

Numerically-aware Nested Dissection Ordering

Jonathan Hogg, Jennifer Scott and Sue Thorne

STFC Rutherford Appleton Laboratory

1 July 2016 Sparse Days at CERFACS 2016 Toulouse, France

Introduction

Solve: Ax = b

A is:

- Sparse
- Large
- Symmetric
- ▶ Indefinite may need pivoting



Sparse factorization phases

Traditionally:

- 1. Find fill-reducing ordering
- 2. Find diagonal scaling
- 3. Perform numerical factorization



Sparse factorization phases

Traditionally:

- 1. Find fill-reducing ordering
- 2. Find diagonal scaling
- 3. Perform numerical factorization

For difficult problems:

- 1. Find diagonal scaling using Hungarian algorithm (MC64)
- 2. Use matching from Hungarian algorithm to compress matrix
- 3. Find fill-reducing ordering on compressed matrix
- 4. Uncompress ordering to one on original matrix
- 5. Perform numerical factorization



Sparse factorization phases

Traditionally:

- 1. Find fill-reducing ordering
- 2. Find diagonal scaling
- 3. Perform numerical factorization

For difficult problems:

- 1. Find diagonal scaling using Hungarian algorithm (MC64)
- 2. Use matching from Hungarian algorithm to compress matrix
- 3. Find fill-reducing ordering on compressed matrix
- 4. Uncompress ordering to one on original matrix
- 5. Perform numerical factorization

Aim: replace steps 2-4 with something more intelligent.



	,	1	2	3	4	5	6
1			0.9			1.0	0.2
2		0.9	0.0			0.1	1.0
3	İ			1.0	0.2	0.4	0.9
4				0.2	1.0	0.2	0.6
5			0.1				
6		0.2	1.0	0.9	0.6	0.2	8.0

► Simple nested dissection structure



		1	2	3	4	5	6	
1		0.0	0.9			(1.0)		'
2		0.9	0.0				1.0	
3	İ			(1.0)	0.2	0.4	0.9	
4				0.2	(1.0)	0.2	0.6	
5		(1.0)	0.1	0.4	0.2	0.5	0.2	
6		0.2	(1.0)	0.9	0.2	0.2	8.0	
	`							′

- Simple nested dissection structure
- ► Hungarian scaled



		1	2	3	4	5	6		
1		0.0	0.9			1.0	0.2		
2		0.9	0.0			0.1	1.0		
3	İ			1.0	0.2	0.4	0.9		
4				0.2	1.0	0.2	0.6		
5					0.2				
6		0.2	1.0	0.9	0.6	0.2	8.0		
But what if we force compression									

But what if we force compression...

- Simple nested dissection structure
- ► Hungarian scaled



	,	1	2	3	4	5	6	
1		0.0	0.9			1.0	0.2	
2		0.9	0.0			0.1	1.0	
3				1.0	0.2	0.4	0.9	
4					1.0			
5		1.0	0.1	0.4	0.2	0.5	0.2	

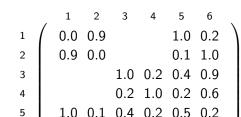
But what if we force compression...

 $0.2\ 1.0\ 0.9\ 0.6\ 0.2\ 0.8$

- Simple nested dissection structure
- Hungarian scaled

- Forced pivots
- More numerically stable/Less pivoting





But what if we force compression...

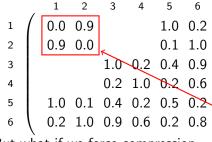
0.2 1.0 0.9 0.6 0.2 0.8

- Simple nested dissection structure
- Hungarian scaled

- Forced pivots
- More numerically stable/Less pivoting
- ► More fill!



6



But what if we force compression...

1 5 2 6 3 4

1.0 0.9

- Simple nested dissection structure
- Hungarian scaled

But wasn't that a "good enough" pivot?

- Forced pivots
- More numerically stable/Less pivoting
- ► More fill!



1

Assumptions

- ▶ Only want to work with entries of A.
- "Large" entries stay large.
- Only concerned with "small" diagonals.



Assumptions

- Only want to work with entries of A.
- "Large" entries stay large.
- Only concerned with "small" diagonals.

Define diagonal entry a_{ii} to be:

```
large if \max_{k \neq i} |a_{ik}| < u_{ord}^{-1} |a_{ii}|, small otherwise.
```



Assumptions

- ▶ Only want to work with entries of A.
- "Large" entries stay large.
- Only concerned with "small" diagonals.

