The University of Florida Sparse Matrix Collection

Timothy A. Davis¹ and Yifan Hu^2

The University of Florida Sparse Matrix Collection is a large, widely available, and actively growing set of sparse matrices that arise in real applications. Its matrices cover a wide spectrum of domains, include those arising from problems with underlying 2D or 3D geometry (such as structural engineering, computational fluid dynamics, model reduction, electromagnetics, semiconductor devices, thermodynamics, materials, acoustics, computer graphics/vision, robotics/kinematics, and other discretizations) and those that typically do not have such geometry (such as optimization, circuit simulation, economic and financial modeling, theoretical and quantum chemistry, chemical process simulation, mathematics and statistics, power networks, and other networks and graphs). The collection is widely used by the sparse matrix algorithms community for the development and performance evaluation of sparse matrix algorithms. The collection includes software for accessing and managing the collection, from MATLAB, Fortran, and C, as well as online search capability. Graph visualization of the matrices is provided, and a new multilevel coarsening scheme is proposed to facilitate this task.

Categories and Subject Descriptors: G.1.3 [Numerical Analysis]: Numerical Linear Algebra—linear systems (direct methods), sparse and very large systems; G.4 [Mathematics of Computing]: Mathematical Software—algorithm analysis, efficiency; G.2 [Discrete Mathematics]: Graph Theory

General Terms: Algorithms, Experimentation, Performance

Additional Key Words and Phrases: sparse matrices, performance evaluation, graph drawing, multilevel algorithms

1. INTRODUCTION

Although James Wilkinson's foundational work in numerical analysis touched only lightly upon sparse matrix computations, his definition of a sparse matrix is widely used ([Gilbert et al. 1992], for example). Wilkinson defined a matrix as "sparse" if it has enough zeros that it pays to take advantage of them. He actually stated his definition in the negation:

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The matrix may be sparse, either with the non-zero elements concentrated on a narrow band centered on the diagonal or alternatively they may be distributed in a less systematic manner. We shall refer to a matrix as dense if the percentage of zero elements or its distribution is such as to make it uneconomic to take advantage of their presence. [Wilkinson 1971]

In other words, if you can save time or memory (usually both) by exploiting the zeros, then the matrix is sparse. An interesting aspect of this definition is that it is dependent not only on the matrix, but on the algorithm used on the matrix. For example, a matrix may be "sparse" for an iterative method for solving linear systems or for a graph theoretic algorithm, but not for a sparse factorization method

This article describes the University of Florida Sparse Matrix Collection (hereafter referred to as the UF Collection), which contains sparse matrices arising in a wide range of applications. Section 2 gives the motivation for collecting sparse matrices from real applications and making them widely available. Section 3 describes the current state of the collection and the breadth of problems the matrices represent. Section 4 describes the algorithm used, and new techniques developed, for visualizing the matrices. Section 5 describes the three data formats used for storing the matrices, and the kinds of auxiliary information available for each matrix. Section 6 describes the four methods for searching and downloading matrices of interest: a MATLAB interface (UFget), a Java interface (UFgui), the matrix web pages (via a standard browser and a web-based search tool), and Amazon Web ServicesTM. Examples of how the UF Collection can be used for performance evaluation are given in Section 7. The future of the UF Collection depends critically upon the submission of new matrices, as discussed in Section 8. Finally, Section 9 summarizes the contributions of the UF Collection and its associated software.

In this paper, a graph or mesh is said to have 2D or 3D geometry if its vertices have a position on an xy or xyz plane that naturally arises from the problem being solved. A sparse matrix is said to have 2D or 3D geometry if its nonzero pattern is the adjacency matrix of such a graph. The notation |A| refers to the number of nonzeros in a matrix.

2. MOTIVATION

The role of sparse matrices from real applications in the development, testing, and performance evaluation of sparse matrix algorithms has long been recognized. The first established collection was started by Duff and Reid (1970 to 1979, [Duff and Reid 1979]), and then compiled into the Harwell-Boeing collection by Duff, Grimes, and Lewis [Duff et al. 1989]. This collection provided the starting point of University of Florida Sparse Matrix Collection. Since the start of our collection in 1992, additional matrices have been added over the years, and other collections have been made, many of which have also been incorporated into the UF Collection (such as [Bai et al. 1996; 2008; Batagelj and Mrvar 2008; Boisvert et al. 2008; Boisvert et al. 1997; Dumas 2008; Gay 2008; Gould et al. 2008; Koster 2008; Mészáros 2008; Mittelmann 2008; Resende et al. 1995; Rudnyi 2008; Rudnyi et al. 2006; Saad 2008; Schenk 2008]).

The Matrix Market [Boisvert et al. 1997] is the most similar collection to the UF Collection. Both collections include a search tool, and both categorize the matrices by application domain and problem source. Both provide matrices in similar file formats. Both provide a web page for each matrix, with basic statistics and figures. They differ in size, with the UF Collection containing much larger matrices and 4.5 times as many matrices. The latest matrix added to the Matrix Market was in 2000, whereas UF collection is constantly being updated with new matrices. The largest matrix in the Matrix Market has dimension 90,449 with 2.5 million nonzeros, whereas the largest matrix in the UF Collection has a dimension of 28 million with 760 million nonzeros. Nearly every matrix in the Matrix Market is also included in the UF Collection. However, the Matrix Market does include matrix generators; the UF Collection has no matrix generators.

Nearly all research articles that include a section on the performance analysis of a sparse matrix algorithm include results on matrices from real applications or parametrized matrices that mimic those that could arise in practice. Since maintaining a large collection of matrices from real applications is not trivial, an alternative is first considered, namely, parametrized and random matrix generators.

2.1 Parameterized and random matrices

Randomized or repeatable parametrized sequences of matrices can be easily constructed via simple matrix generators. Examples are listed below, as a comparison and contrast with the UF Collection, which does not include any matrix generators.

- (1) Simple discretizations of the Laplace operator on square 2D and 3D meshes.
- (2) The L-shaped meshes of [George and Liu 1981].
- (3) Least-squares problems from square 2D finite-element meshes [George et al. 1983].
- (4) The LAPACK test matrix generators [Anderson et al. 1999], which can generate banded matrices and sparse matrices with random nonzero pattern. These also appear in the Matrix Market.
- (5) The Non-Hermitian Eigenvalue Problem (NEP) matrix generators [Bai et al. 1996; 2008]. These include regular 2D meshes and random patterns; additional matrices are made available only as operators (y = Ax, where A is not explicitly represented).
- (6) Zlatev's matrix generators, which create a sparse Toeplitz structure (where selected diagonals are all nonzero) [Zlatev 1991].
- (7) Higham's Matrix Computational Toolbox [Higham 2002], part of which appears as the gallery function in MATLAB. The gallery contains three functions that generate parametrized sparse matrices from regular 2D meshes (neumann, poisson, and wathen) and two that generate banded matrices (toeppen and tridiag). No randomization is used, except in the values (but not pattern) of the wathen matrices. Many of these matrix generators also appear in the Matrix Market.
- (8) Matrices with purely random nonzero patterns [Erdös and Rényi 1959; Gilbert 1959]. They can be generated by sprand, sprand, and sprandsym in MATLAB [Gilbert et al. 1992].

