Dense Matrix Algorithms

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Chapter 8
Topic Overview

- Matrix-Vector Multiplication
- Matrix-Matrix Multiplication
- Solving a System of Linear Equations
Matix Algorithms: Introduction

- Due to their regular structure, parallel computations involving matrices and vectors readily lend themselves to data-decomposition.

- Typical algorithms rely on input, output, or intermediate data decomposition.

- Most algorithms use one- and two-dimensional block, cyclic, and block-cyclic partitionings.
Matrix-Vector Multiplication

- We aim to multiply a dense $n \times n$ matrix $A$ with an $n \times 1$ vector $x$ to yield the $n \times 1$ result vector $y$.
- The serial algorithm requires $n^2$ multiplications and additions.

\[ W = n^2. \]  \hfill (1)
Matrix-Vector Multiplication: Rowwise 1-D Partitioning

- The $n \times n$ matrix is partitioned among $n$ processors, with each processor storing complete row of the matrix.

- The $n \times 1$ vector $x$ is distributed such that each process owns one of its elements.
Matrix-Vector Multiplication: Rowwise 1-D Partitioning

(a) Initial partitioning of the matrix and the starting vector $x$

(b) Distribution of the full vector among all the processes by all-to-all broadcast

(c) Entire vector distributed to each process after the broadcast

(d) Final distribution of the matrix and the result vector $y$

Multiplication of an $n \times n$ matrix with an $n \times 1$ vector using rowwise block 1-D partitioning. For the one-row-per-process case, $p = n$. 
Matrix-Vector Multiplication: Rowwise 1-D Partitioning

- Since each process starts with only one element of $x$, an all-to-all broadcast is required to distribute all the elements to all the processes.

- Process $P_i$ now computes $y[i] = \sum_{j=0}^{n-1} (A[i, j] \times x[j])$.

- The all-to-all broadcast and the computation of $y[i]$ both take time $\Theta(n)$. Therefore, the parallel time is $\Theta(n)$. 
Matrix-Vector Multiplication: Rowwise 1-D Partitioning

• Consider now the case when $p < n$ and we use block 1D partitioning.

• Each process initially stores $n/p$ complete rows of the matrix and a portion of the vector of size $n/p$.

• The all-to-all broadcast takes place among $p$ processes and involves messages of size $n/p$.

• This is followed by $n/p$ local dot products.

• Thus, the parallel run time of this procedure is

$$T_P = \frac{n^2}{p} + t_s \log p + t_w n.$$  \hspace{1cm} (2)

This is cost-optimal.
Matrix-Vector Multiplication: Rowwise 1-D Partitioning

Scalability Analysis:

- We know that $T_o = pT_P - W$, therefore, we have,

  $$T_o = t_sp \log p + t_w np.$$  \hspace{1cm} (3)

- For isoefficiency, we have $W = KT_o$, where $K = E/(1 - E)$ for desired efficiency $E$.

- From this, we have $W = O(p^2)$ (from the $t_w$ term).

- There is also a bound on isoefficiency because of concurrency. In this case, $p < n$, therefore, $W = n^2 = \Omega(p^2)$.

- Overall isoefficiency is $W = O(p^2)$. 
Matrix-Vector Multiplication: 2-D Partitioning

- The $n \times n$ matrix is partitioned among $n^2$ processors such that each processor owns a single element.

- The $n \times 1$ vector $x$ is distributed only in the last column of $n$ processors.
Matrix-Vector Multiplication: 2-D Partitioning

(a) Initial data distribution and communication steps to align the vector along the diagonal

(b) One-to-all broadcast of portions of the vector along process columns

(c) All-to-one reduction of partial results

(d) Final distribution of the result vector

Matrix-vector multiplication with block 2-D partitioning. For the one-element-per-process case, \( p = n^2 \) if the matrix size is \( n \times n \).
Matrix-Vector Multiplication: 2-D Partitioning

- We must first align the vector with the matrix appropriately.

- The first communication step for the 2-D partitioning aligns the vector $x$ along the principal diagonal of the matrix.