Define diagonal entry a_{ii} to be:

large if
$$\max_{k \neq i} |a_{ik}| < u_{ord}^{-1} |a_{ii}|$$
, small otherwise.

Define off-diagonal entry a_{ii} to be:

large if
$$\begin{vmatrix} a_{ii} & a_{ij} \\ a_{ji} & a_{jj} \end{vmatrix} \begin{vmatrix} \max_{k \neq i,j} |a_{ik}| \\ \max_{k \neq i,j} |a_{jk}| \end{vmatrix} \le u_{ord}^{-1} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$
, small otherwise.



Assumptions

- ▶ Only want to work with entries of A.
- "Large" entries stay large.
- ▶ Only concerned with "small" diagonals.

Define diagonal entry a_{ii} to be:

large if
$$\max_{k \neq i} |a_{ik}| < u_{ord}^{-1} |a_{ii}|$$
, small otherwise.

Define off-diagonal entry a_{ii} to be:

large if
$$\begin{vmatrix} a_{ii} & a_{ij} \\ a_{ji} & a_{jj} \end{vmatrix} \begin{vmatrix} \max_{k \neq i,j} |a_{ik}| \\ \max_{k \neq i,j} |a_{jk}| \end{vmatrix} \le u_{ord}^{-1} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$
, small otherwise.

Note: can ignore large a_{ij} if both a_{ii} and a_{ji} are large.

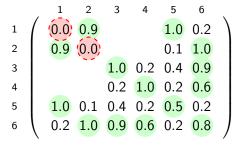


Back to our example

```
1 2 3 4 5 6
1 (0.0) 0.9 1.0 0.2
2 0.9 (0.0) 0.1 1.0
3 1.0 0.2 0.4 0.9
4 0.2 1.0 0.2 0.6
5 1.0 0.1 0.4 0.2 0.5 0.2
6 0.2 1.0 0.9 0.6 0.2 0.8
```



Back to our example



Problem reduces to:

- For every red diagonal
- Ensure it can be paired with a green off-diagonal
- Without messing up fill-reducing order



WARNING!

"Ensure there is a large entry in column" is insufficient.

$$\left(\begin{array}{ccc}
\mathbf{x} & \mathbf{x} & \mathbf{x} \\
\mathbf{x} & \mathbf{x} & \mathbf{x} \\
\mathbf{x} & \mathbf{x} & \mathbf{x}
\end{array}\right)$$

WARNING!

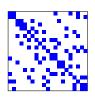
"Ensure there is a large entry in column" is insufficient.

$$\left(\begin{array}{ccc}
\mathbf{x} & \mathbf{x} & \mathbf{x} \\
\mathbf{x} & \mathbf{x} & \mathbf{x} \\
\mathbf{x} & \mathbf{x} & \mathbf{x}
\end{array}\right)$$

Big entries in row 3 can only be paired with a_{11} or a_{22} , not both!

Need a matching!



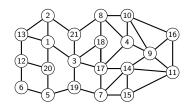


1. Original matrix



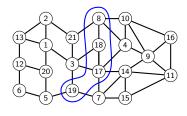
1. Original matrix (with fill)





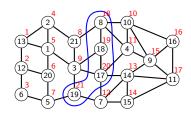
- 1. Original matrix (with fill)
- 2. Represent as graph





- 1. Original matrix (with fill)
- 2. Represent as graph
- 3. Find separator

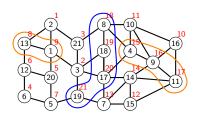




- 1. Original matrix (with fill)
- 2. Represent as graph
- 3. Find separator
- 4. Reorder to end







- 1. Original matrix (with fill)
- 2. Represent as graph
- 3. Find separator
- 4. Reorder to end
- Recurse



Compatible matchings

Matching \mathcal{M}

- ▶ Set of pairs (i,j) such that i and j occur in a most one pair.
- ▶ Pairs represent 2×2 pivots, i.e. a_{ij} must be large.
- Need not have full cardinality.



Compatible matchings

Matching \mathcal{M}

- ▶ Set of pairs (i, j) such that i and j occur in a most one pair.
- ▶ Pairs represent 2×2 pivots, i.e. a_{ij} must be large.
- Need not have full cardinality.

Partition $(\mathcal{B}, \mathcal{W}, \mathcal{S})$

- ▶ Disjoint sets such that $i \in \mathcal{B}, j \in \mathcal{W} \Rightarrow a_{ij} = 0$.
- S is the separator.



