### EFFICIENTLY COMPUTING WITH DESIGN STRUCTURE MATRICES

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### **1** INTRODUCTION

The design structure matrix or dependency structure matrix (DSM) provides an effective tool for the representation and analysis of complex system models. In a majority of application areas these matrices are almost invariably sparse in that a large proportion of the entries are identically zero. Algorithms for sparse matrices arising in large-scale problems must exploit the sparsity structure for computational efficiency. Combinatorial structures play an important role in the design of sparse matrix algorithms (Gilbert et. al., 2008). In this paper we borrow novel ideas from combinatorial scientific computing literature and illustrate how they can be applied in DSM computations to build new and efficient software tools for analysing the DSM. Some of the existing publicly available DSM research software use MATLAB – an integrated development environment for technical computing. McGill (2005) and Thebeau (2001) discuss MATLAB implementation of DSM partitioning and clustering where matrices are stored as dense matrices. It is to be noted that MATLAB, however, does implement sparse matrix operations using a column-oriented sparse storage of the matrix. Our objective here is to use a general-purpose high-level programming language (e.g., C++) for the implementation of computationally intensive DSM algorithms for large-scale problems, thus ensuring maximum portability and extensibility.

Many problems in numerical and combinatorial computing can be modelled by sparse matrices as well as graphs as both of these tools depict dependency relationship among the system elements (Hossain and Steihaug, 2006, 2010; Hossain, 2009). The increasing complexity of product architectures and the large-scale nature of the design processes for new products pose considerable challenges in the planning and realization of their development (Sharman and Yassine, 2004). Some of these challenges are addressed by choosing a suitable representation (or abstraction) of the problem so that novel algorithmic techniques that are successfully applied in solving similar problems in other scientific areas can be used on the problems under discussion. Braha and Bar-Yam (2004, 2007) study statistical properties of directed graphs or networks representing large-scale, complex distributed product development. The duality between sparse matrices and graphs can be exploited in the design and analysis of algorithmic tasks for the underlying computational problems - e.g. in the analysis of complex networks. In this note, the main focus is to identify and explore algorithmic techniques and data structures for efficient representation and computations as required in major DSM applications (Braha and Bar-Yam, 2004, 2007; Browning, 2001; Jebala and Eppinger, 1991; Kusiak and Wang, 1993). We propose Compressed Sparse Row (CSR) as a unifying data layout scheme for both the DSM and its underlying graph, and present precise computational complexity estimates for the DSM partitioning algorithms. Specifically, we view the DSM computation as two related but separate problems: one that is concerned with the visualization of the pattern of dependencies among the process elements and one that is concerned with the computational tasks of analyzing these relationships. This viewpoint is necessary as for large-scale problems (MacCormack et. al., 2006; Braha and Bar-Yam, 2004, 2007) even storing the DSM as a dense matrix may not be feasible.

The two main categories of DSM identified in Browning (2001) are the static DSM where the interacting system elements represent organizational entities or product components and the taskbased DSM where the system elements are constrained by precedence relationship. In either case the main computational task can be viewed as a rearrangement of rows and columns of the matrix that optimizes certain objective function. Let  $A \in \Re^{n \times n}$  be a *DSM* where the entry in row *i* and column *j*, written a(i,j) or  $a_{ij}$ , denotes the strength of the interaction between the system elements *i* and *j* with a(i,j) = 0 implying no interaction. Without loss of generality, we assume only nonnegative interactions. Let  $e_i = (0 \ 0 \ \dots \ 0 \ 1 \ 0 \ \dots \ 0)^T$  be a vector in  $\{0,1\}^n$  where the *i*th entry of the vector,  $e_i(i)$ , is *1* and all other entries are 0. Then  $P \in \{0, 1\}^{n \times n}$  is called a permutation matrix if its *j*th column  $P(:,j) = e_k$  for some  $k \in \{1, 2, \dots, n\}$  and  $P(:,j) \neq P(:1)$ ,  $j \neq l$ .

