Sequential Sparse Matrix–Vector Multiplication

Section 4.1 of Parallel Scientific Computation, 2nd edition

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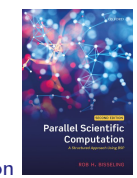
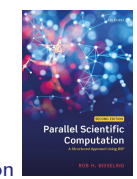
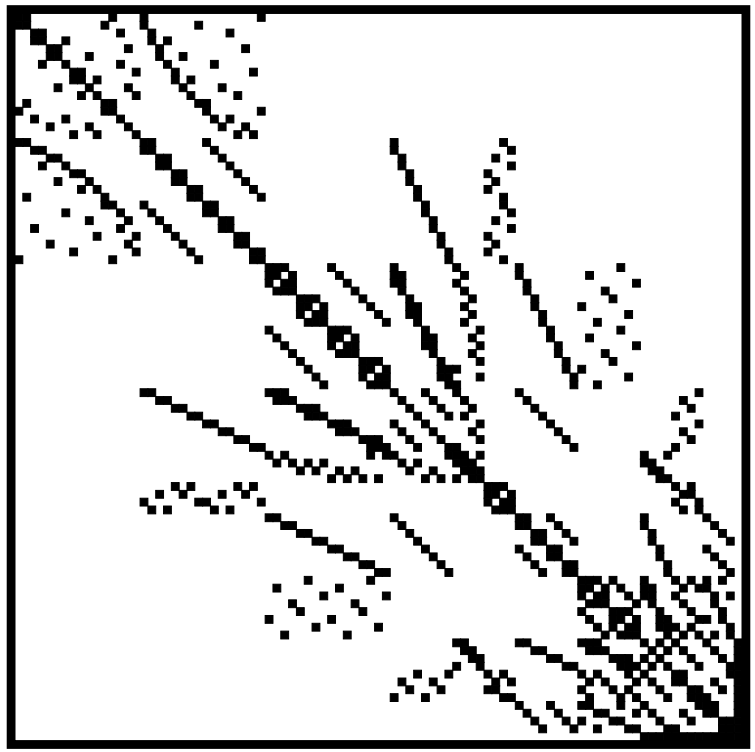


Sparse and dense matrices

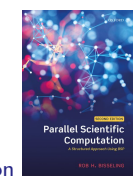
- Sparse matrices are sparsely populated by nonzero elements.
- Dense matrices are densely populated by nonzeros.
- Sparse matrix computations save time: operations with zeros can be skipped or simplified; only the nonzeros must be handled.
- Sparse matrix computations also save memory: only the nonzeros need to be stored (together with their location).



Sparse matrix cage6



- $n = 93$ rows/columns
- $nz = 785$ nonzeros
- $c = 8.4$ nonzeros per row
- $d = 9.1\%$ density



Matrix statistics

- Number of nonzeros is

$$nz = nz(A) = |\{a_{ij} : 0 \leq i, j < n \wedge a_{ij} \neq 0\}|.$$

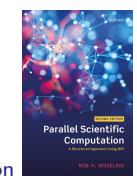
- Average number of nonzeros per row or column is