- The second step copies the vector elements from each diagonal process to all the processes in the corresponding column using $n$ simultaneous broadcasts among all processors in the column.

- Finally, the result vector is computed by performing an all-to-one reduction along the columns.
Matrix-Vector Multiplication: 2-D Partitioning

- Three basic communication operations are used in this algorithm: one-to-one communication to align the vector along the main diagonal, one-to-all broadcast of each vector element among the $n$ processes of each column, and all-to-one reduction in each row.

- Each of these operations takes $\Theta(\log n)$ time and the parallel time is $\Theta(\log n)$.

- The cost (process-time product) is $\Theta(n^2 \log n)$; hence, the algorithm is not cost-optimal.
Matrix-Vector Multiplication: 2-D Partitioning

- When using fewer than $n^2$ processors, each process owns an $(n/\sqrt{p}) \times (n/\sqrt{p})$ block of the matrix.

- The vector is distributed in portions of $n/\sqrt{p}$ elements in the last process-column only.

- In this case, the message sizes for the alignment, broadcast, and reduction are all $(n/\sqrt{p})$.

- The computation is a product of an $(n/\sqrt{p}) \times (n/\sqrt{p})$ submatrix with a vector of length $(n/\sqrt{p})$.
Matrix-Vector Multiplication: 2-D Partitioning

- The first alignment step takes time $t_s + t_w n / \sqrt{p}$.
- The broadcast and reductions take time $(t_s + t_w n / \sqrt{p}) \log(\sqrt{p})$.
- Local matrix-vector products take time $t_c n^2 / p$.
- Total time is

$$T_P \approx \frac{n^2}{p} + t_s \log p + t_w \frac{n}{\sqrt{p}} \log p$$

(4)
Matrix-Vector Multiplication: 2-D Partitioning

Scalability Analysis:

- $T_o = pT_p - W = t_s p \log p + t_w n \sqrt{p} \log p$.

- Equating $T_o$ with $W$, term by term, for isoeficiency, we have, $W = K^2 t_w^2 p \log^2 p$ as the dominant term.

- The isoeficiency due to concurrency is $O(p)$.

- The overall isoeficiency is $O(p \log^2 p)$ (due to the network bandwidth).

- For cost optimality, we have, $W = n^2 = p \log^2 p$. For this, we have, $p = O\left(\frac{n^2}{\log^2 n}\right).$
Matrix-Matrix Multiplication

- Consider the problem of multiplying two $n \times n$ dense, square matrices $A$ and $B$ to yield the product matrix $C = A \times B$.

- The serial complexity is $O(n^3)$.

- We do not consider better serial algorithms (Strassen’s method), although, these can be used as serial kernels in the parallel algorithms.

- A useful concept in this case is called block operations. In this view, an $n \times n$ matrix $A$ can be regarded as a $q \times q$ array of blocks $A_{i,j}$ ($0 \leq i, j < q$) such that each block is an $(n/q) \times (n/q)$ submatrix.

- In this view, we perform $q^3$ matrix multiplications, each involving $(n/q) \times (n/q)$ matrices.
Matrix-Matrix Multiplication

- Consider two $n \times n$ matrices $A$ and $B$ partitioned into $p$ blocks $A_{i,j}$ and $B_{i,j}$ ($0 \leq i, j < \sqrt{p}$) of size $(n/\sqrt{p}) \times (n/\sqrt{p})$ each.

- Process $P_{i,j}$ initially stores $A_{i,j}$ and $B_{i,j}$ and computes block $C_{i,j}$ of the result matrix.

- Computing submatrix $C_{i,j}$ requires all submatrices $A_{i,k}$ and $B_{k,j}$ for $0 \leq k < \sqrt{p}$.

- All-to-all broadcast blocks of $A$ along rows and $B$ along columns.

- Perform local submatrix multiplication.
Matrix-Matrix Multiplication

- The two broadcasts take time $2(t_s \log(\sqrt{p}) + t_w (n^2/p)(\sqrt{p} - 1))$.

- The computation requires $\sqrt{p}$ multiplications of $(n/\sqrt{p}) \times (n/\sqrt{p})$ sized submatrices.

