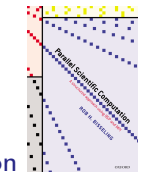
Parallel Sparse Matrix–Vector Multiplication (PSC §4.3)

original slides by Rob Bisseling, Universiteit Utrecht,
accompanying the textbook *Parallel Scientific Computation*

adapted for the lecture *HPC – Algorithms and Applications*,
Michael Bader, TUM, Winter 2016/17



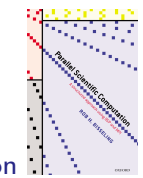
How to build a distributed sparse-matrix data structure

Basically two options:

1. Start with a global data structure for the sparse matrix; then add&distribute elements over the processors
2. (Logically) distribute the matrix first, and then let each processor represent the local nonzeros

Preferred approach: "distribute first"

- 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.



Most general matrix distribution

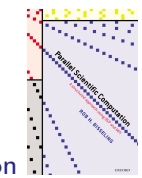
Crucial question for *distribute first approach*:
→ how to define partitioning of the matrix elements?

- The most general scheme maps nonzeros to processors,

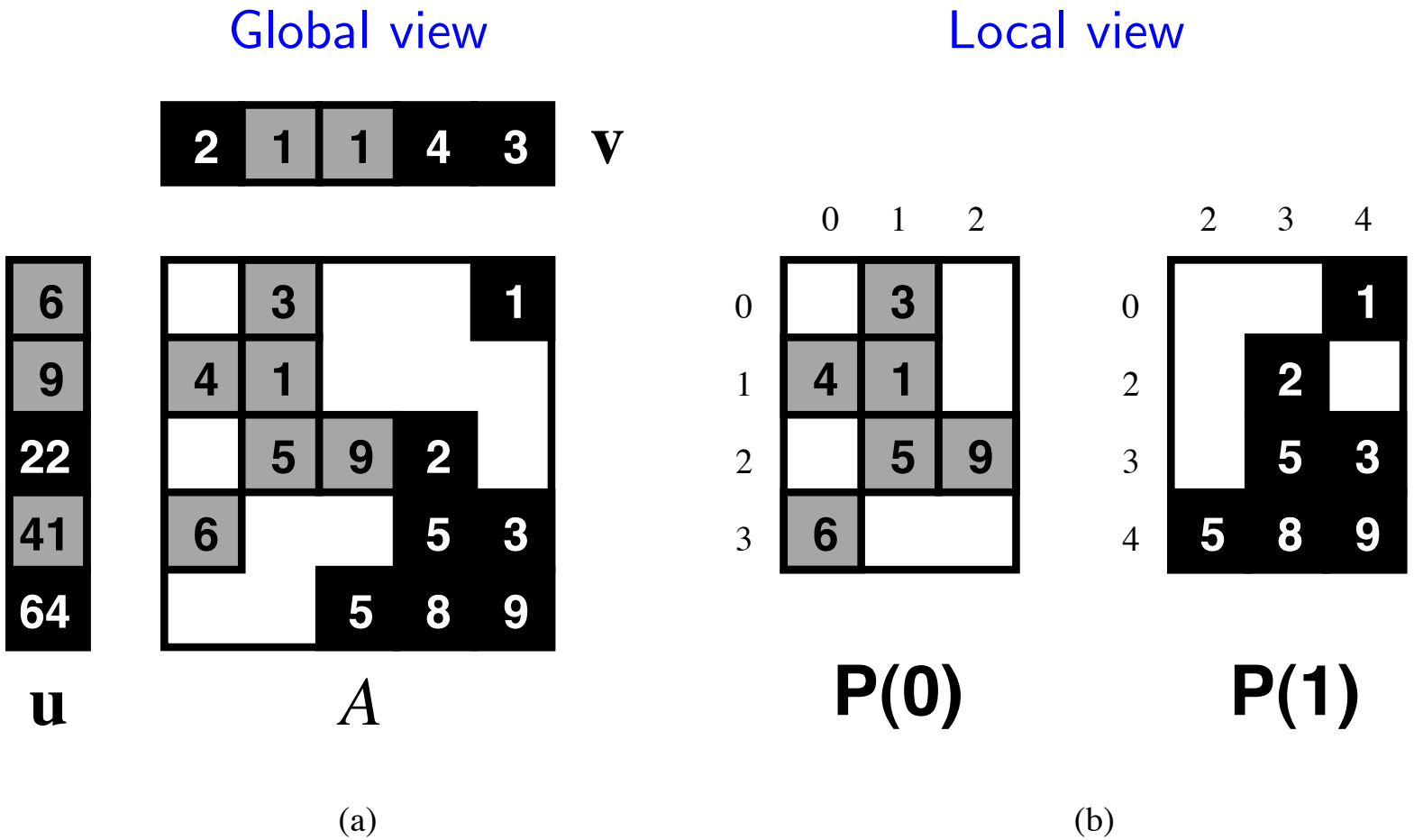
$$a_{ij} \longmapsto P(\phi(i,j)), \text{ for } 0 \leq i,j < n \text{ and } a_{ij} \neq 0,$$