#### 2 SPARSE DATA STRUCTURES AND GRAPHS

The CSR scheme is one of the common data structures for representing matrices whose sparsity patterns have no known regular structure. This storage scheme can be implemented using three arrays: value to store the nonzero entries row-by-row, colind that stores the column indices of the nonzero entries in value, and rowptr that contains the (array) index of the first nonzero element of each row of the sparse matrix in colind and value arrays. In the *CSR* storage scheme the sparse matrix is compressed by moving the nonzero entries in each row to the left as shown in Figure 1.

1	$(a_{11})$	0	$a_{13}$	$a_{14}$	0	0)	(a <sub>11</sub>	$a_{13}$	$a_{14}$	0	0	0)
	0	$a_{22}$	0	0	0	$a_{26}$	$a_{22}$	$a_{26}$	0	0	0	0
	$a_{31}$	0	$a_{33}$	0	$a_{35}$	0	$a_{31}$	$a_{33}$	$a_{35}$	0	0	0
	0	$a_{42}$	0	$a_{44}$	0	0	$a_{42}$	$a_{44}$	0	0	0	0
	$a_{51}$	0	$a_{53}$	0	$a_{55}$	0	$a_{51}$	$a_{53}$	$a_{55}$	0	0	0
	0	$a_{62}$	0	$a_{64}$	0	$a_{66}$	$a_{62}$	$a_{64}$	$a_{66}$	0	0	0)

Figure 1: A sparse matrix (left) and its row-compressed form (right).

The data structures to store the example matrix under the CSR scheme are shown in Figure 2.



 $Figure \ 2: \ CSR \ data \ structure.$ 

Array value stores the nonzero entries in each row contiguously; array colind stores the column indices of the nonzero entries of value; array rowptr indexes into colind array and stores the index location of the first nonzero entry in each row of the matrix. The nonzero entries in row *i* can then be accessed as value(rowptr(i))  $\cdots$  value(rowptr(i+1)-1). Note that the *CSR* scheme stores only the nonzero entries of the matrix. Let nnz(A) denote the number of nonzero entries in matrix *A*. The storage requirement in the *CSR* scheme for  $A \in \Re^{n \times n}$  is therefore  $2 \times nnz(A) + n + 1$  units of computer memory with row-wise access to the nonzero entries of the matrix. A companion data structure, the *Compressed Sparse Column* (*CSC*), can be defined to provide column-wise access

to the matrix nonzero entries using arrays rowind that stores the row indices of the nonzero entries in value and colptr that indexes into rowind and stores the index location of the first nonzero entry in each column of the matrix. The access to the nonzero entries in column j is provided as value (colptr(j))  $\cdots$  value (colptr(j+1)-1). With both column- and row-wise accesses the storage requirement for a sparse matrix using the compressed row/column scheme is therefore  $3 \times nnz(A) + 2 \times n + 2$  units of computer memory, which is consistent with the design principle for sparse linear algebra (Gilbert et. al., 2008). Associated with matrix A is a directed graph G = (V, E) where V is the set of n vertices and there is a directed edge from vertex  $v_i$  to vertex  $v_j$ , denoted  $(v_i, v_j) \in E$  whenever  $a_{ij} \neq 0$ ,  $i \neq j$ . Then nnz(A) = |E|. The first DSM computational problem, known in the literature as partitioning, is to sequence the tasks in a task-based DSM so as to minimize the feedback marks. As a sparse matrix problem the partitioning problem can be stated as,

find a permutation matrix P such that  $P^{T}AP$  is block lower triangular.

$$P^{T}AP = \begin{pmatrix} A_{11} & 0 & 0 & 0 & 0 & 0 \\ A_{21} & A_{22} & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \ddots & 0 & 0 & 0 \\ A_{i1} & \dots & \dots & A_{ii} & 0 & 0 \\ \vdots & \vdots & \vdots & \dots & \ddots & 0 \\ A_{k1} & A_{k2} & \dots & \dots & A_{kk} \end{pmatrix}$$

Figure 3. A sparse matrix in block lower triangular form (bltf).