$$c = c(A) = \frac{nz(A)}{n}.$$

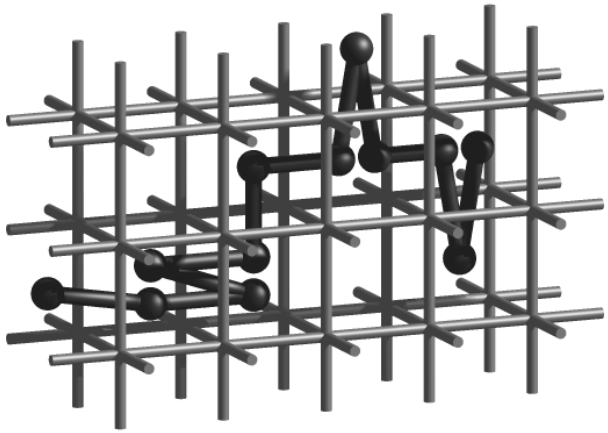
- Density is

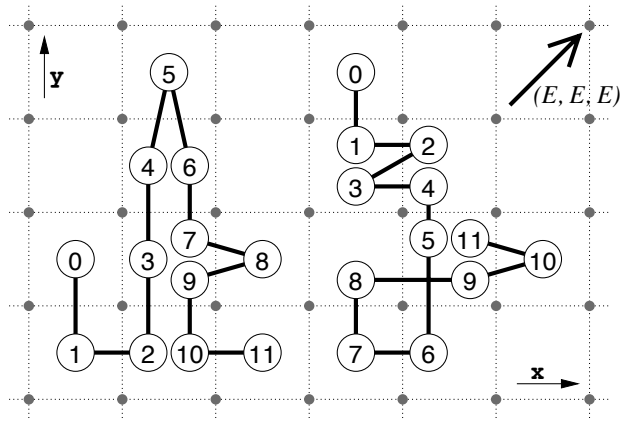
$$d = d(A) = \frac{nz(A)}{n^2}.$$

- Matrix is sparse if $nz(A) \ll n^2$, or $c(A) \ll n$, or $d(A) \ll 1$.



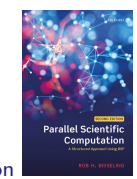
Application: cage model for gel electrophoresis of DNA



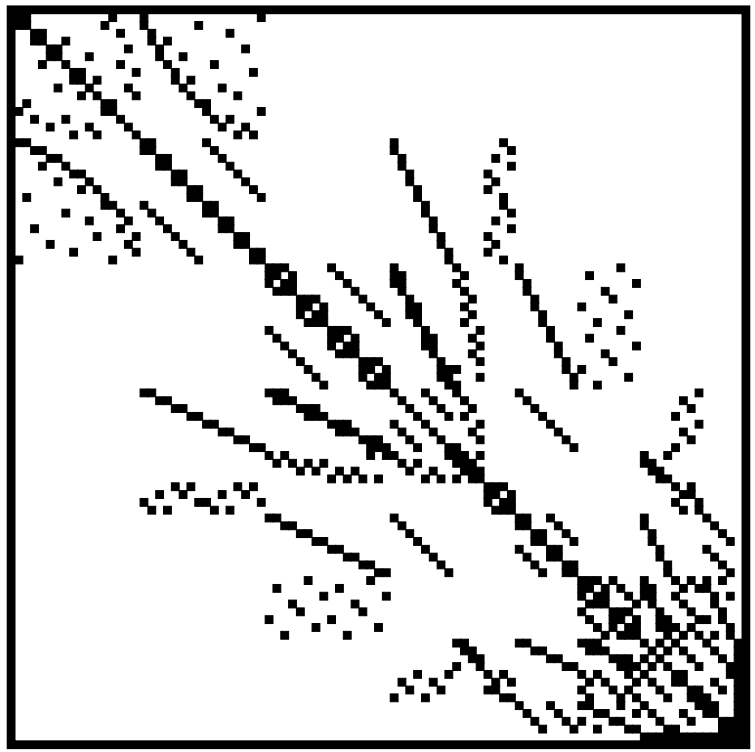


- 3D cubic lattice models a gel, in which a DNA polymer moves.
- DNA reptates, i.e., moves like a snake: its kinks and end points move under the influence of an electric field E.
- Gel electrophoresis was used in first-generation DNA sequencing to separate DNA fragments by length.
- Shorter fragments move faster.