- (9) The YM11 subroutine in HSL can generate random sparse matrices, with options for ensuring structural nonsingularity and bandedness (a matrix is structurally nonsingular if there exists a permutation so that the matrix has a zero-free diagonal) [Duff 2001].
- (10) In between the purely-random and purely-parametrized classes of matrices are partially randomized matrices with specific structure, as exemplified by the CONTEST toolbox [Taylor and Higham 2009]. They provide a set of graph generators, some of which use an underlying 2D or 3D geometry and some that do not. For example, they include an implementation of the small-world graphs of [Kleinberg 2000], which are 2D meshes with additional randomized edges to distant vertices in the plane. Network generators in CONTEST that do not have geometry include the scale-free graph models of [Barabási and Albert 1999].

The prime advantage of random and parametrized matrices is that they are very easy to generate in any size desired. Matrices from real applications are very difficult to generate and it is hard to vary them in size.

Another key advantage of random and parametrized matrices is that asymptotic results can sometimes be derived. For example, the nested dissection ordering applied to a 2D s-by-s mesh leads to an asymptotically optimal ordering for sparse Cholesky factorization, with $31(n\log_2 n)/8 + O(n)$ nonzeros in the Cholesky factor L, and requiring $829(n^{3/2})/84 + O(n\log n)$ floating point operations to compute, where $n=s^2$ is the dimension of the matrix [George and Liu 1981].

Purely random matrices may be useful for testing some sparse matrix applications. For example, they can be useful for testing the convergence of iterative methods, assuming the generator has some control over the eigenvalue spectra (as is the case for sprandsym, for example). However, under Wilkinson's definition they are not truly sparse when factorized by direct methods. With modest assumptions, purely random n-by-n matrices with O(n) nonzero entries require $O(n^3)$ time and $O(n^2)$ memory to factorize, because of catastrophic fill-in [Duff 1974]. Catastrophic fill-in very rarely occurs in matrices arising in real applications, and even when it does it is an indication that direct factorization methods are not applicable to that problem. Thus, performance obtained on purely random matrices will not indicate how well a sparse matrix factorization method will work on matrices from real applications. Purely random networks also do not accurately model the characteristics of real networks [Watts and Strogatz 1998].

In between the two extremes of highly structured matrices (banded, or square 2D and 3D meshes, for example) and purely randomized matrices is another class of matrix generators that can create matrices with some regular structure and a carefully selected random structure. The small-world graphs from the CONTEST toolbox are one such example. These are constructed to capture essential properties of large networks, such as the small-world property, scale-free degree distribution, motifs, and graphlet frequency [Taylor and Higham 2009]. These models are very useful for network algorithms, but they have not yet been shown to mimic the performance of sparse matrix factorization methods on matrices from real applications.

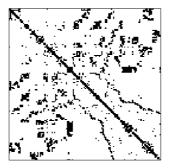


Fig. 1. Sparse matrix pattern of a RAH-66 Comanche helicopter

2.2 Sparse matrices from real applications

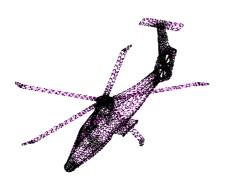
While useful, random and parametrized matrices have their limitations. This motivates the development of the UF Collection, which focuses on matrices from real applications¹.

One of the matrices in the UF Collection is a complete representation of a Boeing/Sikorsky RAH-66 Comanche helicopter, with 3D geometry (obtained from Alex Pothen). Figure 1 shows the sparsity pattern of the matrix. Nested dissection is still useful for this problem, but asymptotic results cannot be derived for a complex structure such as this one. A simple square 3D mesh would not be a good approximation to this graph, since it would not capture the properties of the long helicopter rotors, or the topology of the hole where the rear rotor is located. This matrix is one of the few in the collection where the 3D coordinates of the vertices are given; a picture of the graph drawing when these coordinates are used is shown in Figure 2, on the left. For comparison, a force-directed graph drawing [Hu 2005], which recreates these coordinates based only on the connectivity of the graph, is shown on the right. The method for creating this figure is discussed in Section 4. The structure is warped, with the tail rotor twisted out of its housing (to the right) and its five main rotors shrunken (on the top), but it is still clear that the graph represents some kind of 3D problem. Edge colors in the force-directed graphs represent the distance between two vertices.

Figure 3 is the nonzero pattern of matrix arising from circuit simulation (left) and its force-directed graph drawing (right). The graphs of the Comanche helicopter and this electronic circuit indicate that one is a 3D problem and the other is a network with no 2D or 3D geometry. This difference is not clear by merely comparing the nonzero patterns of their matrices.

Parameterized matrices can capture many key properties of matrices from real applications, such as the regularity of a 3D mesh, or the small-world properties of a network, but they cannot capture the rich and complex structure of matrices such

 $^{^{1}\}mathrm{The}$ UF Collection does include a handful of random matrices, which remain in the collection for historical reasons.



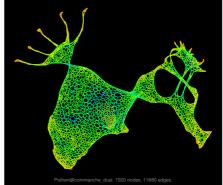
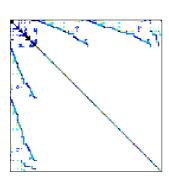


Fig. 2. Graph of a RAH-66 Comanche helicopter, using given 3D coordinates (left) and its force-directed graph drawing (right)



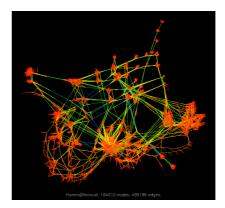


Fig. 3. Sparse matrix pattern of an electronic circuit from Steve Hamm, Motorola (left) and its force-directed graph (right)

as those presented above.

2.3 Collecting the matrices

The ideal matrix collection would be informally representative of matrices that arise in practice. It should cast a broad net so as to capture matrices from every application domain that relies on sparse matrix methods. For example, matrices arising in circuit simulation (and other network-related domains) differ greatly from matrices arising from the discretization of 2D and 3D physical domains; this can be clearly seen in the preceding figures. Computational fluid dynamics matrices differ from structural engineering matrices, and both are vastly different from matrices arising in linear programming or financial portfolio optimization. The collection should be kept up to date, since matrices of interest grow in size each year as computer memories get larger. New application domains also appear, such as eigenvalue problems arising in web connectivity matrices [Kamvar 2008; Kamvar et al. 2004; Page et al. 1998], which have existed only since the mid 1990's.