Figure 3 shows a sparse matrix symmetrically permuted to block lower triangular form in which the diagonal blocks are square submatrices. Without loss of generality we assume that the diagonal entries of the *DSM* are nonzero (see e.g. MacCormack, 2006). Clearly, if the diagonal blocks are scalar quantities ( $1 \times 1$  matrix), then *A* can be permuted into a lower triangular form i.e.,  $P^{T}AP$  is lower triangular and there are no feedback marks - the ideal arrangement of the tasks in a project. It is therefore of interest to know whether the *bltf* of a *DSM* is unique and if the diagonal blocks themselves can be permuted to a *bltf*. Answers to the above questions as well as other *DSM*-related questions are most conveniently provided using graph theory.

A directed path from vertex  $v_i$  to vertex  $v_j$ , written,  $v_i \mapsto v_j$  is a sequence of vertices ( $v_i \equiv v_{i_1}, v_{i_2}, \dots, v_{i_l} \equiv v_j$ ) such that  $(v_{i_k}, v_{i_{k+l}}) \in E$ ,  $k \equiv 1 \dots l - 1$  and that the vertices in the path are all distinct. A directed path  $v_i \mapsto v_j$  is called a *directed cycle* whenever  $v_i = v_j$ . A graph H = (V', E') is a subgraph of graph G = (V, E) if  $V' \subseteq V$ ,  $E' \subseteq E$  and  $(u, v) \in E'$  implies  $u, v \in V'$ . A subgraph H is said to be *strongly connected* if for each pair of vertices  $u, v \in V', u \mapsto v, v \mapsto u$ . A subgraph H is said to be a *strongly connected component (scc)* if H is strongly connected and no other strongly connected subgraph of graph G properly contains H. Since each vertex can belong to exactly one strongly connected component, strongly connected components of a graph partitions the vertices of the graph and the partition is unique. With the concept of matrix reducibile if there is a permutation P for which the *bltf*, as in Figure 3, has at least two diagonal blocks. A matrix is *irreducible* if it is not reducible. The following result (see Brualdi and Herbert, 1991) characterizes the *DSM* partitioning as a graph problem.

**Theorem 1.** Matrix  $A \in \mathcal{R}^{n \times n}$  with nonzero diagonal entries is irreducible if and only if G(A) is strongly connected.

From Theorem 1 we can deduce that each diagonal block  $A_{ii}$  represents a strongly connected component of G(A) and therefore cannot itself be permuted into a block triangular form. Several algorithms exist for finding the *bltf* for sparse matrices with varying asymptotic computational

complexity. One method, due originally to Harary (see Duff and Reid, 1978), involves computing the power of the 0-1 matrix (a matrix where the nonzero entries are replaced with a 1) associated with matrix A requiring  $O(n^3)$  computational effort (Gebala and Eppinger, 1991). A  $O(n^2)$  algorithm, due to Sargent and Westerberg (1964), finds sccs utilizing the fact that the vertices in a cycle must belong to the same strongly connected component. The first asymptotically optimal algorithm requiring only O(|V| + |E|) computational effort for partitioning a directed graph into its strongly connected components is due to Tarjan (1972). Duff and Reid (Duff and Reid, 1978) discuss an implementation of Tarjan's algorithm. Central to this elegant algorithm is to use a vertex stack to identify and incrementally build strongly connected components during a depth-first search (dfs) of the graph. As each vertex is visited (via an edge) for the first time by the *dfs* algorithm it is pushed onto the stack. Using an auxiliary array of size n = |V| the so called *root* of each strongly connected component is computed. Whenever a root vertex is discovered during the return from a recursive call to the dfs, all the vertices in the same connected component (including the root vertex) are found in the stack. These vertices, together with the root vertex, are popped from the stack and are assigned a component number. In our example matrix, the vertices labelled 1 and 4 are the root vertices corresponding to the two strongly connected components as depicted in Figure 4. The order in which the depth-first traversal visits the vertices defines the permutation matrix which can be efficiently represented by a permutation vector. For our example matrix A the graph G(A) consists of two strongly connected components: the first consisting of vertices  $\{v_6, v_2, v_4\}$  with  $v_4$  as the root and the second consisting of vertices { $v_5$ ,  $v_3$ ,  $v_1$ } with  $v_1$  as the root. The corresponding permutation matrix P defined by  $P(:, 1) = e_6$ ,  $P(:,2) = e_2, P(:,3) = e_4, P(:,4) = e_5, P(:5) = e_3, P(:,6) = e_1$  can be represented by the vector (6 2 4 5 3 1).