A. van Heukelum, G. T. Barkema, R. H. Bisseling, *Journal of Computational Physics* **180** (2002) pp. 313–326.

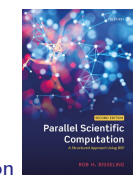


Transition matrix for the cage model

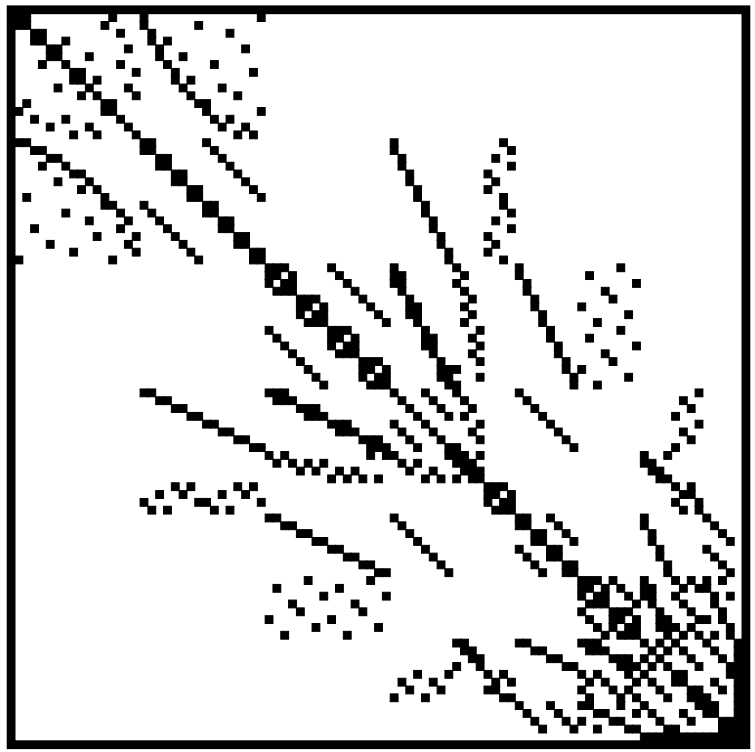


- Matrix element a_{ij} is the probability that a polymer in state j moves to a state i.
- Hence, the matrix is stochastic, i.e. $0 \leq a_{ij} \leq 1$ and

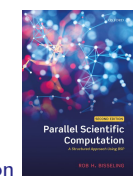
$$\sum_{i=0}^{n-1} a_{ij} = 1, \text{ for all } j.$$



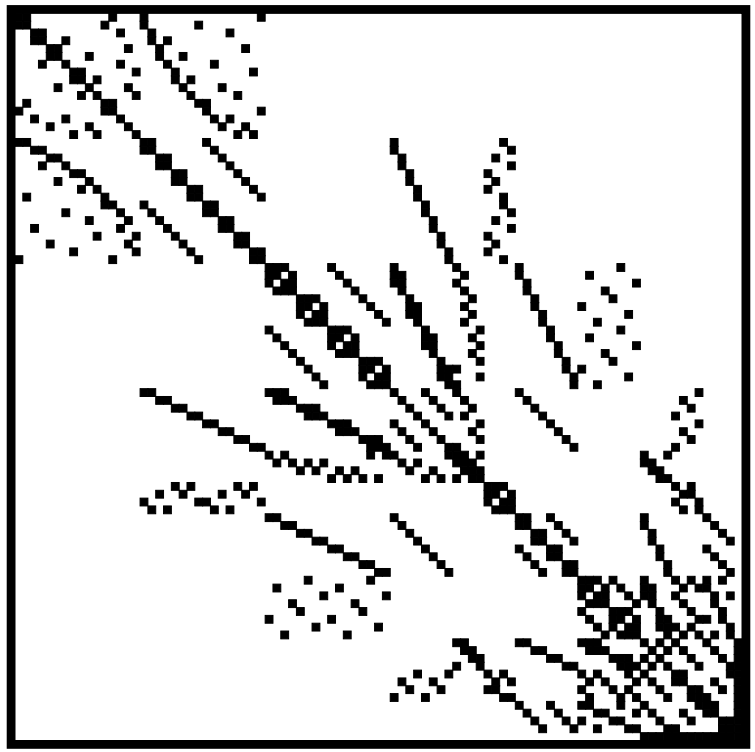
Transition matrix is sparse



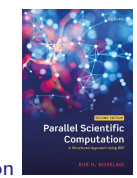
- Polymer has 6 monomers for cage6. We can move only one monomer at a time.
- Hence, each state has only a few connected states and the matrix is sparse.



