

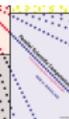
Parallel Sparse Matrix–Vector Multiplication (PSC §4.3)



Option 1: represent first, distribute later

First build a global data structure to represent the sparse matrix, then distribute it over the processors:

- ▶ A parallelising compiler would do this.
- ▶ Requires **global collaboration** between the processors.
- ▶ Simple operations become complicated: in a linked list, 3 processors must work together and communicate to insert a new nonzero.



Option 2: distribute first, represent later

Distribute the matrix first, and then let each processor represent the local nonzeros:

- ▶ This assigns subsets of nonzeros to processors.
- ▶ The subsets form a **partitioning** of the nonzero set: subsets are disjoint and together they contain all nonzeros.
- ▶ Sequential sparse data structures can be used.
- ▶ Simple operations remain **simple**: insertion and deletion are local operations without communication.
- ▶ This is the **preferred approach**.

Most general matrix distribution

- ▶ The most general scheme maps **nonzeros** to processors,

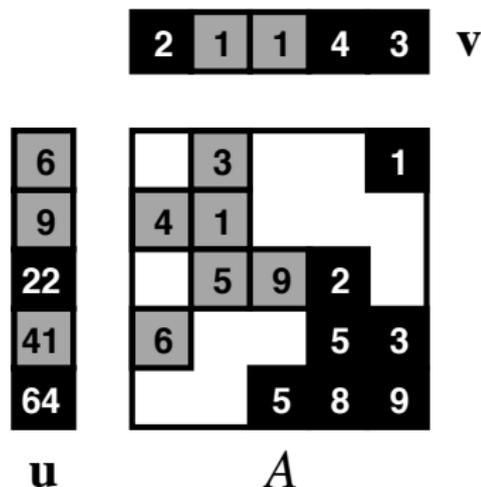
$$a_{ij} \mapsto P(\phi(i,j)), \text{ for } 0 \leq i,j < n \text{ and } a_{ij} \neq 0,$$

where $0 \leq \phi(i,j) < p$.

- ▶ **Zeros** are not assigned to processors. For convenience, we define $\phi(i,j) = -1$ if $a_{ij} = 0$.
- ▶ Here, we use a 1D processor numbering.

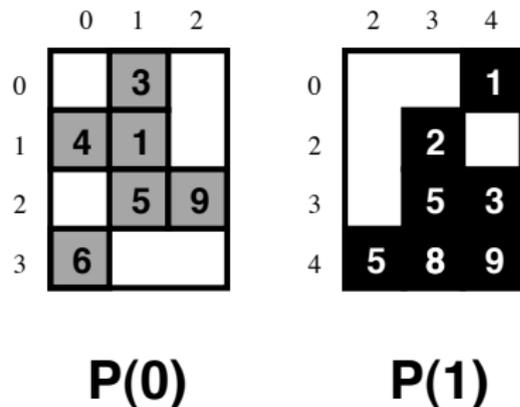
Distribution of matrix and vectors

Global view



(a)

Local view

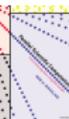


(b)

$p = 2$, $n = 5$, $nz = 13$. $P(0)$ grey cells, $P(1)$ black cells.
Matrix distribution is non-Cartesian.

Where to compute $a_{ij} \cdot v_j$?

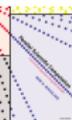
- ▶ Usually, there are many more nonzeros than vector components, $\text{nz}(A) \gg n$, so move the vector components v_j to the nonzeros a_{ij} , not vice versa.
- ▶ Add local products $a_{ij}v_j$ belonging to the same row i . Result on $P(s)$ is the **local contribution** u_{is} to u_i
- ▶ Result u_{is} is sent to the owner of u_i .
- ▶ Thus, we do not communicate elements of A , but only components of \mathbf{v} and contributions to components of \mathbf{u} .



How to distribute the vectors?