Compatible matchings

Matching \mathcal{M}

- ▶ Set of pairs (i,j) such that i and j occur in a most one pair.
- ▶ Pairs represent 2×2 pivots, i.e. a_{ij} must be large.
- Need not have full cardinality.

Partition $(\mathcal{B}, \mathcal{W}, \mathcal{S})$

- ▶ Disjoint sets such that $i \in \mathcal{B}, j \in \mathcal{W} \Rightarrow a_{ii} = 0$.
- \triangleright S is the separator.

Definition: \mathcal{M} compatible with $(\mathcal{B}, \mathcal{W}, \mathcal{S})$ if

- ▶ $(i,j) \in \mathcal{M} \Rightarrow i$ and j in same subset.
- ▶ $i \notin S \Rightarrow a_{ii}$ is large or some j such that $a_{ij} \in \mathcal{M}$.



Observations

Definition: \mathcal{M} compatible with $(\mathcal{B}, \mathcal{W}, \mathcal{S})$ if

- ▶ $(i,j) \in \mathcal{M} \Rightarrow i$ and j in same subset.
- ▶ $i \notin S \Rightarrow a_{ii}$ is large or some j such that $a_{ij} \in \mathcal{M}$.

Observations

- ▶ Don't care about small diagonals in S. Either:
 - 1. They have a partner; or
 - 2. Must be updated by a large entry before elimination.



Observations

Definition: \mathcal{M} compatible with $(\mathcal{B}, \mathcal{W}, \mathcal{S})$ if

- ▶ $(i,j) \in \mathcal{M} \Rightarrow i$ and j in same subset.
- ▶ $i \notin S \Rightarrow a_{ii}$ is large or some j such that $a_{ij} \in \mathcal{M}$.

Observations

- ▶ Don't care about small diagonals in S. Either:
 - 1. They have a partner; or
 - 2. Must be updated by a large entry before elimination.
- Otherwise, all small diagonals have a matched entry in the same partition.
- ► As we only match on large entries, we have a 2 × 2 pivot for each small diagonal.



Observations

Definition: \mathcal{M} compatible with $(\mathcal{B}, \mathcal{W}, \mathcal{S})$ if

- ▶ $(i, j) \in \mathcal{M} \Rightarrow i$ and j in same subset.
- ▶ $i \notin S \Rightarrow a_{ii}$ is large or some j such that $a_{ii} \in \mathcal{M}$.

Observations

- ▶ Don't care about small diagonals in S. Either:
 - 1. They have a partner; or
 - 2. Must be updated by a large entry before elimination.
- ▶ Otherwise, all small diagonals have a matched entry in the same partition.
- As we only match on large entries, we have a 2×2 pivot for each small diagonal.
- ⇒ Compatibility is exactly what we want



Outline Algorithm

- 2. Find a partition $(\mathcal{B}, \mathcal{W}, \mathcal{S})$.
- 4. Order S to end.
- 5. Restrict matrix to \mathcal{B} and recurse.
- 6. Restrict matrix to \mathcal{W} and recurse.



Outline Algorithm

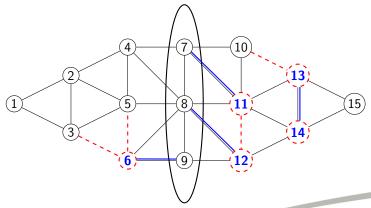
- 1. Be supplied a matching \mathcal{M} .
- 2. Find a partition $(\mathcal{B}, \mathcal{W}, \mathcal{S})$.
- 3. Adjust \mathcal{M} and $(\mathcal{B}, \mathcal{W}, \mathcal{S})$ to be compatible.
- 4. Order S to end.
- 5. Restrict matrix and matching to \mathcal{B} and recurse.
- 6. Restrict matrix and matching to \mathcal{W} and recurse.



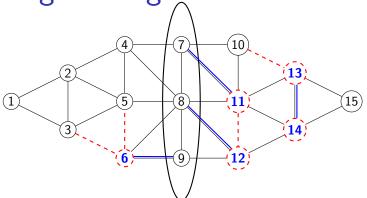
Moving to compatibility

Given incompatible \mathcal{M} and $(\mathcal{B}, \mathcal{W}, \mathcal{S})$:

- ▶ Assume \mathcal{M} is compatible on entire matrix.
- ▶ There must exist some edge $(i,j) \in \mathcal{M}$ cut by \mathcal{S} .