Sparsity structure of cage6

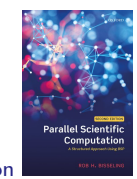


- Each move can be reversed, hence $a_{ij} \neq 0 \Longleftrightarrow a_{ji} \neq 0$, i.e., the matrix is structurally symmetric.
- A move against the electric field has a different probability than a move with the field. Hence $a_{ij} \neq a_{ji}$, so that the matrix is unsymmetric.



Power method

- Let $\mathbf{x}$ be the vector of state frequencies: component x_i represents the relative frequency of state i, with $0 \leq x_i \leq 1$ and $\sum_i x_i = 1$.
- The power method computes $A\mathbf{x}, A^2\mathbf{x}, A^3\mathbf{x}, \ldots$, until convergence.
- The final component x_i represents the frequency of state i in the steady-state situation, where $A\mathbf{x} = \mathbf{x}$.
- Main operation: multiplication of sparse matrix A and dense vector $\mathbf{x}$.



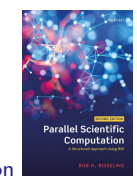
Sparse matrix–vector multiplication (SpMV)

- Let A be a sparse $n \times n$ matrix and $\mathbf{v}$ a dense input vector of length n.
- We consider the problem of computing the dense output vector $\mathbf{u}$,

$$\mathbf{u} := A\mathbf{v}.$$

- The components of $\mathbf{u}$ are

$$u_i = \sum_{j=0}^{n-1} a_{ij} v_j, \quad \text{for } 0 \leq i < n.$$

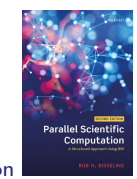


Sparse matrix–vector multiplication algorithm

input: A : sparse $n \times n$ matrix,
$\mathbf{v}$: dense vector of length n.
output: $\mathbf{u}$: dense vector of length n, $\mathbf{u} = A\mathbf{v}$.

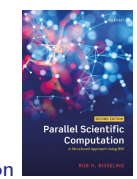
for $i := 0$ **to** $n - 1$ **do**
  $u_i := 0$;
for all $(i, j) : 0 \leq i, j < n \wedge a_{ij} \neq 0$ **do**
  $u_i := u_i + a_{ij} v_j$;

- The sparsity of A is expressed by the test $a_{ij} \neq 0$.
- Such a test is never executed in practice, and instead a sparse data structure is used.