- ▶ In many iterative solvers, the same vector is **repeatedly multiplied** by a matrix A .
- ▶ Usually, a few vector operations are interspersed, such as DAXPYs $\mathbf{y} := \alpha \mathbf{x} + \mathbf{y}$ or inner products $\alpha := \mathbf{x}^T \mathbf{y}$.
- ▶ All vectors should then be distributed in the same way: $\text{distr}(\mathbf{u}) = \text{distr}(\mathbf{v})$ for the operation $\mathbf{u} := A\mathbf{v}$.
- ▶ Sometimes, however, we compute $A^T A \mathbf{v}$. The **output vector for A** is then taken as the **input vector for A^T** .
- ▶ Now, we do not need to revert immediately to the input distribution. We allow $\text{distr}(\mathbf{u}) \neq \text{distr}(\mathbf{v})$.
- ▶ We map vector components to processors by

$$u_i \mapsto P(\phi_{\mathbf{u}}(i)), \text{ for } 0 \leq i < n.$$

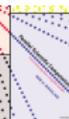


Deriving a parallel algorithm

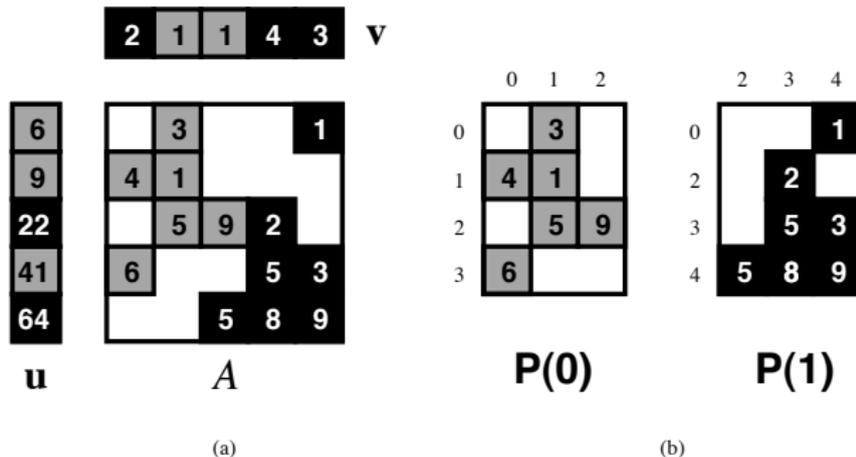
- ▶ Once we have chosen the data distribution and decided to compute the products $a_{ij}v_j$ on the processor that owns a_{ij} , the **parallel algorithm follows naturally**.
- ▶ The main computation for processor $P(s)$ is multiplying each local nonzero element a_{ij} by v_j and adding the result into a local partial sum,

$$u_{is} = \sum_{0 \leq j < n, \phi(i,j)=s} a_{ij}v_j.$$

- ▶ Sparsity is exploited:
 - ▶ only terms with $a_{ij} \neq 0$ are summed;
 - ▶ only local partial sums u_{is} are computed for which $\{j : 0 \leq j < n \wedge \phi(i,j) = s\} \neq \emptyset$.



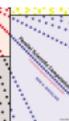
Row index set



- ▶ On $P(0)$, row 4 is empty. On $P(1)$, row 1 is empty.
- ▶ Index set I_s of rows that are locally nonempty in $P(s)$ is

$$I_s = \{i : 0 \leq i < n \wedge (\exists j : 0 \leq j < n \wedge \phi(i, j) = s)\}$$

- ▶ $I_0 = \{0, 1, 2, 3\}$ and $I_1 = \{0, 2, 3, 4\}$.



Local sparse matrix–vector multiplication

$$I_s = \{i : 0 \leq i < n \wedge (\exists j : 0 \leq j < n \wedge \phi(i, j) = s)\}$$