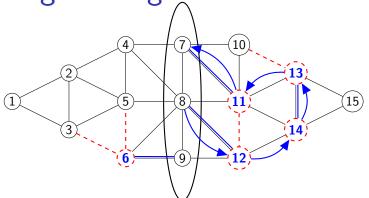






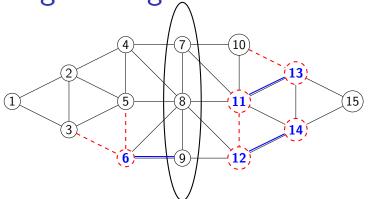
- ▶ Find alternating path starting with cut edge (i, j).
- ▶ Finish in S with an edge in M; or
- ▶ Finish outside S with edge not in M.
- ightharpoonup WITHOUT intermediate vertex in \mathcal{S} .
- ▶ Otherwise move j into S.





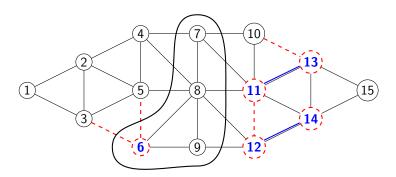
- ▶ Find alternating path starting with cut edge (i, j).
- ▶ Finish in S with an edge in M; or
- ▶ Finish outside S with edge not in M.
- ightharpoonup WITHOUT intermediate vertex in \mathcal{S} .
- ▶ Otherwise move j into S.





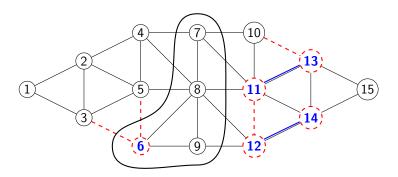
- ▶ Find alternating path starting with cut edge (i, j).
- ▶ Finish in S with an edge in M; or
- ▶ Finish outside S with edge not in M.
- ightharpoonup WITHOUT intermediate vertex in S.
- ▶ Otherwise move j into S.





- ▶ Find alternating path starting with cut edge (i, j).
- ▶ Finish in S with an edge in M; or
- ▶ Finish outside S with edge not in M.
- ▶ WITHOUT intermediate vertex in S.
- ▶ Otherwise move j into S.

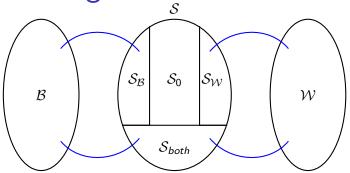




But now we don't need $9 \in S$?



Trimming



- ▶ Try pulling nodes out of S_B into B.
- ▶ If they have a small diagonal, find a partner from $S_B \cup S_0$.
- ▶ Same for S_W .
- Update sets and repeat until nothing moves.
- lacktriangle Can allow alternating paths in ${\cal B}$ and ${\cal W}$ too: complicated



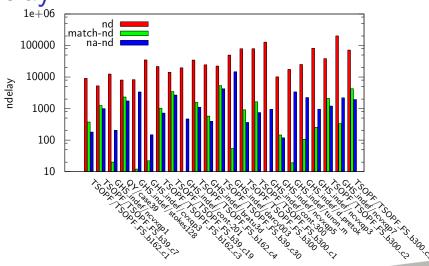
Numerical results

- 23 very difficult problems from UFL (just scaling doesn't work)
- Ordering with in-house Nested Dissection code
- Pre-scaled by symmetrized Hungarian scaling (MC64)
- Factorized with HSL_MA97
- Consider:

```
ndelay — number of delayed pivots (i.e. how far from predicted order) fflop — number of floating point operation to calculate L
```

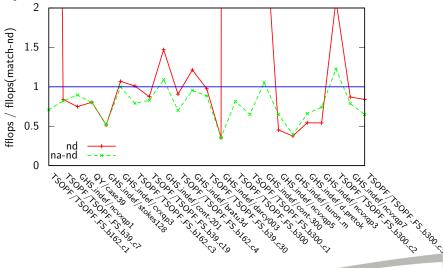


ndelay





fflops





For AMD

Modifying Approximate Minimum Degree

- Approach by Duff and Pralet in 2005
- Relaxed version of "compress then order" approach
- Rather than glue pivots together, constrain them
- Only allow small pivots to be ordered after update by big off-diagonal.

Reasonable results obtained.

Unclear if used by any solvers in practice.



Summary

- Post processing to a dissection algorithm
- But part of a nested dissection algorithm
- Could be put into any ND code with a little work
- Effective at reducing delays without significantly increasing size/work for factors
- ► More details in technical report: RAL-P-2016-004





Thanks for listening!

Questions?

http://www.numerical.rl.ac.uk/spral

Funded by ESPRC grant EP/M025179/1

Say what now

An appendix?