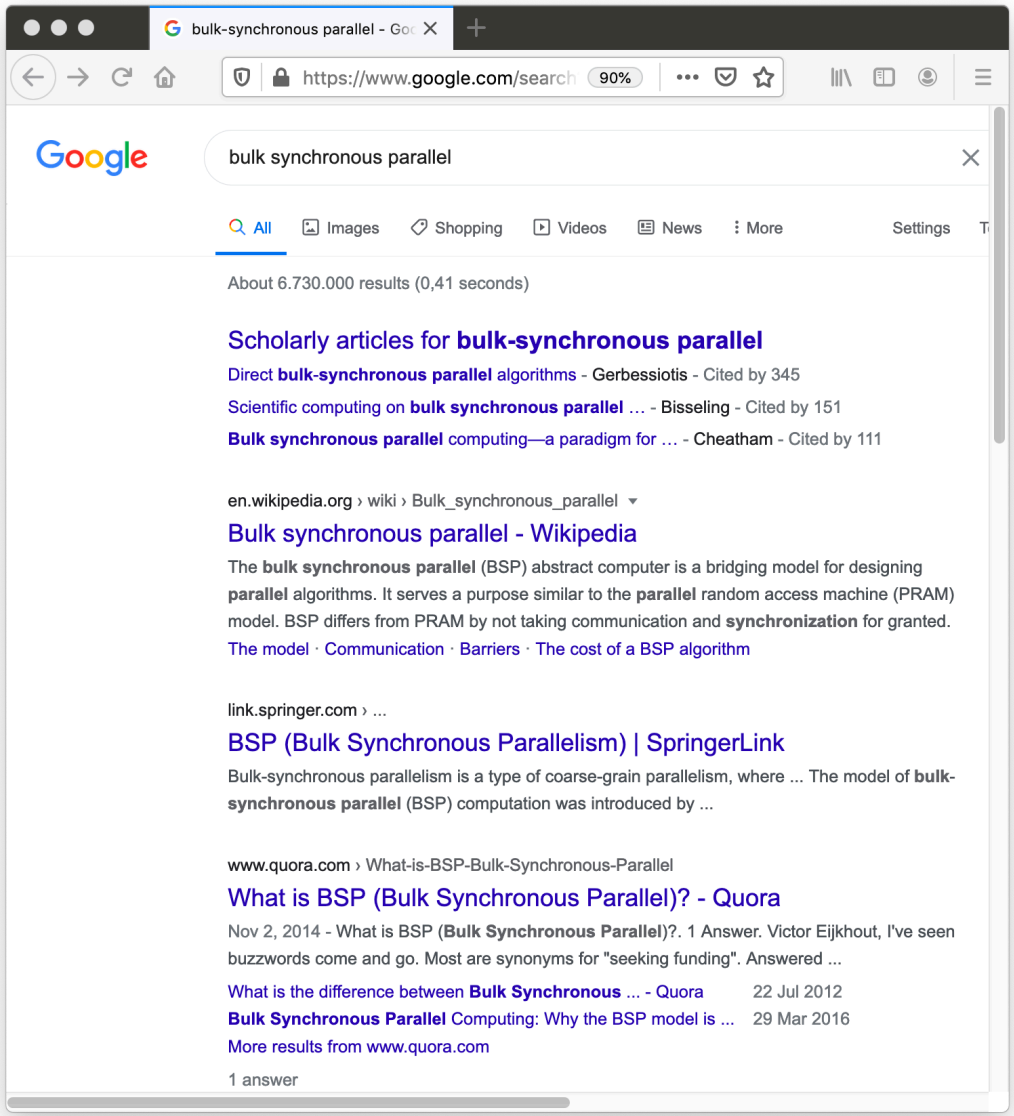


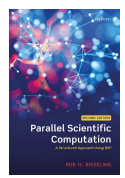
Application of SpMV: iterative solution methods

- Sparse matrix–vector multiplication is the main computation step in iterative solution methods for linear systems or eigensystems.
- Iterative methods start with an initial guess $\mathbf{x}^0$ and then successively improve the solution by finding better approximations $\mathbf{x}^k$, $k = 1, 2, \ldots$, until the error is tolerable.
- Examples:
  - Linear systems $A\mathbf{x} = \mathbf{b}$, solved by the conjugate gradient (CG) method or MINRES, GMRES, QMR, BiCG, Bi-CGSTAB, IDR, IDR(s), SOR, FOM, ...
  - Eigensystems $A\mathbf{x} = \lambda\mathbf{x}$ solved by the Lanczos method, Jacobi–Davidson, ...
- One size does not fit all. Different applications require different iterative methods.



Web searching: which page ranks first?





The weblink matrix A

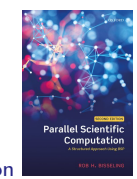
- Given n web pages with hyperlinks between them, we can define the sparse $n \times n$ weblink matrix A by

$$a_{ij} = \begin{cases} 1 & \text{if there is a hyperlink from page } j \text{ to page } i \\ 0 & \text{otherwise.} \end{cases}$$

- Let $\mathbf{e} = (1, 1, \ldots, 1)^{\mathrm{T}}$, represent an initial uniform importance (rank) of all web pages. Then

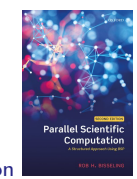
$$(A\mathbf{e})_i = \sum_j a_{ij} e_j = \sum_j a_{ij}$$

  is the total number of hyperlinks pointing to page i.
- The vector $A\mathbf{e}$ represents the importance of the pages; $A^2\mathbf{e}$ takes the importance of the pointing pages into account as well; and so on.



Weblink matrix bspww500

- This matrix with $n = 500$ and $nz = 13\,400$ represents 500 web pages and the hyperlinks connecting them.
- It was obtained by a breadth-first search in 2017 of the World Wide Web starting at `http://www.bsp-worldwide.org` and using the web crawler `surfer.m` by Cleve Moler.