(1) { Local sparse matrix–vector multiplication }

for all $i \in I_s$ **do**

$u_{is} := 0;$

for all $j : 0 \leq j < n \wedge \phi(i, j) = s$ **do**

$u_{is} := u_{is} + a_{ij}v_j;$

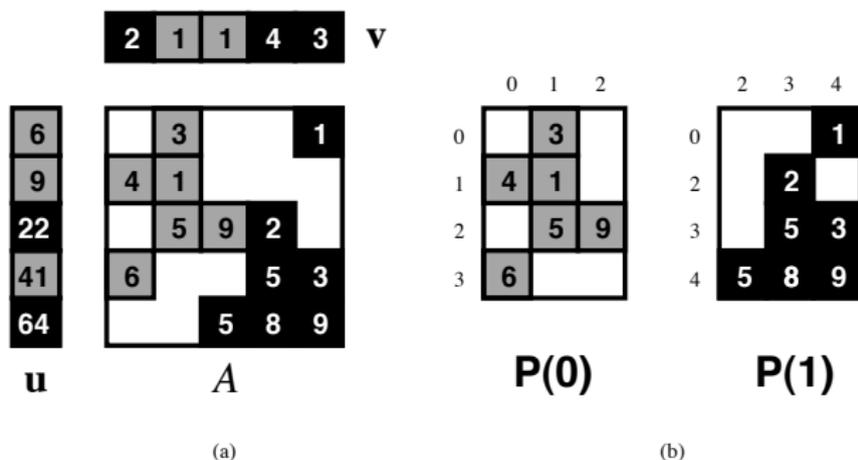
Data structure for local sparse matrix

- ▶ Compressed row storage (CRS) suits row-oriented local matrix–vector multiplication.
- ▶ CRS must be adapted to avoid overhead of many empty rows, which typically occurs if $c \ll p$.
- ▶ We number the nonempty local rows from 0 to $|I_s| - 1$. The corresponding indices i are the **local indices**.
- ▶ The original **global indices** from the set I_s are stored in increasing order in an array *rowindex* of length $|I_s|$:

$$i = \text{rowindex}[i].$$

- ▶ Address of first local nonzero of row i is *start*[i].

Column index set



- ▶ Index set J_s of columns that are locally nonempty in $P(s)$ is

$$J_s = \{j : 0 \leq j < n \wedge (\exists i : 0 \leq i < n \wedge \phi(i, j) = s)\}$$

- ▶ $J_0 = \{0, 1, 2\}$ and $J_1 = \{2, 3, 4\}$.

Fanout

$$J_s = \{j : 0 \leq j < n \wedge (\exists i : 0 \leq i < n \wedge \phi(i, j) = s)\}$$

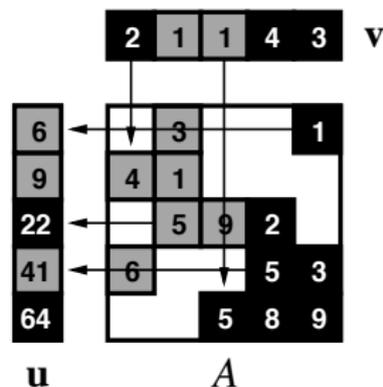
(0) { Fanout }
 for all $j \in J_s$ **do**
 get v_j from $P(\phi_{\mathbf{v}}(j))$;

- ▶ The **receiver knows** (from its index set J_s) that it needs the vector component v_j . The sender is unaware of this. Thus, the receiver initiates the communication by using a 'get'.
- ▶ In **dense algorithms**, communication patterns are predictable and thus known to every processor, so that we only need 'put' primitives.
- ▶ In **sparse algorithms**, we also have to use 'get' primitives.

Fanin and final summation

- (2) { Fanin }
for all $i \in I_s$ **do**
 put u_{iS} in $P(\phi_{\mathbf{u}}(i))$;
- (3) { Summation of nonzero partial sums }
for all $i : 0 \leq i < n \wedge \phi_{\mathbf{u}}(i) = s$ **do**
 $u_i := 0$;
 for all $t : 0 \leq t < p \wedge u_{it} \neq 0$ **do**
 $u_i := u_i + u_{it}$;

Communication



- ▶ **Vertical** arrows: communication of **components** v_j .
- ▶ v_0 is sent from $P(1)$ to $P(0)$, because of the nonzeros $a_{10} = 4$ and $a_{30} = 6$ owned by $P(0)$.
- ▶ v_1, v_3, v_4 need not be sent.
- ▶ **Horizontal** arrows: communication of **partial sums** u_{is} .