Sparse matrix algorithm developers use the matrices in the UF Collection to develop their methods, since theoretical asymptotic time/memory complexity analysis only goes so far. If there are no matrices available to developers from a given application domain, it is quite possible that when their methods are used in that domain, the performance results will be disappointing. This provides a strong motivation for computational scientists to submit their matrices to a widely available collection such as this one, so that gaps can be avoided. Thus, new application areas are always being added to the collection.

Our strategy for adding matrices to the collection is simple, although admittedly ad hoc. The first author maintains a collection of codes for the direct solution of sparse linear systems. End-users of this software are uniformly requested to submit matrices to the collection. Additional matrices are requested when they are found cited in articles and conference presentations, which includes a wider range of matrices (such as graphs arising in network analysis). Any matrices received are included, unless they are clear duplications of matrices already in the collection. Small matrices are not included, unless they are subsets of a larger collection (such as the Pajek data set).

This strategy does introduce an unavoidable source of bias, but we have attempted to avoid this bias by relying on matrices collected by others. The UF Collection includes many sets of matrices collected in this way, such as those collected by Saad, who develops iterative methods for sparse linear systems [Saad 2003]. Not all matrices in the collection arise from a sparse linear system. For example, many linear programming problems have been included in the UF Collection [Gay 2008; Mészáros 2008; Mittelmann 2008; Resende et al. 1995]. Network and combinatorial problems are also included, such as a matrix of prime numbers from Problem 7 of Trefethen's 100-digit challenge [Trefethen 2002].

Once a matrix is collected, its maintenance is the responsibility of the first author. This guards against arbitrary modifications in the matrices, which can occur when the matrix submitters modify their matrix problems. Repeatability of experiments based on the UF Collection is thus ensured.

DESCRIPTION OF THE COLLECTION

As of March 2010 the UF Sparse Matrix Collection consists of 2272 problems, each of which contains at least one sparse matrix (typically just one). It often represents a sparse linear system of the form Ax = b, where b is sometimes provided as well as the sparse matrix A. Many other problems are eigenvalue problems, and many matrices come from unstructured graphs and networks with no associated linear system. In some cases, a problem consists of a sequence of closely related matrices, such as Jacobian matrices arising in the solution of a nonlinear system. Some problems include two sparse matrices, such as a stiffness matrix and a mass matrix from a structural engineering eigenvalue problem. In this case, A is the stiffness matrix, and the mass matrix appears as an auxiliary matrix in the problem.

3.1 Application areas

The collection is divided into 157 different matrix *groups*, with more groups added as new matrices are submitted to the collection. A complete list of these groups is too long to include here; details are given on the collection's web site. Each group

Table I. Partial list of sources of matrices

[Gav 2008]

[Gould et al. 2008] [Gupta 1996]

[Kamvar et al. 2004]

[Kemelmacher 2005] [Koster 2008]

[Miller and Wang 1991]

[Keiter et al. 2003]

[Mészáros 2008]

[Mittelmann 2008]

Non-Hermitian Eigenvalue Problems [Bai et al. 1996]
Pajek Networks [Batagelj and Mrvar 2008]
Multistage stochastic financial modeling [Berger et al. 1995]
The Matrix Market (collection) [Boisvert et al. 1997]
Univ. of Utrecht circuit simulation [Bomhof and van der Vorst 2000]

MRI reconstruction M. Bydder, UCSD
Harwell-Boeing Collection [Duff et al. 1989]
Combinatorial problems [Dumas 2008]
Frequency domain, nonlinear analog circuits [Feldmann et al. 1996]

NETLIB Linear Programming Test Problems
Symmetric sparse matrix benchmarks
Linear programming problems
Stanford/Berkeley Web Matrices
Xyce circuit simulation matrices
Computer vision problems
PARASOL Matrix Collection
Linear programming test set
2D and 3D semiconductor physics
Linear programming test set
QAPLIB, quadratic assignment

QAPLIB, quadratic assignment [Resende et al. 1995]
Oberwolfach Model Reduction Benchmarks [Rudnyi et al. 2006]
SPARSKIT matrix collection [Saad 2008]
Univ. of Basel Collection [Schenk 2008]
DNA electrophoresis matrices [van Heukelum et al. 2002]

Chemical engineering problems [van Heukelum et al. 2002] [Zitney 1992; Zitney et al. 1996]

typically consists of a set of matrices from a single source. A few of the matrix groups in the UF Collection consist of entire sets of matrices from another sparse matrix collection. In this case, the group may consist of matrices from very different application areas. For example, the Harwell-Boeing collection forms a single group [Duff and Reid 1979; Duff et al. 1989]. Sources (papers and web sites) for some of the matrix groups are listed in Table I, which gives a flavor of the range of problems the collection contains.

The group of a problem forms part of the full name of the problem. For example, the full name of the west0479 problem in the Harwell-Boeing collection (the HB group in the UF sparse matrix collection) is HB/west0479. In addition, all problems are tagged with a string, kind, which indicates the application domain of the problem. The group and kind of a problem are not the same. Some groups have many different kinds of problems, and problems of the same kind can appear in different groups. For example, the HB/west0479 problem is in the HB group, and its kind is tagged as a "chemical process simulation problem." Five other groups include chemical process simulation problems, namely, the Bai, Grund, Mallya, VanVelzen, and Zitney groups, all of which are named after the person from whom the matrices were obtained.

A complete list of the kind strings for all problems is given in Table II. The table is split into two categories: problems with no underlying geometry and problems with 2D or 3D geometry.

The collection contains 68 matrices with random nonzero pattern. They appear in the collection only because they already occur as widely-used test problems in

Table II.	Summary of Problem.kind for all 2272 problems		
problems with no 2D/3D geometry			
70	chemical process simulation problem		
251	circuit simulation problem		
299	combinatorial problem		
11	counter-example problem		
68	economic problem		
4	frequency-domain circuit simulation problem		
23	least squares problem		
342	linear programming problem		
135	optimization problem		
56	power network problem		
10	statistical/mathematical problem		
61	theoretical/quantum chemistry problem		
88	directed graph		
8	bipartite graph		
23	undirected graph		
68	random graph		
756 problems with 2D/3D geometry			
13	acoustics problem		
166	computational fluid dynamics problem		
12	computer graphics/vision problem		
44	electromagnetics problem		
28	materials problem		
42	model reduction problem		
3	robotics problem		
35	semiconductor device problem		
288	structural problem		
31	thermal problem		
94	2D/3D problem (other than those listed above)		

another collection that was subsequently added to the UF sparse matrix collection. In retrospect, their inclusion in the UF Collection was a mistake, but matrices are never removed once added, since this would cause confusion when replicating results that use the collection. We guarantee statements such as "all matrices with property X in the collection as of date Y" always give a single consistent answer.