Figure 4. The directed graph associated with the matrix of Figure 1

$(a_{11})$	0	$a_{13}$	$a_{14}$	0	0)	$(a_{66})$	$a_{62}$	$a_{64}$	0	0	0)
0	$a_{22}$	0	0	0	$a_{26}$	$a_{26}$	$a_{22}$	0	0	0	0
$a_{31}$	0	$a_{33}$	0	$a_{35}$	0	0	$a_{42}$	$a_{44}$	0	0	0
0	$a_{42}$	0	$a_{44}$	0	0	0	0	0	$a_{55}$	$a_{53}$	$a_{51}$
$a_{51}$	0	$a_{53}$	0	$a_{55}$	0	0	0	0	$a_{35}$	$a_{33}$	$a_{31}$
0	$a_{62}$	0	$a_{64}$	0	$a_{66}$	0	0	$a_{14}$	0	$a_{13}$	$a_{11}$

Figure 5: Block triangular form (on the right) of the example matrix (on the left).

In Figure 5 the original matrix on the left is symmetrically permuted into a block lower triangular form. The top-left diagonal block represents the first strongly connected component and the bottom-right diagonal block represents the second strongly connected component. It is also easy to see that the algorithm sketched above can be used to perform related computation – e.g., *tearing* (Kusiak and Wang, 1993; Gebala and Eppinger, 1991) – without a second pass over the graph vertices. With respect to the implementation of Tarjan's algorithm for DSM partitioning we first note that since G(A) is a directed graph, for each vertex  $v_i$  we need access to edges of the form  $(v_i, v_j)$ ,  $a_{ij} \neq 0$  (also known as outgoing edges) only; therefore, the CSR representation of the sparse matrix suffices. Secondly, the main computational step in the algorithm is to access the outgoing edges at each vertex. This is efficiently done by j = colind(k),  $k = \text{rowptr}(i) \cdots \text{rowptr}(i+1) - 1$  to access the vertices adjacent to vertex  $v_i$  via the outgoing edges. Therefore, the CSR storage scheme provides an efficient implementation of Tarjan's algorithm.

#### **3 CONCLUDING REMARKS**

In this paper we have proposed a sparse data structure for efficiently computing with *DSM* matrices and have provided a precise characterization of the computational complexity of the *DSM* partitioning. Although our discussion is centred around partitioning, our proposal extends to other computations such as tearing and clustering (MacCormack et al., 2006). We have also sketched Tarjan's asymptotically optimal partitioning algorithm. For sparse rectangular matrices, a more general partitioning procedure based on bipartite graph matching that utilizes strong Hall property can be found in Pothen and Fan (1990). The research presented in this paper is a preliminary report on the design of a software toolkit for *DSM* partitioning and tearing.

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### Outline

- Motivation and Background
- Efficient Computer Representation for Large-scale DSM
- Problem Formulation
- Strongly-connected Components in Linear Time
- Concluding Remarks





# The DSM

The DSM depicts pair-wise dependency between system elements

- Only a small fraction of the possible dependencies are actually present
- The dimension of the matrix is large  $(10^2 \sim 10^6 \text{ or more})$
- Important DSM computations have combinatorial components
  - Partitioning: Rearrange the columns and rows to reduce the feedback marks.
  - Tearing: Remove a subset of marks that optimizes certain objective function



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## Large-scale Problems (1)

A. MacCormack, J. Rusnak and C. Y. Baldwin, Exploring the Structure of Complex Software Designs: An Empirical Study of Open Source and Proprietary Code, *Management Science*, 52(7):1015-1030, 2006.

	Mozilla	Linux
Number of source files	1684	1778
Function/source file	17.7	12.8
Memory to store full matrix (4 bytes/element)	13.5 GB	7 GB





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### Large-scale Problems (2)

The Statistical Mechanics of Complex Product Development: Empirical and Analytical Results. *Management Science*. Vol. 53 (7). pp. 1127-1145. July 2007.