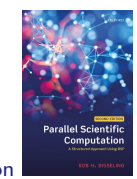


The random surfer model

- A random web surfer chooses each of the c_j outgoing hyperlinks from page j with equal probability $\frac{1}{c_j}$.
- To incorporate this behaviour, we define the $n \times n$ diagonal scaling matrix D by

$$d_{jj} = c_j,$$

  and multiply the weblink matrix A from the right by D^{-1}.
- This divides each column j of A by c_j.



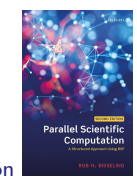
The Google matrix

- Let α be the probability that a surfer follows an outlink of the current page. Typically $\alpha = 0.85$. The surfer jumps to a random page with probability $1 - \alpha$.
- The Google matrix is defined by

$$G = \alpha A D^{-1} + (1 - \alpha)\frac{1}{n}\mathbf{e}\mathbf{e}^{\mathrm{T}}.$$

- Note that this definition is under the assumption that all $c_j > 0$.
- The PageRank of a set of web pages is obtained by repeated multiplication by G, involving sparse matrix–vector multiplication by A and some vector operations.

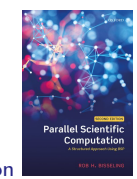
S. Brin and L. Page, *Computer Networks and ISDN Systems*, **30**(1–7) (1998) pp. 107–117.



Vector operation

- The vector $\mathbf{e}$ can be viewed as an $n \times 1$ matrix of all ones and the vector $\mathbf{e}^{\mathrm{T}}$ as a $1 \times n$ matrix.
- The matrix $\mathbf{e}\mathbf{e}^{\mathrm{T}}$ is an $n \times n$ matrix with all elements equal to 1.
- Multiplication of a vector $\mathbf{x}$ by $\mathbf{e}\mathbf{e}^{\mathrm{T}}$ is cheap:

$$\mathbf{e}\mathbf{e}^{\mathrm{T}}\mathbf{x} = \mathbf{e}(\mathbf{e}^{\mathrm{T}}\mathbf{x}) = (\sum_{i=0}^{n-1} x_i)\mathbf{e}.$$



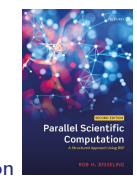
Escaping from dangling nodes

- If $c_j = 0$, column j must be empty and page j a dangling node; it could be a PDF file or an image file.
- To avoid division by zero, the diagonal element is then redefined as $d_{jj} = 1$.
- To make the Google matrix stochastic (with all column sums equal to 1), we must add to G an extra term

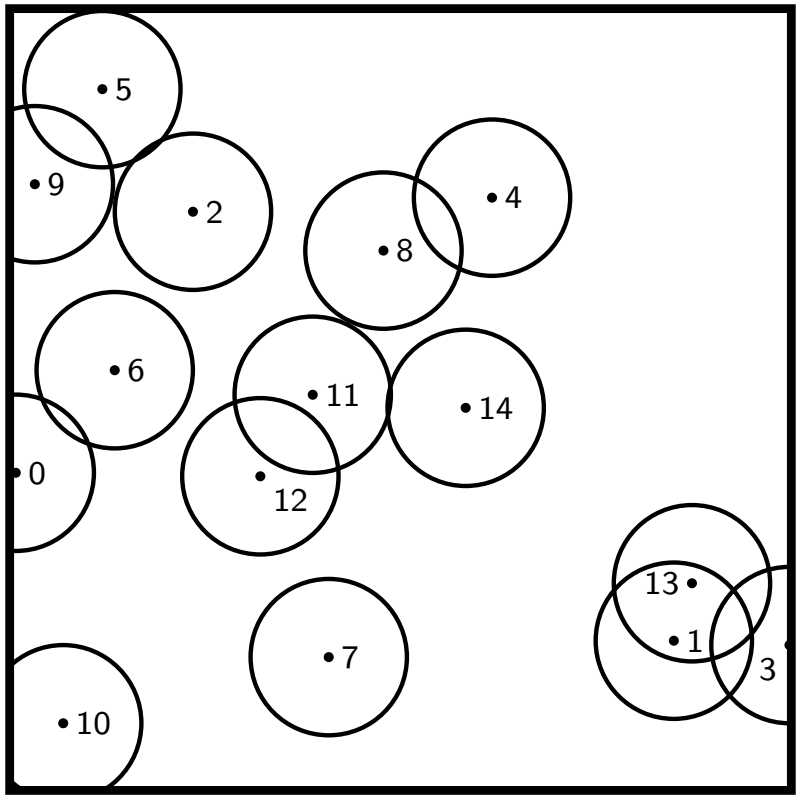
$$\alpha \frac{1}{n} \mathbf{e}\hat{\mathbf{e}}^{\mathrm{T}}.$$