- The parallel run time is approximately

  $$T_P = \frac{n^3}{p} + t_s \log p + 2t_w \frac{n^2}{\sqrt{p}}. \quad (5)$$

- The algorithm is cost optimal and the isoefciency is $O(p^{1.5})$ due to bandwidth term $t_w$ and concurrency.

- Major drawback of the algorithm is that it is not memory optimal.
Matrix-Matrix Multiplication: Cannon’s Algorithm

- In this algorithm, we schedule the computations of the $\sqrt{p}$ processes of the $i$th row such that, at any given time, each process is using a different block $A_{i,k}$.

- These blocks can be systematically rotated among the processes after every submatrix multiplication so that every process gets a fresh $A_{i,k}$ after each rotation.
Matrix-Matrix Multiplication: Cannon’s Algorithm

(a) Initial alignment of A

(b) Initial alignment of B

(c) A and B after initial alignment

(d) Submatrix locations after first shift

(e) Submatrix locations after second shift

(f) Submatrix locations after third shift

communication steps in Cannon’s algorithm on 16 processes.
Matrix-Matrix Multiplication: Cannon’s Algorithm

- Align the blocks of $A$ and $B$ in such a way that each process multiplies its local submatrices. This is done by shifting all submatrices $A_{i,j}$ to the left (with wraparound) by $i$ steps and all submatrices $B_{i,j}$ up (with wraparound) by $j$ steps.

- Perform local block multiplication.

- Each block of $A$ moves one step left and each block of $B$ moves one step up (again with wraparound).

- Perform next block multiplication, add to partial result, repeat until all $\sqrt{p}$ blocks have been multiplied.
Matrix-Matrix Multiplication: Cannon’s Algorithm

- In the alignment step, since the maximum distance over which a block shifts is $\sqrt{p} - 1$, the two shift operations require a total of $2(t_s + t_w n^2 / p)$ time.

- Each of the $\sqrt{p}$ single-step shifts in the compute-and-shift phase of the algorithm takes $t_s + t_w n^2 / p$ time.

- The computation time for multiplying $\sqrt{p}$ matrices of size $(n/\sqrt{p}) \times (n/\sqrt{p})$ is $n^3 / p$.

- The parallel time is approximately:

$$T_P = \frac{n^3}{p} + 2\sqrt{p} t_s + 2t_w \frac{n^2}{\sqrt{p}}. \quad (6)$$

- The cost-efficiency and isoefficiency of the algorithm are identical to the first algorithm, except, this is memory optimal.
Matrix-Matrix Multiplication: DNS Algorithm

- Uses a 3-D partitioning.

- Visualize the matrix multiplication algorithm as a cube – matrices $A$ and $B$ come in two orthogonal faces and result $C$ comes out the other orthogonal face.

- Each internal node in the cube represents a single add-multiply operation (and thus the complexity).

- DNS algorithm partitions this cube using a 3-D block scheme.
Matrix-Matrix Multiplication: DNS Algorithm

- Assume an $n \times n \times n$ mesh of processors.

- Move the columns of $A$ and rows of $B$ and perform broadcast.

- Each processor computes a single add-multiply.

- This is followed by an accumulation along the $C$ dimension.

- Since each add-multiply takes constant time and accumulation and broadcast takes $\log n$ time, the total runtime is $\log n$.

- This is not cost optimal. It can be made cost optimal by using $n/\log n$ processors along the direction of accumulation.
Matrix-Matrix Multiplication: DNS Algorithm

The communication steps in the DNS algorithm while multiplying 4 × 4 matrices $A$ and $B$ on 64 processes.
Matrix-Matrix Multiplication: DNS Algorithm

Using fewer than $n^3$ processors.

- Assume that the number of processes $p$ is equal to $q^3$ for some $q < n$.

- The two matrices are partitioned into blocks of size $(n/q) \times (n/q)$. Each matrix can thus be regarded as a $q \times q$ two-dimensional square array of blocks.