3.2 Matrix statistics

The 2272 matrices in the collection come from 359 different authors and 50 different editors. A matrix *editor* is the one who collected the matrix for inclusion into any established collection (not just the UF Collection², but also for others such as the Harwell/Boeing collection³, the Matrix Market⁴, or the GRID/TSLE collection⁵). A matrix *author* is the one who created the matrix. Each matrix has an editor and an author (sometimes the same person). Editors contributing at least 10 matrices are listed in Table III (sorted by the number of matrices collected).

Figures 4 and 5 plot the matrix size (dimension and number of nonzeros) versus

 $^{^2 {\}rm UF~Sparse~Matrix~Collection:~http://www.cise.ufl.edu/research/sparse/matrices}$

 $^{^3} Harwell/Boeing\ collection:\ http://www.cse.scitech.ac.uk/nag/hb/hb.shtml$

 $^{^4 {\}it Matrix~Market:~http://math.nist.gov/MatrixMarket}$

 $^{^5\}mathrm{GRID}/\mathrm{TLSE}$ collection: http://gridtlse.enseeiht.fr:8080/websolve/

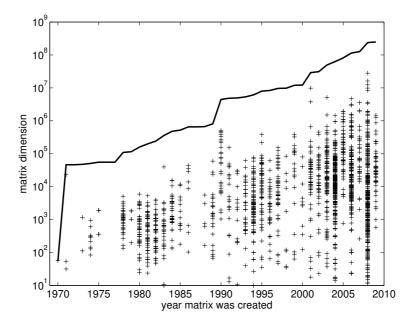


Fig. 4. Matrix dimension (the largest of row/column dimension if rectangular) versus year created. The solid line is the cumulative sum.

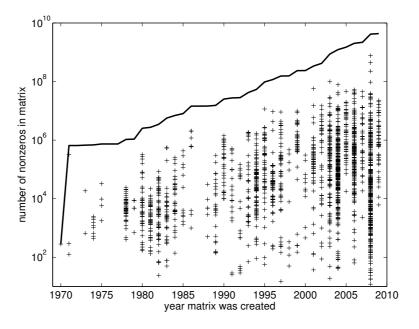


Fig. 5. Number of nonzeros in each matrix versus year created. The solid line is the cumulative sum

Table III. Primary editors of the UF Collection

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# matrices	editor	
720	T. Davis	
293	JG. Dumas	
255	I. Duff, R. Grimes, J. Lewis	
166	C. Meszaros	
103	O. Schenk	
78	Z. Bai, D. Day, J. Demmel, J. Dongarra	
72	V. Batagelj	
67	Y. Ye	
61	A. Baggag, Y. Saad	
48	D. Gay	
43	R. Fourer	
39	N. Gould, Y. Hu, J. Scott	
38	E. Rudnyi	
35	G. Kumfert, A. Pothen	
34	A. Curtis, I. Duff, J. Reid	
28	J. Chinneck	
27	N. Gould	
25	H. Mittelmann	
23	R. Boisvert, R. Pozo, K. Remington, B. Miller,	
	R. Lipman, R. Barrett, J. Dongarra	
23	F. Grund	
22	J. Koster	
13	I. Lustig	
12	H. Simon	
11	M. Resende	

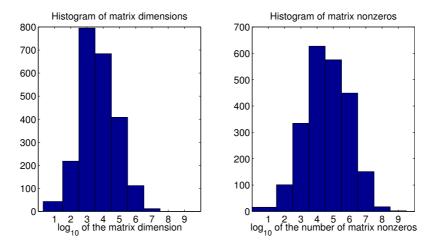


Fig. 6. Overall histograms of matrix dimensions and nonzeros

the year in which the matrices were created. The solid line in the figures is the cumulative sum of the data plotted. Both figures show an exponential growth in problem sizes, similar to how computer memory sizes have grown since 1970.

Note that small problems are still being added to the collection. This is because a matrix group often includes a range of related problems, from small test cases to the largest problems of interest.

The outlier matrix in 1971 is from the Edinburgh Associative Thesaurus, located at www.eat.rl.ac.uk and obtained from the Pajek data set [Batagelj and Mrvar 2008]. It is a graph with 23,219 vertices and 325,592 edges that was first constructed in 1971 [Kiss et al. 1973].

Figure 6 plots two histograms of the overall distribution of matrices in the collection.

4. VISUALIZING THE COLLECTION

Many basic facts, including symmetry, structural rank, ordering statistics, as well as a plot of the sparsity pattern, are given for each matrix in the collection. However these facts alone do not always give sufficient information about the matrix. For example, does this matrix come from an application involving 2D or 3D mesh? Or from a small-world network? Are there other structures in the applications that are not discernible from a plot of the sparsity pattern?

To help answer these questions, a visualization of each matrix in the form of graph drawing is provided. If the matrix is structurally symmetric, it is taken as the adjacency matrix of an undirected graph, where two vertices i and j are connected if the (i,j)-th entry of the matrix is nonzero. Rectangular or structurally unsymmetric matrices are treated as bipartite graphs. More specifically, the augmented matrix

$$\left(\begin{array}{cc} 0 & A \\ A^T & 0 \end{array}\right)$$

is used as the adjacency matrix of an undirected bipartite graph whose vertices are composed of the rows and columns of the matrix. We provide two graphs for square matrices with unsymmetric structure: the graph of $A+A^T$ and the augmented matrix above. The graph drawings depend only on the nonzero pattern, not the values.

The basic algorithm used for drawing the graphs is a multilevel force-directed algorithm [Hu 2005]. However this algorithm fails to produce informative drawings for some matrices. We propose here a new coarsening scheme to deal with these cases. In the following we briefly describe the basic algorithm, followed by the new coarsening scheme.

4.1 The graph drawing algorithm

The basic algorithm [Hu 2005] employs a force-directed model [Fruchterman and Reingold 1991]. Vertices are treated as particles with electrical charges that push each other away. This repulsive force $F_r(i,j)$ between any two vertices i and j is proportional to the inverse of their distance,

$$F_r(i,j) = \frac{K^2}{\|x_i - x_j\|}, \ i \neq j.$$

Here K is a parameter, and x_i is the location of vertex i. At the same time, vertices that share an edge are attracted to each other by a spring force,

$$F_a(i,j) = \frac{\|x_i - x_j\|^2}{K}$$
, i and j share an edge,

that is proportional to the square of their distance. The minimal energy configuration of this physical system is taken as the optimal drawing of the graph.

An iterative algorithm is used to attempt to find the optimal configuration. Starting from a random layout, for each vertex, the combined repulsive and attractive forces are calculated, and the vertex is moved along the direction of the force, with the distance moved controlled by a step length. This process is repeated, with the step length gradually reduced, until the positions stabilize. This simple force-directed process works well for small graphs. However, for large graphs, the process is likely to give suboptimal layout, due to the fact that this physical system of springs and electrical charges has many local minimum configurations. Therefore we employ a multilevel scheme to provide a "global view" and to help find a global optimum.

