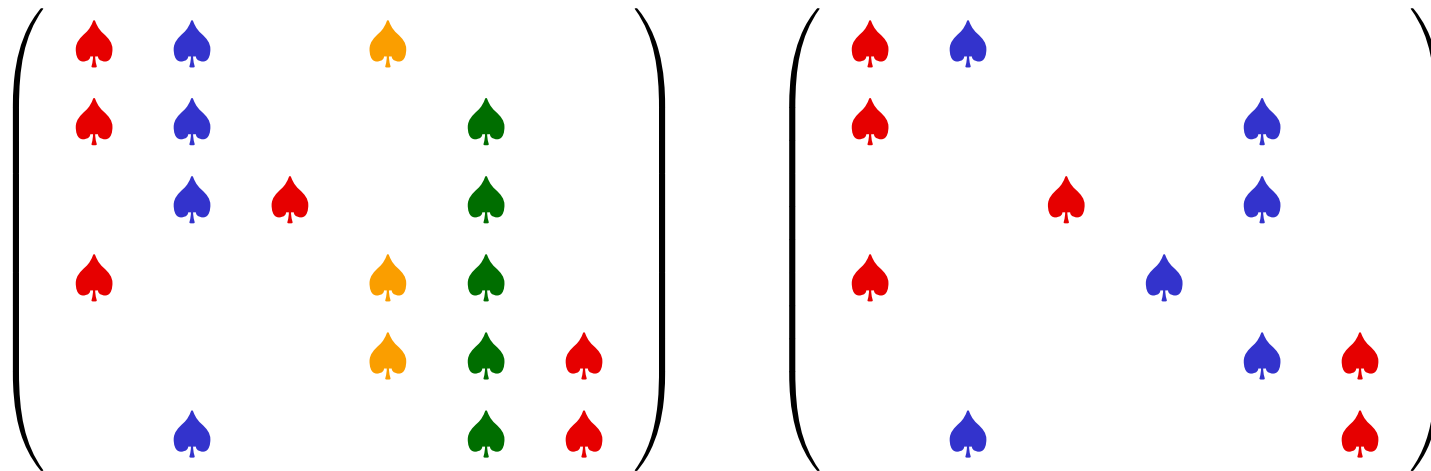






### 3. Reuse of matrix patterns: Proposal 1

large (coloured ♠) & small (♣) entries  $\rightarrow$  only two matvecs needed





### 3. Reuse of matrix patterns: Proposal 2: Results

**Proposal 2:** Freezing the matrix pattern in a matrix-free environment: use of the sparsified pattern of a **different** matrix from a sequence.

Driven cavity flow,  $n = 8603$ ,  $R = 500$ , ILUT( $1.0 * 10^{-6}$ , 25); Newton

No. A-matrix	No. P-matrix	<i>CG – its</i>
$A^1$	$M^1$ via $A^1$ and pattern of $\hat{A}^1$	44
$A^2$	$M^2$ via $A^2$ and pattern of $\hat{A}^1$	38
$A^3$	$M^3$ via $A^3$ and pattern of $\hat{A}^1$	41
$A^4$	$M^4$ via $A^4$ and pattern of $\hat{A}^1$	42
$A^5$	$M^5$ via $A^5$ and pattern of $\hat{A}^1$	43
$A^2$	$M^2$ via $A^2$ and pattern of $\hat{A}^2$	42
$A^3$	$M^3$ via $A^3$ and pattern of $\hat{A}^3$	38
$A^4$	$M^4$ via $A^4$ and pattern of $\hat{A}^4$	43
$A^5$	$M^5$ via $A^5$ and pattern of $\hat{A}^5$	42



## 3. Reuse of matrix patterns: Proposal 3

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**Proposal 3:** Freezing the preconditioner pattern (for preconditioners with pattern input)

- Determination of a suitable pattern of preconditioner may be sometimes rather difficult

Our approach:

- Find a pattern for  $A_0$  by a sophisticated / time-consuming method using both symbolic/numeric information
- Use the pattern to get preconditioners  $M_0, M_1, \dots$
- Restart if necessary



### 3. Reuse of matrix patterns: Proposal 3

old SPAI versus old LS based on old SPAI pattern

The 2D nonlinear convection-diffusion problem (Kelley, 1995); 5-point finite differences; uniform grid  $70 \times 70$ ; first 8 systems; SPAI(0.0,5,5); preconditioner size = 87300

$$\Delta u - Ru \nabla u = 2000x(1-x)y(1-y), \quad R = 500$$

NO UPDATES		
<i>Matrix</i>	<i>old_SPAI_its</i>	<i>old_LS/SPAI_its</i>
$A^1 / M^1$	50	49
$A^2 / M^1$	76	71
$A^3 / M^1$	89	79
$A^4 / M^1$	113	134
$A^5 / M^1$	138	147
$A^6 / M^1$	157	161
$A^7 / M^1$	201	173
$A^8 / M^1$	238	179