- Here, the vector $\hat{\mathbf{e}}$ is defined by

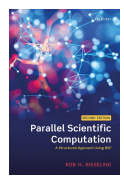
$$\hat{e}_j = \begin{cases} 1 & \text{if } c_j = 0 \\ 0 & \text{otherwise.} \end{cases}$$



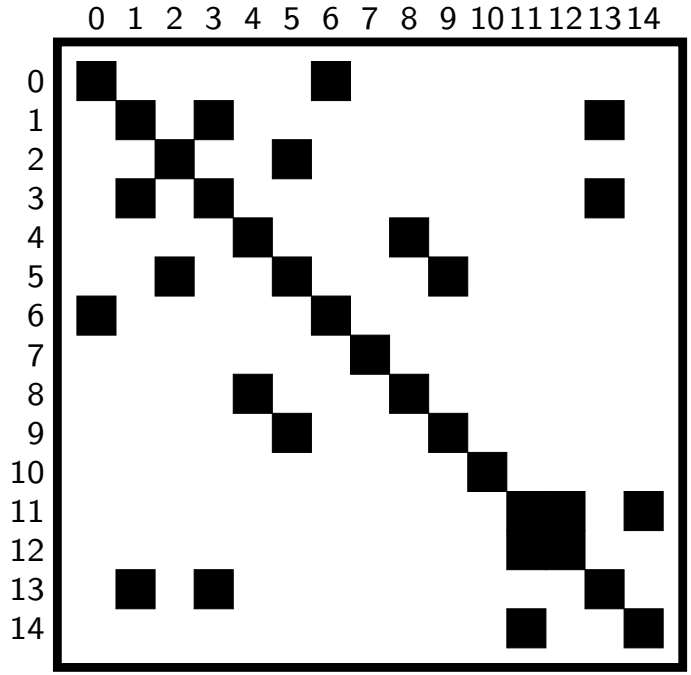
Insight into other applications



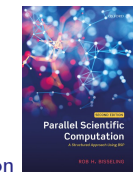
- A molecular dynamics domain of size 1.0×1.0 with 15 particles.
- The cut-off radius for interaction between particles is $r_c = 0.2$. The circles shown have radius $r_c/2 = 0.1$.
- Particles interact if their circles intersect.



Force matrix F represents particle interactions



- Shown is the matrix $F + I$, where F is the sparse 15×15 force matrix corresponding to the particle interactions.
- If particles i and j interact, nonzeros f_{ij} and f_{ji} appear in F.
- Row i of $F + I$ expresses the information needed to compute the next position of particle i in a molecular dynamics simulation: forces $f_{ij} \neq 0$ and the current position and velocity of i.



Summary

- Sparse matrices are the rule, rather than the exception. In many applications, variables are connected to only a few others, leading to sparse matrices.
- Sparse matrices occur in many application areas:
  - transition matrices in Markov models;
  - finite-element matrices in engineering;
  - linear programming matrices in optimization;
  - weblink matrices in Google PageRank computation.
- Sparse matrix–vector multiplication is important for iterative solvers and it is the workhorse of the PageRank computation.
- It can also capture other applications such as molecular dynamics.
- The sequential computation is simple, but its parallelization is a challenge.