The multilevel approach has three distinctive phases: coarsening, coarsest graph layout, and finally, prolongation and refinement. In the coarsening phase, a series of coarser and coarser graphs, $\mathcal{G}^0, \mathcal{G}^1, \ldots, \mathcal{G}^l$, are generated, the aim is for each coarser graph \mathcal{G}^{k+1} to encapsulate the information needed to layout its "parent" \mathcal{G}^k , while containing roughly a fraction t, or less, of vertices (we set t=0.75). The coarsening continues until a graph with only a small number of vertices is reached. The optimal layout for the coarsest graph can be found cheaply. The layout on the coarser graphs are recursively interpolated to the finer graphs, with further refinement at each level.

Another important ingredient to allow very large graphs to be drawn is the Barnes-Hut force approximation scheme [Barnes and Hut 1986]. In this scheme, a nested space partitioning data structure is used to approximate the all-to-all repulsive force so as to reduce the quadratic complexity to log-linear, under certain assumptions.

4.2 A new coarsening scheme

The aforementioned multilevel algorithm was found to work well for many test graphs from the graph drawing literature [Hu 2005]. However, when applied to the UF Collection, we found that for some matrices, the multilevel process broke down, and the resulting drawing was poor. An example is shown in Figure 7. On the left of the figure is the sparsity pattern of the gupta1 matrix. From this plot we can conclude that this matrix describes a graph of three groups of vertices: those represented by the top 1/3 of the rows in the plot, the middle 1/3 of the rows, and the rest. Vertices in each group are all connected to a selected few in that group, these links are seen as dense horizontal and vertical bars in the matrix plot. At the same time, vertices in the top group are connected to those in middle group, which in turn are connected to those in the bottom group, as represented by the off-diagonal lines parallel to the diagonal. However, the graph drawing in the middle of Figure 7 shows none of these structures.

Analyzing the multilevel process (Table IV), we found that while up to level 2,

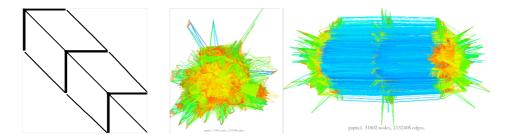


Fig. 7. Matrix plot of gupta1 matrix (left) and the initial graph drawing (middle). After applying the new coarsening scheme, the graph drawing reflects the structure of the matrix much better (right)

level	V	E
0	31802	2132408
1	20861	2076634
2	12034	1983352
3	11088	stopped

Table IV. The process of coarsening on gupta1 matrix

a significant reduction in the number of vertices were achieved as the graphs were coarsened (a reduction from 31802 vertices to 12034 vertices), between level 2 and level 3, the number of vertices hardly changed (11088/12034 = 0.92 > t). Consequently we had to stop the coarsening process and use the iterative force-directed algorithm on the large coarsest level graph with 11088 vertices. As expected, the result (middle of Figure 7) was very poor.

This matrix exemplifies many of the problematic matrices: they contain star-graph like substructures, with many vertices all connected to a few vertices. Such structures pose a challenge to the popular graph coarsening schemes, in that these schemes are not able to coarsen them adequately. One of these schemes is based on maximal independent edge set (MIES). An MIES is the largest set of edges that does not share a vertex. An MIES-based coarsening scheme works by finding an MIES, then merging the end vertex pairs of the edges in the set. This gives us a graph with less vertices and edges. Unfortunately for star-graph like structure, this scheme does not coarsen sufficiently. For example, Figure 8 (left) shows such a graph, with k = 10 vertices on the out-skirts all connected to two vertices at the center. Because of this structure, any MIES can only contain two edges (the two thick red edges in Figure 8). When the end vertices of the MIES are merged at the center of each edge, the resulting graph has only two less vertices. Therefore if k is large enough, the coarsening can be arbitrarily slow $(k/(k+2) \rightarrow 1 \text{ as } k \rightarrow \infty)$.

Having found the root cause of the problem, we propose a new coarsening scheme in the following. The scheme works by finding of vertices that share the same neighbors (these vertices are known as supervariables in the numerical analysis literature [Duff and Reid 1996], or as modules in the graph theory literature [McConnell and Spinrad 1999]), then matching pairs of these vertices. A usual MIES scheme then matches the remaining unmatched vertices. Finally the matched vertices are merged

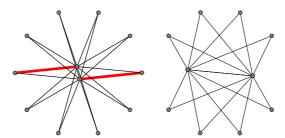


Fig. 8. A maximal independent edge set based coarsening scheme fails to coarsen sufficiently a star-graph like structure: a maximal independent edge set (thick and red edges) (left); when merging the end vertices of the edge set at the middle of these edges, the resulting coarsened graph only has 2 less vertices (right)

to get the coarsened graph. The scheme is able to overcome the slow coarsening problem associated with graphs having star-graph like substructures. Applying this scheme to the graph in Figure 9 (left) resulted in a graph with 1/2 the number of vertices (Figure 9 right). With this new coarsening scheme, we are able to layout many more graphs aesthetically. For example, when applied to the gupta1 matrix, the drawing at Figure 7 (right) reveals the correct visual structures as we expected, with three groups of vertices, each connected to a few within the group, and a linear connectivity relation among the groups.

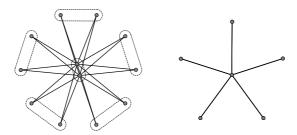


Fig. 9. Matching and merging vertices with the same neighborhood structure (left, with dashed line enclosing matching vertex pairs) resulted in a new graph (right) with 1/2 the number of vertices

A complete run of the graph drawing algorithm on the entire collection of 2272 matrices in March 2010 takes in the order of 18 days of CPU time on one Intel Xeon E7330 2.4 GHz processor (the machine itself has 60 processors and 132 GB of memory). The median number of vertices is 5185, and median CPU time 4.8 seconds. Figure 10 gives the log-log plot of CPU time over n, versus the number of vertices (n). If the run time scaled linearly with n, the plot would be flat. As can be seen, the time scales slightly super-linearly to the number of vertices. The best-fit line is a run time of $O(n^{1.28})$. This complexity is higher than the expected log-linear, albeit based on results from matrices of different structures, instead of a true asymptotic study. We intend to investigate it further.