### 3. Reuse of matrix patterns: Proposal 3

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#### SPAI versus LS with old SPAI pattern

The same 2D nonlinear convection-diffusion problem (Kelley, 1995);  
SPAI(0.0,5,5)

#### new SPAI versus new LS with old SPAI pattern

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Number of iterations in SPAI:	$50 \pm 8$
Number of iterations in LS with old SPAI pattern:	$50 \pm 8$
Time for computing SPAI preconditioner	=0.62 – 0.69 s
Time for computing LS preconditioner with old SPAI pattern	=0.22 s
Sequential time for 50 iterations	$\approx 0.1$ s

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## 4. Reuse of matrix: Entrywise updates

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Exploiting both pattern and numerical values

$$A_0 \rightarrow A_1 = A_0 + B$$



## 4. Reuse of matrix: Entrywise updates

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Exploiting both pattern and numerical values

$$A_0 \rightarrow A_1 = A_0 + B$$

**Case I:** Simple one-entry off-diagonal updates

$$B = uv^T = \alpha e_i e_j^T$$



## 4. Reuse of matrix: Entrywise updates

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Exploiting both pattern and numerical values

$$A_0 \rightarrow A_1 = A_0 + B$$

**Case I: Simple one-entry off-diagonal updates**

$$B = uv^T = \alpha e_i e_j^T$$

$$A_1^{-1} = (A_0 + B)^{-1} = (A_0 + xy^T)^{-1} = (LDU + xy^T)^{-1} = \\ (L(D + L^{-1}xy^T U^{-1})U)^{-1} \approx U^{-1}(I + \alpha D^{-1}e_i e_j^T)^{-1} D^{-1} L^{-1} =$$

$$\frac{U^{-1}(I - \alpha D^{-1}e_i e_j^T)D^{-1}L^{-1}}{1 + \alpha e_j^T D^{-1}e_i}$$





## 4. Reuse of matrix: Entrywise updates

Exploiting both pattern and numerical values

$$A_0 \rightarrow A_1 = A_0 + B$$

**Case I: Simple one-entry off-diagonal updates**

$$B = uv^T = \alpha e_i e_j^T$$

$$A_1^{-1} = (A_0 + B)^{-1} = (A_0 + xy^T)^{-1} = (LDU + xy^T)^{-1} = \\ (L(D + L^{-1}xy^T U^{-1})U)^{-1} \approx U^{-1}(I + \alpha D^{-1}e_i e_j^T)^{-1} D^{-1} L^{-1} =$$

$$\frac{U^{-1}(I - \alpha D^{-1}e_i e_j^T)D^{-1}L^{-1}}{1 + \alpha e_j^T D^{-1}e_i}$$

- Approximation good if there is a **strong matrix diagonal** – it can be forced by a weighted matching applied to the matrix graph
- Inversion of a Gauss-Jordan transform
- More Gauss-Jordan transforms can be accumulated in one sweep (using pattern-based conditions) ... **next slide**



## 4. Reuse of matrix: Entrywise updates II.

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### More Gauss-Jordan transforms

- Entries for a sweep with Gauss-Jordan transforms can be (e.g.) found from a **weighted spanning forest**  $T$  of the graph  $G_B$  of a (sparsified) difference matrix  $B = A_1 - A_0$ .



## 4. Reuse of matrix: Entrywise updates II.

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### More Gauss-Jordan transforms

- Entries for a sweep with Gauss-Jordan transforms can be (e.g.) found from a **weighted spanning forest**  $T$  of the graph  $G_B$  of a (sparsified) difference matrix  $B = A_1 - A_0$ .

### The procedure

1. Find the weighted forest  $T$  of  $G_B$
2. Find the order of Gauss-Jordan transforms corresponding to the edges of  $T$  (It can be proved that it is feasible)
3. Add to the product of the Gauss-Jordan transforms other nonzeros entries of  $B$  (It can be shown which entries, based on simple structural conditions)



## 4. Reuse of matrix: Entrywise updates III.

Updates of diagonal + subdiagonal representing convection changes in a 2D convection-diffusion problem,  $n = 10000$

2D CD problems with a 1D - convection shift		
<i>Shift</i>	<i>NO_updates_its</i>	<i>CONV_updates_its</i>
0.1	52	54
0.2	58	60
0.3	67	60
0.4	68	61
0.5	75	65
0.6	81	73
0.7	100	76
0.8	121	78
0.9	146	81
1.0	186	82