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

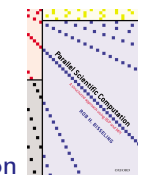
  → *Notation: "a_{ij} is stored on the processor given by $\phi(i,j)$."*
- Zeros are not assigned to processors.
  For convenience, we define $\phi(i,j) = -1$ if $a_{ij} = 0$.
- Here, we use a 1D processor numbering.



Example: Distribution of matrix and vectors

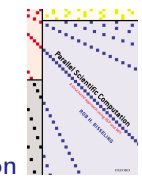


$p = 2$, $n = 5$, $nz = 13$. $P(0)$ grey cells, $P(1)$ black cells.



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

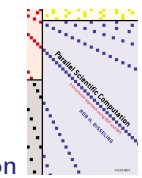
- Usually, there are many more nonzeros than vector components, $nz(A) \gg n$, so move the vector components v_j to the nonzeros a_{ij}, not vice versa.
- Accumulate/Add local products $a_{ij} v_j$ belonging to the same row i.
  Result on $P(s)$ is the local contribution u_{is} to u_i
- Result u_{is} 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 $A^TA\mathbf{v}$. 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

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

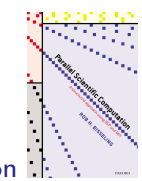


Deriving a parallel algorithm

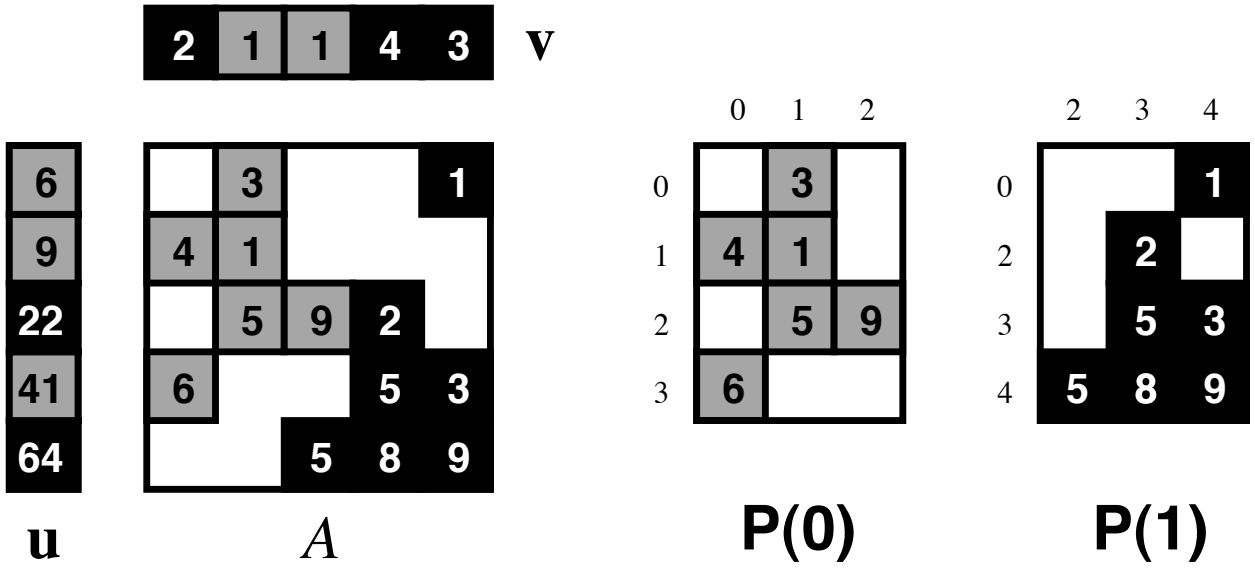
- Once we have chosen the data distribution and decided to compute the products $a_{ij}v_j$ on the processor that owns a_{ij}, the parallel algorithm follows naturally.
- The main computation for processor $P(s)$ is multiplying each local nonzero element a_{ij} by v_j and adding the result into a local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