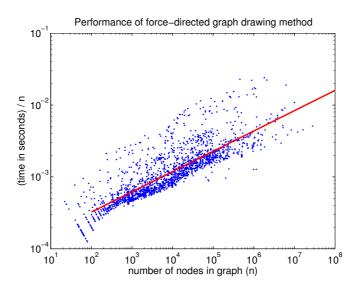


Fig. 10. Performance of the graph drawing method, with each dot represent a matrix

5. MATRIX DATA FORMATS

The matrix problems appear in three formats: MATLAB MAT-file, Matrix Market (MM) [Boisvert et al. 1997], and Rutherford-Boeing (RB) [Duff et al. 1997]. The matrices and all auxiliary data are identical in all three formats, down to the very last bit. The following data appears each matrix problem:

- —name: the matrix name (HB/west0479, for example).
- —title: a short descriptive title.
- —A: the sparse matrix itself.
- —id: the matrix id.
- —date: the date the matrix was created.
- —author: the matrix author (left blank if unknown).
- —ed: the matrix editor (Table III).
- —kind: the matrix kind-string (Table II).

The following optional fields are present in some problems:

- —Zeros: a binary matrix of numerically-zero entries provided by the matrix author. In the MM and RB formats, these are held in the matrix itself. They cannot be held in the MAT form, because MATLAB drops these entries.
- —b: a right-hand side (sparse or dense).
- —x: the solution to Ax = b (sparse or dense).
- —notes: additional text describing the problem.
- —aux: any additional data. The contents of this are problem-dependent. Examples include the l, h, and c vectors for a linear-programming problem (minimize c^Tx subject to Ax = b and $l \le x \le h$), an n-by-3 array of xyz coordinates of the vertices, an array of n strings with the names of each vertices, a sparse mass

matrix for a generalized eigenvalue problem, etc.

In the MAT-format, the entire problem is held as a MATLAB struct, and stored in its own MAT-file.

The MM format [Boisvert et al. 1997] stores a sparse matrix as a collection of triplets (i, j, a_{ij}) , with the row index, column index, and numerical value. In the MM format, triplets appear one per line in any order and duplicates are permitted. However, our MM files are all sorted, with no duplicate entries. The MM format permits comments in the matrix file, and most of the additional problem characteristics (name, id, notes, etc.) appear as structured comments.

The RB format [Duff et al. 1997] stores a sparse matrix in compressed-column form, as three vectors Ap, Ai, and Ax. The row indices and numerical values of entries in the jth column are located in positions Ap(j) through Ap(j+1)-1 of Ai and Ax, respectively. This format does not allow for structured comments, so this information is held in a separate file.

For the MM and RB formats, the matrix file and any auxiliary matrices are all kept in a single directory, then archived as a single ZIP file.

The SuiteSparse package (http://www.cise.ufl.edu/research/sparse) includes software in MATLAB, C, and Fortran, for reading and writing the matrices and for creating and maintaining the collection.

ACCESSING THE COLLECTION

There are four methods for accessing matrices in the collection on the web.

6.1 UFgui: Java interface

UFgui is a Java-based application for browsing, selecting, and downloading matrices from the primary web site for the collection. A screenshot is shown in Figure 11. It provides a selection mechanism for choosing matrices with specific features (size, symmetry, number of nonzeros, whether it has 2D/3D geometry or not, matrix group, and matrix kind). The selected matrices act as a set of id's, where clicking select acts as a set union, and deselect acts as a set difference. For example, to select all real square matrices except for those arising in circuit simulation, select real and square, and then click select. Then select chemical process simulation and click deselect. Clicking download then downloads all selected matrices that have not yet been downloaded. Right-clicking the table of matrices provides options for exporting the list of selected matrix id's as a spreadsheet or a MATLAB M-file. As matrices are selected in the table, an image of the nonzero pattern of the most recently-selected matrix is displayed. The table also indicates which matrices have already been downloaded, under the mat, MM, and RB column headings. In Figure 11, the HB/will199 matrix has already been downloaded into /Users/davis/sparse/UFget, in both MAT and MM formats, but not in RB for-

Clicking on a column heading sorts the table by that column. The sort is stable, in the sense that ties are broken according to the previous sort. Thus, to view matrices grouped by their 2D/3D characteristic, and then sorted by the number of rows, the user can first click to sort on the number of rows, and then click the 2D/3D column heading to sort by that characteristic.

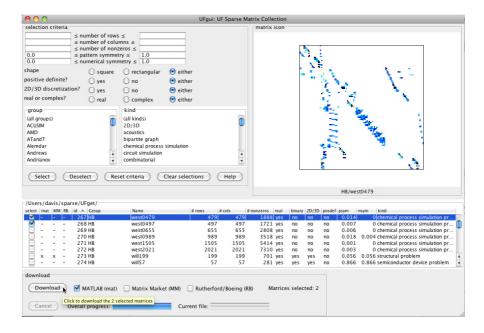


Fig. 11. UFgui: Java interface to the UF Collection

6.2 UFget: MATLAB interface

UFget is the MATLAB interface to the collection. Problem=UFget('HB/west0479') loads the matrix of that name into the MATLAB workspace, downloading it if necessary. Problem=UFget(267) does the same, using the problem id instead. The index of the entire collection is loaded with index=UFget, which automatically updates itself every 90 days so that new matrices can be included. This index contains statistics about each matrix and can be searched via simple MATLAB expressions. For example, the following MATLAB code downloads all square matrices with full structural rank whose nonzero pattern is at least 50% symmetric, in increasing order of number of nonzeros. It then computes a fill-reducing ordering with AMD [Amestoy et al. 1996; 2004] on the pattern of $A + A^T$ (ignoring numerical cancellation), and determines the number of nonzeros in the Cholesky factorization.

```
index = UFget ;
matrices = find (index.nrows == index.ncols & ...
    index.sprank == index.nrows & ...
    index.pattern_symmetry > 0.5) ;
[ignore i] = sort (index.nnz (matrices)) ;
matrices = matrices (i) ;
nmat = length (matrices) ;
for k = 1:nmat
    Problem = UFget (matrices (k)) ;
    A = spones (Problem.A) + spones (Problem.A') ;
    p = amd (A) ;
    anz = nnz (A) ;
    lnz = sum (symbfact (A (p,p))) ;
end
```

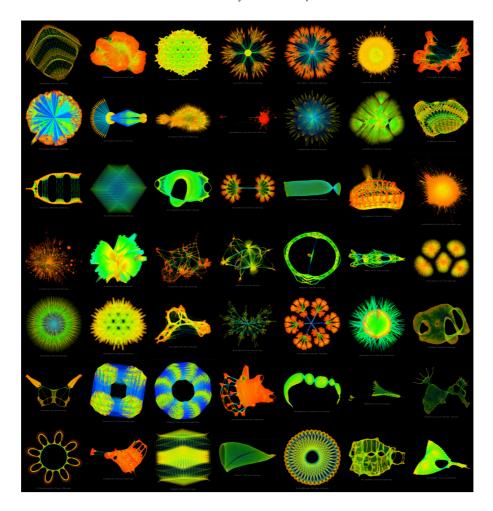


Fig. 12. A sample of matrices from the collection, for the purpose of illustrating the complexity and diversity of matrices arising in real applications

6.3 Via a web browser

The collection's primary web site is http://www.cise.ufl.edu/research/sparse/matrices, with a link to an online form that allow the users to search by keywords, as well as by matrix type, structure, dimensions or other statistics.