New preconditioner: 34 iterations



## 4. Reuse of matrix: Entrywise updates IV.

Updates of diagonal + subdiagonal representing convection changes in a 2D convection-diffusion problem (different from the previous one),

$$n = 10000$$

2D CD problems with a 1D - convection shift		
<i>Shift</i>	<i>NO_updates_its</i>	<i>CONV_updates_its</i>
0.1	34	33
0.2	36	35
0.3	39	34
0.4	38	33
0.5	44	34
0.6	56	38
0.7	53	34
0.8	63	34
0.9	69	30

New preconditioner: 35 iterations



## 4. Reuse of matrix: Triangular updates

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Exploiting both pattern and numerical values

$$A_0 \rightarrow A_1 = A_0 + B$$



## 4. Reuse of matrix: Triangular updates

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Exploiting both pattern and numerical values

$$A_0 \rightarrow A_1 = A_0 + B$$

**Case II: Triangular updates**

$$B = L_B + D_B + U_B$$



## 4. Reuse of matrix: Triangular updates

---

Exploiting both pattern and numerical values

$$A_0 \rightarrow A_1 = A_0 + B$$

**Case II: Triangular updates**

$$B = L_B + D_B + U_B$$

$$\begin{aligned} A_1^{-1} &= (A_0 + B)^{-1} = (A_0 + L_B + D_B + U_B)^{-1} = \\ &= (LDU + L_B + D_B + U_B)^{-1} = (L(D + L^{-1}(L_B + D_B + U_B)U^{-1})U)^{-1} \approx \\ &= U^{-1}(I + D(D_B + U_B)U^{-1})^{-1}D^{-1}L^{-1} = (DU + D_B + U_B)^{-1}L^{-1} \end{aligned}$$





## 4. Reuse of matrix: Triangular updates

Exploiting both pattern and numerical values

$$A_0 \rightarrow A_1 = A_0 + B$$

**Case II: Triangular updates**

$$B = L_B + D_B + U_B$$

$$\begin{aligned} A_1^{-1} &= (A_0 + B)^{-1} = (A_0 + L_B + D_B + U_B)^{-1} = \\ &= (LDU + L_B + D_B + U_B)^{-1} = (L(D + L^{-1}(L_B + D_B + U_B)U^{-1})U)^{-1} \approx \\ &= U^{-1}(I + D(D_B + U_B)U^{-1})^{-1}D^{-1}L^{-1} = (DU + D_B + U_B)^{-1}L^{-1} \end{aligned}$$

- Approximation good in many practical situations
- It can be shown **theoretically** that it behaves well if  $\|L - I\|$  is small
- ... but not only in this case, as the subsequent experiments show
- $L$  or  $U$  based



## 4. Reuse of matrix: Triangular updates II.

### Triangular update versus no update

The 2D nonlinear convection-diffusion problem (Modified from Kelley, 1995); **upwind** FD; uniform grid  $50 \times 50$ ; BiCgstab ( $10^{-7}$ ), ILU(0.001)

$$\Delta u - Ru\nabla u = x(1-x)y(1-y), \quad R = 50$$

matrix / precond	CG its / no update	CG its / L-based update	CG its / U-based update
$A^1 / M^1$	4	4	4
$A^2 / M^1$	8	6	6
$A^3 / M^1$	11	8	10
$A^4 / M^1$	16	11	16
$A^5 / M^1$	23	17	24
$A^6 / M^1$	32	22	24
$A^7 / M^1$	70	37	32
$A^8 / M^1$	68	40	32
$A^9 / M^1$	67	41	32
$A^{10} / M^1$	74	42	32
$A^{1-10} / M^{1-10}$	$4 \pm 2$	$4 \pm 2$	$4 \pm 2$



## 4. Reuse of matrix: Triangular updates III.

### Triangular update versus no update

The 2D nonlinear convection-diffusion problem (Modified from Kelley, 1995); **upwind** FD; uniform grid  $50 \times 50$ ; BiCgstab ( $10^{-7}$ ), ILU(0.001)

$$\Delta u - Ru\nabla u = x(1-x)y(1-y), R = 100$$

matrix / preconditioner	CG its / no update	CG its / L-based update	CG its / U-based update
$A^1 / M^1$	4	4	4
$A^2 / M^1$	8	5	5
$A^3 / M^1$	12	7	10
$A^4 / M^1$	16	8	13
$A^5 / M^1$	19	10	13
$A^6 / M^1$	23	13	16
$A^7 / M^1$	32	16	21
$A^8 / M^1$	44	25	21
$A^9 / M^1$	50	28	23
$A^{10} / M^1$	48	27	23
$A^{1-11} / M^{1-11}$	$4 \pm 2$	$4 \pm 2$	$4 \pm 2$