Problem	Dimension	Number of nonzeros	Density (%)
Vehicle	120	417	2.89
Operating Software	466	1245	3 X 10 <sup>-2</sup>
Pharma. Facility	582	4123	3.4 X 10 <sup>-3</sup>
Hospital Facility	889	8178	1.3 X 10 <sup>-3</sup>



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### Sparse Matrix Representation and Computation

- Computer representation of a sparse matrix should be proportional to max(n, nnz) computer words
  - Coordinate storage: three arrays I (row index), J (column index), v (value) of size  $\mathtt{nnz},$  each;
  - Compressed row (column) storage: three arrays rowptr of size n+1, colind of size nnz, and value of size nnz
  - Compressed diagonal storage
  - ...
- Running time of a basic sparse matrix operation (e.g., sparse matrix multiplied by a dense vector) should be proportional to the size of the data accessed and the number of nonzero floating point operations.





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### Compressed Sparse Row (CRS) Representation

$\begin{pmatrix} a_{11} \\ 0 \\ a_{31} \\ 0 \end{pmatrix}$	$a_{22}$	$a_{13} \\ 0 \\ a_{33} \\ 0$	$a_{14} \\ 0 \\ 0 \\ a_{14}$	0 0 a <sub>35</sub>	$0 \\ a_{26} \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ $		$a_{22} \\ a_{31}$	$a_{26} \\ a_{33}$	a <sub>14</sub> 0 a <sub>35</sub>	0 0	0 0	0 0			• nnz = 2	
$\begin{bmatrix} 0 \\ a_{51} \\ 0 \end{bmatrix}$	$a_{42}$ 1 0 $a_{62}$	$a_{53}$	$a_{44} \\ 0 \\ a_{64}$	0 a <sub>55</sub> 0	0 0 a <sub>66</sub>			$a_{53}$	$a_{55}$ $a_{66}$	0	0	0			•	Column indices of the nonzeros in
Figure 1	1: A s	parse	e mat	trix (	left) a	and its	row-	comp	resse	d fo	rm	(righ	t).		col	<pre>row i: ind(l)coli</pre>
	1: A s	parse	e mat	rix (	left) a	und its	row-	comp	resse	ed fo	rm	(righ	t).			<pre>row i: ind(l)coli d(h)</pre>
Figure 1					left) (			<i>comp</i>		ed fo a <sub>62</sub>	rm a61		t).			<pre>row i: ind(l)coli</pre>
Figure 1										_			t).		1 =	<pre>row i: ind(l)coli d(h)</pre>

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rowptr

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Figure 2: CSR data structure.

## A DSM and its Graph

(a <sub>11</sub>	0	$a_{13}$	$a_{14}$	0	0)
0	$a_{22}$	0	0	0	$a_{26}$
$a_{31}$	0	$a_{33}$	0	$a_{35}$	0
0	$a_{42}$	0	$a_{44}$	0	0
$a_{51}$	0	$a_{53}$	0	$a_{55}$	0
0	$a_{62}$	0	$a_{64}$	0	$a_{66}$



- For a sparse matrix A define a directed graph G(A) = (V, E) where
  - There are n vertices:
  - $V = \{v_{1}, v_{2}, ..., v_{n}\}$
  - for  $a_{ij} \neq 0$ ,  $i \neq j$  there is a directed edge from  $v_i$  to  $v_{j,}$ denoted  $(v_i, v_j)$  in *E*
- |V| = n, |E| = nnz



# **DSM** Partitioning

Matrix Partitioning Problem

Given a task-based *DSM* A find a permutation matrix P such that the number of feed-back marks in  $P^{T}AP$  is minimized (over all such permutation of the rows and columns of A).

Observations:

- A permutation matrix is a (column/row) permuted identity matrix.
- If  $P^TAP$  is lower triangular then the permutation P results in optimum arrangement of the tasks.
  - Not all DSM can be permuted to lower triangular form.

# "Find a Permutation Matrix P Such that $P^{T}AP$ is Block Lower Triangular"



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 $P^{T}AP = \begin{pmatrix} A_{11} & 0 & 0 & 0 & 0 & 0 & 0 \\ A_{21} & A_{22} & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \ddots & 0 & 0 & 0 \\ A_{i1} & \dots & \dots & A_{ii} & 0 & 0 \\ \vdots & \vdots & \vdots & \dots & \ddots & 0 \end{pmatrix}$ 

Figure 3. A sparse matrix in block lower triangular form (bltf).