Cost analysis

Wat kost het? (Dutch for: How much does it cost?)

- ▶ Answer depends on matrix A and distributions ϕ , $\phi_{\mathbf{v}}$, $\phi_{\mathbf{u}}$.
- ▶ We can obtain an **upper bound on the BSP cost**, assuming:
 - ▶ the matrix nonzeros are evenly spread over the processors, each processor having $\frac{cn}{p}$ nonzeros;
 - ▶ the vector components are also evenly spread, each processor having $\frac{n}{p}$ components.
- ▶ Bound may be **far too pessimistic** for particular distributions that are well-tailored to the matrix.

Cost of separate supersteps

(0): $P(s)$ must receive at most all n components v_j , but not the $\frac{n}{p}$ local components, so that $h_r = n - \frac{n}{p}$. $h_s = \frac{n}{p}(p-1)$, because the $\frac{n}{p}$ local components must be sent to all the other $p-1$ processors.

$$T_{(0)} = \left(1 - \frac{1}{p}\right)ng + l.$$

(1): 2 flops are needed for each local nonzero.

$$T_{(1)} = \frac{2cn}{p} + l.$$

Cost of separate supersteps (cont'd)

(2): Similar to (0).

$$T_{(2)} = \left(1 - \frac{1}{p}\right)ng + l.$$

(3): Each of the $\frac{n}{p}$ local vector components is computed by adding at most p partial sums.

$$T_{(3)} = n + l.$$

Total BSP cost is bounded by

$$T_{MV} \leq \frac{2cn}{p} + n + 2\left(1 - \frac{1}{p}\right)ng + 4l.$$

Efficient computation

$$T_{MV} \leq \frac{2cn}{p} + n + 2\left(1 - \frac{1}{p}\right)ng + 4l.$$

- ▶ Computation is **efficient** if $\frac{2cn}{p} > 2ng$, i.e., $c > pg$. But this happens rarely: **only for very dense matrices**.
- ▶ The number of nonzeros per row c , and not the density d , determines the efficiency directly.
- ▶ To make the computation efficient for smaller c , we can:
 - ▶ use a Cartesian distribution and exploit its **2D** nature;
 - ▶ refine the general distribution using an automatic procedure to detect the **underlying matrix structure**;
 - ▶ exploit properties of **specific matrix classes**, such as random sparse matrices and Laplacian matrices.

Communication volume

- ▶ **Communication volume** V of an algorithm is the total number of data words sent. It depends on ϕ , $\phi_{\mathbf{u}}$, $\phi_{\mathbf{v}}$.
- ▶ For a given ϕ , obtain a **lower bound** V_{ϕ} on V by counting:
 - ▶ the number of processors p_i that have a nonzero a_{ij} in matrix row i ; at least $p_i - 1$ processors must send a contribution u_{is} .
 - ▶ the number of processors q_j that has a nonzero a_{ij} in matrix column j .

$$V_{\phi} = \sum_{0 \leq i < n, p_i \geq 1} (p_i - 1) + \sum_{0 \leq j < n, q_j \geq 1} (q_j - 1).$$

- ▶ An **upper bound** is $V_{\phi} + 2n$, because in the worst case all n components u_i are owned by processors without a nonzero in row i , and similar for the components v_j .

Summary

- ▶ **Distribute first**, represent later.
- ▶ Most general mapping of nonzeros and vector components to processors:

$$a_{ij} \longmapsto P(\phi(i,j)), \text{ for } 0 \leq i,j < n \text{ and } a_{ij} \neq 0,$$

$$u_i \longmapsto P(\phi_{\mathbf{u}}(i)), \text{ for } 0 \leq i < n.$$

- ▶ We have derived a parallel algorithm with 4 supersteps: **fanout**, local matrix–vector multiplication, **fanin**, summation of partial sums.
- ▶ The row index set I_s and column index set J_s are used for exploiting the sparsity in the algorithm.
- ▶ We encountered the first **absolutely necessary** use of a ‘**get**’ primitive.