## 4. Reuse of matrix: Triangular updates IV.

### Triangular update versus no update

The 2D nonlinear convection-diffusion problem (Kelley, 1995); **5-point** finite differences; uniform grid  $70 \times 70$ ; first 8 systems; ILUT(0.1,5)

$$\Delta u - Ru\nabla u = 2000x(1-x)y(1-y), \quad R = 500$$

matrix / preconditioner	CG its / no update	CG its / triangular update
$A^1 / M^1$	25	25
$A^2 / M^1$	98	30
$A^3 / M^1$	90	27
$A^4 / M^1$	135	30
$A^5 / M^1$	179	35
$A^6 / M^1$	229	36
$A^7 / M^1$	275	36
$A^8 / M^1$	345	53
$A^{1-8} / M^{1-8}$	$25 \pm 10$	$25 \pm 10$



## 4. Reuse of matrix: Triangular updates V.

### Triangular update versus no update

The 2D nonlinear convection-diffusion problem (Kelley, 1995); **5-point** finite differences; uniform grid  $70 \times 70$ ; first 8 systems; ILUT(0.1,5)

$$\Delta u - Ru\nabla u = 2000x(1-x)y(1-y), \quad R = 100$$

matrix / preconditioner	CG its / no update	CG its / triangular update
$A^1 / M^1$	25	25
$A^2 / M^1$	33	26
$A^3 / M^1$	46	26
$A^4 / M^1$	67	28
$A^5 / M^1$	80	27
$A^6 / M^1$	113	27
$A^7 / M^1$	117	27
$A^8 / M^1$	147	28
$A^{1-8} / M^{1-8}$	$25 \pm 10$	$25 \pm 10$



## 4. Reuse of matrix: Triangular updates VI.

### Triangular update versus no update

The 2D nonlinear convection-diffusion problem (Kelley, 1995); **5-point** finite differences; uniform grid  $70 \times 70$ ; first 8 systems; ILUT(0.1,5)

$$\Delta u - Ru\nabla u = 2000x(1-x)y(1-y), \quad R = 50$$

matrix / preconditioner	CG its / no update	CG its / triangular update
$A^1 / M^1$	25	25
$A^2 / M^1$	33	26
$A^3 / M^1$	47	27
$A^4 / M^1$	58	27
$A^5 / M^1$	83	27
$A^6 / M^1$	88	28
$A^7 / M^1$	119	28
$A^8 / M^1$	114	27
$A^{1-8} / M^{1-8}$	$25 \pm 10$	$25 \pm 10$



## 5. Conclusions

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- Nonsymmetric preconditioners in the form of decompositions can be **successfully updated** by algebraic techniques.
- Shown to be efficient in **solving nonlinear problems**
- Also **pattern recycling** can help
- A lot of possible combinations with matrix-free environment
- What we **did not show**
  - \* additional scaling by  $\text{diag}(L/U)$  improves the triangular update
  - \* mixing  $L$  and  $U$  based preconditioners; preprocessing for using  $L$  or  $U$
- A lot of **possibilities for improvements** under investigation
  - \* e.g., combination of **rank-1** and **rank-n** updates
  - \* e.g., sparse updates of incomplete factorizations



## 6. Advertisement

Do you know this person?







## 6. Advertisement

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Do you know this person?



Prof. Miroslav Fiedler, \* 1926



## 6. Advertisement

Do you know this person?



**Prof. Miroslav Fiedler, \* 1926**

One of pioneers in  
connecting **linear algebra**,  
**combinatorics**,  
and **Euclidean geometry**:



## 6. Advertisement

Do you know this person?



**Prof. Miroslav Fiedler, \* 1926**

One of pioneers in connecting **linear algebra**, **combinatorics**, and **Euclidean geometry**:

Results on special matrices  
Algebraic connectivity of graphs:  
Fiedler vector for graph partitioning  
Structure of Schur complements  
Structure of matrix inverses  
Aggregation in graphs/matrices



## 6. Advertisement of a special issue of LAA

Do you know this person?



Prof. Miroslav Fiedler, \* 1926

One of pioneers in connecting **linear algebra**, **combinatorics**, and **Euclidean geometry**:

Results on special matrices  
Algebraic connectivity of graphs:  
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Structure of Schur complements  
Structure of matrix inverses  
Aggregation in graphs/matrices

**Special issue of LAA** to celebrate **80th birthday of Prof. Miroslav Fiedler** announced in the latest NA-digest, will cover LAA topics + his interests (i.e., also CSC interests); **deadline** for submissions: **end of 2005**