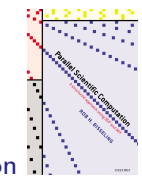
$$I_s = \{i : 0 \leq i < n \wedge (\exists j : 0 \leq j < n \wedge \phi(i,j) = s)\}$$

- $I_0 = \{0,1,2,3\}$ 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**
$u_{is} := u_{is} + a_{ij} v_j;$

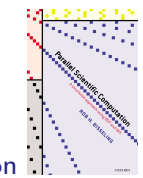


Data structure for local sparse matrix

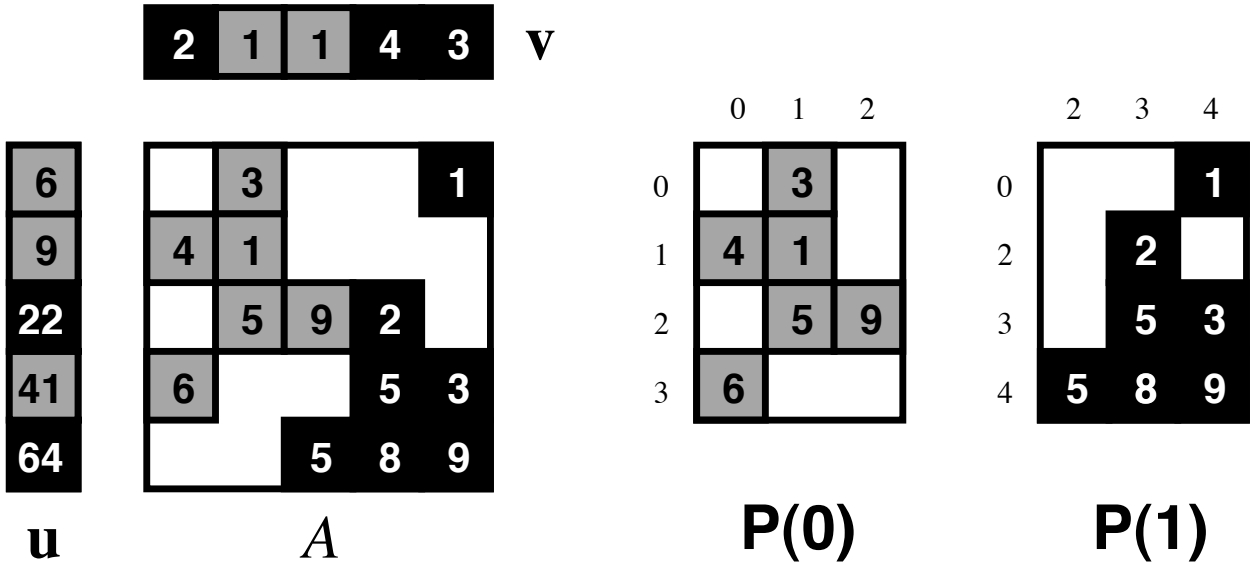
- Compressed row storage (CRS) suits row-oriented local matrix–vector multiplication.
- CRS must be adapted to avoid overhead of many empty rows, which typically occurs if $c \ll p$.
- We number the nonempty local rows from 0 to $|I_s| - 1$. The corresponding indices `i` are the local indices.
- The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

$$i = \mathit{rowindex}[\mathtt{i}].$$

- Address of first local nonzero of row i is $\mathit{start}[\mathtt{i}]$.



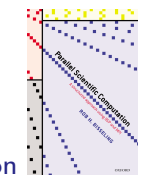
Column index set



- 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 $J_1 = \{2,3,4\}$.

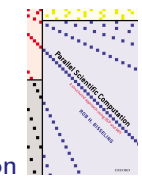


Fanout

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

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

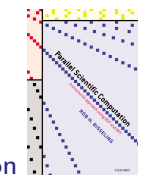
- The receiver knows (from its index set J_s) that it needs the vector component v_j.
- The sender is unaware of this.
- Thus, the receiver needs to initiate the communication
  $\rightarrow$ use 'get' primitive.
- Compare dense algorithms: communication patterns are predictable and thus known to every processor, so that we may use 'get', 'put' or 'send/receive' primitives.