- The algorithm follows from the previous one, except, in this case, we operate on blocks rather than on individual elements.
Matrix-Matrix Multiplication: DNS Algorithm

Using fewer than $n^3$ processors.

- The first one-to-one communication step is performed for both $A$ and $B$, and takes $t_s + t_w(n/q)^2$ time for each matrix.

- The two one-to-all broadcasts take $2(t_s \log q + t_w(n/q)^2 \log q)$ time for each matrix.

- The reduction takes time $t_s \log q + t_w(n/q)^2 \log q$.

- Multiplication of $(n/q) \times (n/q)$ submatrices takes $(n/q)^3$ time.

- The parallel time is approximated by:

$$T_P = \frac{n^3}{p} + t_s \log p + t_w \frac{n^2}{p^{2/3}} \log p. \quad (7)$$

The isoefficiency function is $\Theta(p(\log p)^3)$. 
Solving a System of Linear Equations

Consider the problem of solving linear equations of the kind:

\[ \begin{align*}
    a_{0,0}x_0 & + a_{0,1}x_1 & + \cdots & + a_{0,n-1}x_{n-1} & = b_0, \\
    a_{1,0}x_0 & + a_{1,1}x_1 & + \cdots & + a_{1,n-1}x_{n-1} & = b_1, \\
    & \vdots & & \vdots & \vdots \\
    a_{n-1,0}x_0 & + a_{n-1,1}x_1 & + \cdots & + a_{n-1,n-1}x_{n-1} & = b_{n-1}.
\end{align*} \]

This is written as \( Ax = b \), where \( A \) is an \( n \times n \) matrix with \( A[i, j] = a_{i,j} \), \( b \) is an \( n \times 1 \) vector \([b_0, b_1, \ldots, b_{n-1}]^T\), and \( x \) is the solution.
Solving a System of Linear Equations

Two steps in solution are: reduction to triangular form, and back-substitution. The triangular form is as:

\[ \begin{align*}
    x_0 + u_{0,1}x_1 + u_{0,2}x_2 + \cdots + u_{0,n-1}x_{n-1} &= y_0, \\
    x_1 + u_{1,2}x_2 + \cdots + u_{1,n-1}x_{n-1} &= y_1, \\
    \vdots & \quad \vdots \\
    x_{n-1} &= y_{n-1}.
\end{align*} \]

We write this as: \( Ux = y. \)

A commonly used method for transforming a given matrix into an upper-triangular matrix is Gaussian Elimination.
Gaussian Elimination

procedure GAUSSIAN_ELIMINATION (A, b, y)
begin
for $k := 0$ to $n - 1$ do /* Outer loop */
begin
for $j := k + 1$ to $n - 1$ do

y$[k] := b[k] / A[k, k];$
$A[k, k] := 1;$

for $i := k + 1$ to $n - 1$ do
begin
for $j := k + 1$ to $n - 1$ do

b$[i] := b[i] - A[i, k] \times y[k];$
$A[i, k] := 0;$
endfor; /* Line 9 */
endfor; /* Line 3 */
end GAUSSIAN_ELIMINATION
The computation has three nested loops – in the $k$th iteration of the outer loop, the algorithm performs $(n - k)^2$ computations. Summing from $k = 1..n$, we have roughly $(n^3 / 3)$ multiplications-subtractions.

A typical computation in Gaussian elimination.
Parallel Gaussian Elimination

- Assume $p = n$ with each row assigned to a processor.

- The first step of the algorithm normalizes the row. This is a serial operation and takes time $(n - k)$ in the $k$th iteration.

- In the second step, the normalized row is broadcast to all the processors. This takes time $(t_s + t_w(n - k - 1)) \log n$.

- Each processor can independently eliminate this row from its own. This requires $(n - k - 1)$ multiplications and subtractions.