Each matrix has its own web page, with matrix statistics, any notes about the matrix, download links, an image of the nonzero pattern of the matrix, and a drawing of the graph using the force-directed graph drawing method discussed in Section 4. The main index page includes a sample of 49 thumbnail-sized snapshots of these graphs, shown in Figure 12, which gives a visual indication of the diversity and complexity of matrices in the collection. Each matrix group has a web page, with an index showing thumbnail matrix images and graphs, and basic statistics.

6.4 Amazon Web Services

The entire UF Collection is hosted by Amazon Web ServicesTMas a Public Data Set at http://aws.amazon.com.

7. EXAMPLE USES OF THE COLLECTION

A collection such as the one described here can answer many questions about the design, analysis, and performance of sparse matrix algorithms that cannot be answered by theoretical analyses or artificially-generated matrices. Matrices obtained from (or available in) this collection have been used in a wide range of published experimental results. For a small sample, see [Amestoy et al. 2001; Amestoy et al. 2007; Amestoy and Puglisi 2002; Benzi and Tuma 1998; Brainman and Toledo 2002; Demmel et al. 1999; Duff and Koster 1999; Duff and Pralet 2005; Gupta 2002; Schulze 2001]. As of March 2010, Google Scholar lists 395 papers that cite the UF Collection as it appeared in [Davis 1997] or as a technical report version of this paper. Articles that do not use standard benchmarks such as the UF Collection typically use matrices that could arise in practice, such as the 5-point discrete Laplacian on a regular mesh ([Ruesken 2002], for example).

Three examples of the kinds of questions a set of real matrices can answer are given here: the average-case time complexity of the minimum degree ordering algorithm, the typical fill-in in a Cholesky factorization using the AMD or METIS orderings, and the trade-off between supernodal and non-supernodal sparse Cholesky factorization methods [Chen et al. 2008].

7.1 First example: average-case run time of minimum degree

The minimum degree ordering algorithm is a heuristic for finding a permutation P such that the Cholesky factorization of PAP^T is sparser than that of A. The running time of the minimum degree ordering algorithm is notoriously difficult to analyze. Under modest assumptions, a loose worst-case upper bound on the run time of the approximate-minimum-degree (AMD) variant of this method is given by

$$O\left(\sum_{k=1}^{n} |L_{k*}| \cdot |(PAP^T)_{k*}|\right),\tag{1}$$

where P is the permutation found by AMD, L is the Cholesky factor of PAP^T , and |x| denotes the number of nonzeros in a vector or matrix [Amestoy et al. 1996; 2004]. The bound does not consider the speedup obtained by exploiting supernodes, which has not been analyzed because the graph changes unpredictably during the elimination.

A single dense row or column of A leads to a run time of at least $\Omega(n^2)$, but AMD includes a preprocessing step that removes any row or column with degree $10\sqrt{n}$ or larger (the effect of this step is not accounted for in (1)). Still, a host of nearly-dense rows/columns could lead to unacceptable ordering time. Is the bound (1) reached in practice? What is the average-case time complexity of AMD?

Determining the theoretical average-case time complexity is beyond the scope of any analysis that has been done for this algorithm, so the best that can be done is to test the method on a set of "average" sparse matrices that arise in practice. The

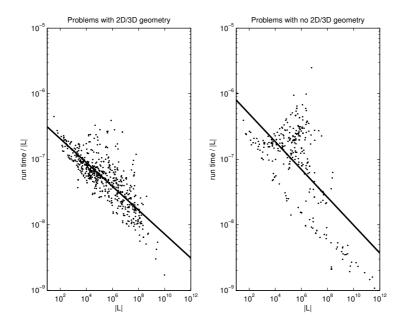


Fig. 13. AMD run time in seconds /|L|, as a function of |L|

results of ordering $A + A^T$ (ignoring numerical cancellation in the matrix addition) on all square matrices in the collection (as of November 2006) whose nonzero pattern is symmetric (or mostly so) are shown in Figures 13 and 14. The selection is the same as shown in Section 6.2. Each matrix is a single dot in Figures 13 and 14. The x-axis is the number of entries in $A + A^T$.

The results are split into two sets: matrices from problems with 2D/3D geometry, and problems without any underlying geometry. A best-fit line is shown (admittedly not a very good fit).

Figure 13 shows that O(|L|) is a very loose upper bound on the average case run time (excluding a few worst-case examples), even though O(|L|) is already a much lower bound than (1). The best-fit line is $O(|L|^{0.66})$ for the 2D/3D case, and $O(|L|^{0.61})$ for problems with no 2D/3D geometry.

Figure 14 indicates that the average-case run time may be slightly super-linear in |A| (at least for 2D/3D problems), with the best-fit line being $O(|A|^{1.1})$ for problems with 2D/3D geometry, and $O(|A|^{1.4})$ otherwise.

7.2 Second example: typical fill-in

To illustrate the importance of the non-random structure in a matrix, consider Figure 15, which plots the quality of the ordering from AMD or METIS [Karypis and Kumar 1998] (whichever gives the best result). For this figure, the y-axis is the number of nonzeros in L divided by the number of nonzeros in the lower triangular part of A, denoted nnz(tril(A)) (the latter is also the x-axis). A metric of 1.0 means that no fill-in occurred. This plot includes all matrices with perfectly symmetric pattern in the collection as of March 2010.

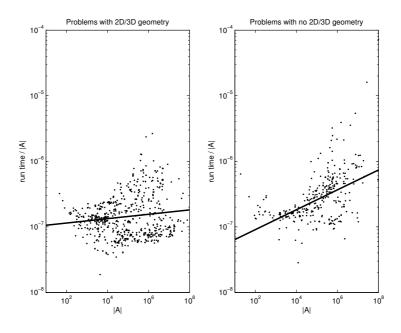


Fig. 14. AMD run time in seconds / |A|, as a function of |A|

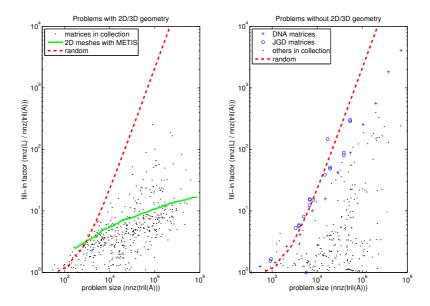


Fig. 15. AMD/METIS fill-in factor, as a function of the number of nonzeros in the lower triangular part of A, $\mathrm{nnz}(\mathrm{tril}(A))$

Superimposed on each of the two plots in Figure 15 is a dashed line for matrices with random nonzero pattern from the MATLAB sprandsym function, with an average of 5 nonzeros per row or column including a zero-free diagonal. This is the same number of entries as a matrix arising from the discretization of a 2D mesh. The left figure includes a solid line which is the METIS result on a square 2D mesh (recall that for these matrices, |A| = 5n and $|L| = 31(n\log_2 n)/8 + O(n)$). The METIS result on square 2D meshes indicates that most matrices from real applications with 2D/3D geometry have a fill-in factor that is not much different than these simple square meshes.