- The diagonal blocks are square
- k = n implies  $P^T A P$  is lower triangular
- k = 1 implies P<sup>T</sup>AP yields no improvement w.r.t. feedback marks
- Matrix *A* is *reducible* if ∃P such that *P<sup>T</sup>AP* has at least two blocks i.e., (k ≥2)
- K = 1 implies irreducible
- Can the diagonal blocks themselves be permuted into *bltf*
- Is *bltf* decomposition unique?





### The Graph Problem

- A *directed path* from vertex  $v_i$  to vertex  $v_j$ , written,  $v_i \mapsto v_j$  is a sequence of vertices  $(v_i \equiv v_{i1}, v_{i2}, \dots, v_{il} \equiv v_j)$  such that  $(v_{ik}, v_{ik+1}) \in E$ ,  $k = 1 \dots l 1$  and that the vertices in the path are all distinct.
- A path is a *cycle* if the start and the end vertices are the same.
- A graph H = (V', E') is a *subgraph* of graph G = (V, E) if  $V' \subseteq V, E' \subseteq E$  and  $(u, v) \in E'$  implies  $u, v \in V'$ .
- A subgraph *H* is said to be *strongly connected* if for each pair of vertices *u*,  $v \in V'$ ,  $u \mapsto v$ ,  $v \mapsto u$ .
- A subgraph *H* is said to be a *strongly connected component (scc)* if *H* is strongly connected and no other strongly connected subgraph of graph *G* properly contains *H*.

Theorem (Brualdi and Herbert, 1991).

Matrix  $A \in \Re^{n \times n}$  with nonzero diagonal entries is irreducible if and only if G(A) is strongly connected.



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### Algorithms and Complexity

- Diagonal blocks cannot themselves be permuted into bltf.
- Strongly connected component *i* corresponds to the diagonal block *A*<sub>*ii*;</sub> Matrix-based Algorithms:
  - O(n<sup>3</sup>) algorithm due to Harary (Harary F., J. Math. Phys. 38, 1959) consists of repeatedly multiplying the binary matrix A with itself.

Graph-based Algorithms:

- O(n<sup>2</sup>) algorithm due to Sargent and Westerberg (Sargent R.W.H. and Westerberg A.W., Trans. Ins. Chem. Engrs. 42, 1964)
- **Optimal Algorithms:** 
  - The first O(n+nnz) algorithm due to Tarjan (R. E. Tarjan, SIAM J. Comput. 1(2), 1972) relies on depth-first search (*dfs*) technique to find strongly connected component.
  - The Kosaraju-Sharir (M. Sharir, Computer and Mathematics with Appl., 7(1), 1981) algorithm performs two *dfs* of the graph; the second *dfs* is performed on the modified graph.
  - The Cheriyan, Melhorn, Gabow algorithm (J. Cheriyan and K. Melhorn, Algorithmica 15, 1996; H.N. Gabow, Inf. Proc. Let. 74(3-4), 2000) maintains all the sccs during dfs





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### Tarjan's Algorithm for finding Strongly Connected Components



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### Notes on Implementation

- For each vertex *v* only the outgoing edges (*v*,*w*) are needed to access *v*'s neighboring vertices *w* 
  - colind(rowptr(v)) .. colind(rowptr(v+1) 1)
- · Each edge (nonzero) is accessed only once
- Depth of recursion can at most be n
- The root finding stack st may never contain more than n elements.
- The number of auxiliary arrays can be reduced and can be lumped together into one large array for better *data locality*



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### Summary and Future Research

#### Summary

- DSM partitioning is equivalent to finding strongly connected components of an associated graph
  - Tarjan's SCC algorithm is asymptotically optimal!
- The CRS scheme provides an efficient implementation for DSM partitioning
  - A graph data structure is not constructed explicitly! same representation suffice for the sparse DSM and its graph.
    - The associated graph being a directed graph allows us to use only row-oriented data access.

#### Future Research

- Numerical testing for large-scale DSM
- Precise computational complexity of other DSM computations
- New heuristics for computationally intractable DSM computation that exploit "special local structures"
- Software tool development