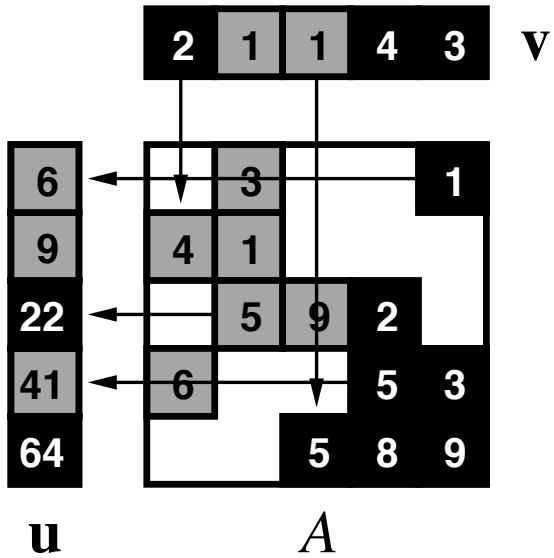
Fanin and final summation

(2) { Fanin }
for all $i \in I_s$ **do**
put u_{is} in $P(\phi_{\mathbf{u}}(i))$;

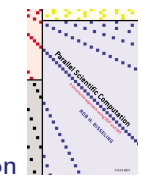
(3) { Summation of nonzero partial sums }
for all $i : 0 \leq i < n \wedge \phi_{\mathbf{u}}(i) = s$ **do**
$u_i := 0$;
for all $t : 0 \leq t < p \wedge u_{it} \neq 0$ **do**
$u_i := u_i + u_{it}$;



Communication



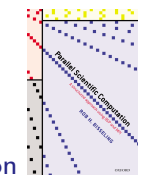
- Vertical arrows: communication of components v_j.
- v_0 is sent from $P(1)$ to $P(0)$, because of the nonzeros $a_{10} = 4$ and $a_{30} = 6$ owned by $P(0)$.
- v_1, v_3, v_4 need not be sent.
- Horizontal arrows: communication of partial sums u_{is}.



Cost analysis

What is the computational/parallel complexity of this algorithm?

- Answer depends on matrix A and distributions $\phi, \phi_{\mathbf{v}}, \phi_{\mathbf{u}}$.
- 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.



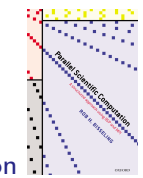
Cost of separate supersteps

(0):
Cost for 'get's: $P(s)$ must receive at most all n components v_j, but not the $\frac{n}{p}$ local components, so that $h_{\mathrm{r}} = n - \frac{n}{p}$.
Cost for remote 'get's that affect $P(s)$: $\frac{n}{p}$ local components must be sent to all the other $p-1$ processors, thus $h_{\mathrm{s}} = \frac{n}{p}(p-1)$.

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

(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).

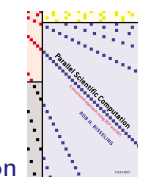
$$T_{(2)} = (1 - \frac{1}{p})ng + l.$$

(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

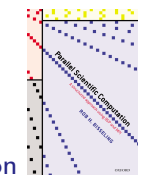
$$T_{\mathrm{MV}} \leq \frac{2cn}{p} + n + 2(1 - \frac{1}{p})ng + 4l.$$



Efficient computation

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

- Computation is efficient if $\frac{2cn}{p} > 2ng$, i.e., $c > pg$.
- But this happens rarely: only for very dense matrices.
- To make the computation efficient for smaller c, we can:
  - use a Cartesian distribution (see later) 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.

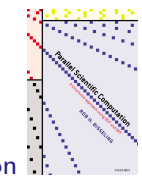


Communication volume

- 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 have a nonzero a_{ij} in matrix column j.

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

- 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:

$$
\begin{aligned}
a_{ij} &\longmapsto P(\phi(i,j)), \text{ for } 0 \leq i,j < n \text{ and } a_{ij} \neq 0, \\
u_i &\longmapsto P(\phi_{\mathbf{u}}(i)), \text{ for } 0 \leq i < n.
\end{aligned}
$$

- 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 an absolutely necessary use of a 'get' primitive.