On the right plot, two sets of matrices are highlighted that have particularly high fill-in. The +'s are from a DNA electrophoresis problem [van Heukelum et al. 2002], and the o's are from J.-G. Dumas' collection of combinatorial mathematical problems [Dumas 2008]. Both sets of matrices have very irregular patterns, and seem to approach the level of fill-in from matrices with random pattern. The DNA and JGD matrices do not have 2D/3D geometry, so they do not appear in the left plot. Other that these two sets of matrices, the fill-in from matrices from real applications seems to be asymptotically lower than fill-in in random matrices.

The outlier in the left plot in Figure 15 with the highest fill-in factor is the GHS_indef/sparsine matrix, a structural optimization matrix [Gould et al. 2008]. It is labeled as a problem with 2D/3D geometry in the collection when added (by this author) to the collection, but this label might be incorrect. Optimization problems often have irregular structure and no underlying geometry, although a mechanical structural optimization problem would presumably have a 2D or 3D geometry. The graph drawing of this matrix can be seen in Figure 12, in the top row, second column. It is very irregular and is visually similar to the linear programming problem in the top right corner of the same figure (the Andrianov/lpl1 matrix). The sparsine graph is very different from the regular structure of a finite-element matrix (Alemdar/Alemdar in the top left corner, for example), which may explain why it is an outlier in the left plot in Figure 15.

7.3 Third example: BLAS trade-off in sparse Cholesky factorization

CHOLMOD is a sparse Cholesky factorization and update/downdate package that appears in x=A\b and chol(A) in MATLAB, when A is sparse and symmetric positive definite [Chen et al. 2008; Davis and Hager 2009]. It includes two sparse Cholesky factorization methods: a BLAS-based supernodal method [Ng and Peyton 1993] and an up-looking non-BLAS-based method [Davis 2005]. The two methods are included because a BLAS-based method is slower for very sparse matrices (tridiagonal ones, for example). The dense matrix operations in the BLAS gain their performance advantage when the ratio of floating-point work to memory traffic is high. Thus, we predicted that the ratio of the number of floating-point operations over the number of nonzeros in L would be a good way to automatically select the appropriate method. Both of these terms are available from the symbolic analysis, prior to numerical factorization. A similar metric was used to compare the BLASbased SuperLU method [Demmel et al. 1999] with its non-BLAS based precursor, GPLU [Gilbert and Peierls 1988]. The primary difference is that for sparse LU factorization, the metric can only be estimated prior to numeric factorization, which limits its use as a simple method for selecting the appropriate method.

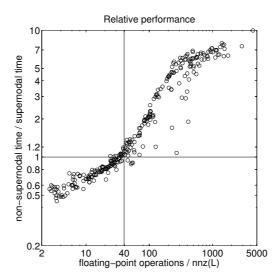


Fig. 16. CHOLMOD relative supernodal and non-supernodal performance

Two questions remain: how useful is this metric, and what should the cutoff value be? We tested both methods with 320 matrices from the September 2006 version of the collection: all symmetric positive definite matrices and all symmetric binary matrices with zero-free diagonals to which values were added to ensure positive-definiteness. The 68 random matrices listed in Table II were excluded. The relative performance of the two methods is plotted versus the flops/|L| ratio, as shown in Figure 16. These results show that the flops/|L| ratio is a remarkably accurate predictor of the relative performance of these two methods (much better than we expected). The outliers in the plot actually strengthen the result, since it shows that most matrices fall along a smooth curve even when it is possible for any given matrix to lie far from the curve. The figure shows that a value of 40 on a Pentium 4 is a good threshold. Even when the wrong method is selected using this approach, at most a 20% performance penalty occurs for matrices in this test set. The threshold of 40 is fairly insensitive to the architecture (it would be 30 on an AMD Opteron, and 35 on a Sun Sparc). It would be impossible to determine this cutoff using random matrices or a theoretical analysis.

8. THE FUTURE

Matrices are continually submitted and are added to the collection every few months. Without the continual influx of new and larger matrices, the collection would become less and less useful over time. As of the writing of this paper in March 2010, we have a back-log of about 60 matrices to be added. No one can predict the future, but we plan on continuing to augment and maintain the collection for as many years as we can.

Computational scientists are encouraged to submit their sparse matrices for inclusion in the collection. Matrices used in published performance evaluations of sparse ACM Transactions on Mathematical Software, Vol. V, No. N, M 20YY.

matrix algorithms are of particular interest, to enable repeatable experiments by other researchers. Matrices can be submitted to http://www.cise.ufl.edu/~web-gfs, for user-name davis. Use a standard format for the matrix, such as a MATLAB MAT-file, a Rutherford-Boeing file, a Matrix Market file, or a list of triplets (where each line of the file contains the row index, column index, and numerical value of one entry in the matrix). Include a description of the matrix, the problem area it arises from, citations (if available), and source (in case the matrix author and submitter are different). Refer to Table II for a list of categories, and select one of them for your matrix or propose a new one.

9. SUMMARY

A large, easily accessible, and actively growing collection of sparse matrices from real applications is crucial for the development and testing of sparse matrix algorithms. The University of Florida Sparse Matrix Collection meets this need, as the largest and most widely-used collection available. We have demonstrated this with just a few examples, but many more can be found via a Google Scholar search for citations to this collection.

We have discussed our strategy for including new matrices in the collection, which is effective although admittedly ad hoc. Four methods of searching and downloading the matrices have been presented: via MATLAB, via a stand-alone Java GUI program, via a standard web browser and search tool, and via Amazon Web ServicesTM.

In addition, the collection has proven to be a valuable resource for development of graph visualization algorithms, prompting us to propose a new coarsening algorithm to handle some matrices with a special substructure. There are still matrices that even the new coarsening scheme does not handle satisfactorily, thus the collection continues to serve as a fertile ground for research on new algorithms.

Acknowledgments

We would like to thank John Gilbert for his comments on random sparse matrices and his feedback on a draft of this paper. We would like to thank Iain Duff for testing and evaluating our UFgui application, and for suggesting features that we then included in that application. We would also like to thank the 359 matrix authors and 49 editors (excluding ourselves) who made this collection possible.

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