- The total parallel time can be computed by summing from $k = 1..n - 1$ as

$$T_P = \frac{3}{2} n(n - 1) + t_s n \log n + \frac{1}{2} t_w n(n - 1) \log n. \quad (8)$$

- The formulation is not cost optimal because of the $t_w$ term.
### Parallel Gaussian Elimination

#### (a) Computation:

(i) \( A[k,j] := A[k,j]/A[k,k] \) for \( k < j < n \)

(ii) \( A[k,k] := 1 \)

#### (b) Communication:

One-to-all broadcast of row \( A[k,*] \)

#### (c) Computation:

(i) \( A[i,j] := A[i,j] - A[i,k] \times A[k,j] \) for \( k < i < n \) and \( k < j < n \)

(ii) \( A[i,k] := 0 \) for \( k < i < n \)

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Gaussian elimination steps during the iteration corresponding to \( k = 3 \) for an \( 8 \times 8 \) matrix partitioned rowwise among eight processes.
Parallel Gaussian Elimination: Pipelined Execution

- In the previous formulation, the \((k+1)\)st iteration starts only after all the computation and communication for the \(k\)th iteration is complete.

- In the pipelined version, there are three steps – normalization of a row, communication, and elimination. These steps are performed in an asynchronous fashion.

- A processor \(P_k\) waits to receive and eliminate all rows prior to \(k\). Once it has done this, it forwards its own row to processor \(P_{k+1}\).
Parallel Gaussian Elimination: Pipelined Execution

Pipelined Gaussian elimination on a $5 \times 5$ matrix partitioned with one row per process.
Parallel Gaussian Elimination: Pipelined Execution

- The total number of steps in the entire pipelined procedure is $\Theta(n)$.

- In any step, either $O(n)$ elements are communicated between directly-connected processes, or a division step is performed on $O(n)$ elements of a row, or an elimination step is performed on $O(n)$ elements of a row.

- The parallel time is therefore $O(n^2)$.

- This is cost optimal.
Parallel Gaussian Elimination: Pipelined Execution

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The communication in the Gaussian elimination iteration corresponding to $k = 3$ for an $8 \times 8$ matrix distributed among four processes using block 1-D partitioning.
Parallel Gaussian Elimination: Block 1D with $p < n$

- The above algorithm can be easily adapted to the case when $p < n$.

- In the $k$th iteration, a processor with all rows belonging to the active part of the matrix performs $(n - k - 1)n/p$ multiplications and subtractions.

- In the pipelined version, for $n > p$, computation dominates communication.

- The parallel time is given by: $2(n/p)\sum_{k=0}^{n-1}(n - k - 1)$, or approximately, $n^3/p$.

- While the algorithm is cost optimal, the cost of the parallel algorithm is higher than the sequential run time by a factor of $3/2$. 
Parallel Gaussian Elimination: Block 1D with $p < n$

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(a) Block 1-D mapping

(b) Cyclic 1-D mapping

Computation load on different processes in block and cyclic 1-D partitioning of an $8 \times 8$ matrix on four processes during the Gaussian elimination iteration corresponding to $k = 3$. 
Parallel Gaussian Elimination: Cyclic 1D Mapping

- The load imbalance problem can be alleviated by using a cyclic mapping.

- In this case, other than processing of the last \( p \) rows, there is no load imbalance.

- This corresponds to a cumulative load imbalance overhead of \( O(n^2 p) \) (instead of \( O(n^3) \) in the previous case).
Parallel Gaussian Elimination: 2-D Mapping

• Assume an $n \times n$ matrix $A$ mapped onto an $n \times n$ mesh of processors.

• Each update of the partial matrix can be thought of as a scaled rank-one update (scaling by the pivot element).

• In the first step, the pivot is broadcast to the row of processors.

• In the second step, each processor locally updates its value. For this it needs the corresponding value from the pivot row, and the scaling value from its own row.

• This requires two broadcasts, each of which takes $\log n$ time.

• This results in a non-cost-optimal algorithm.
Parallel Gaussian Elimination: 2-D Mapping

Various steps in the Gaussian elimination iteration corresponding to $k = 3$ for an $8 \times 8$ matrix on 64 processes arranged in a logical two-dimensional mesh.
Parallel Gaussian Elimination: 2-D Mapping with Pipelining

- We pipeline along two dimensions. First, the pivot value is pipelined along the row. Then the scaled pivot row is pipelined down.


- The computation and communication for each iteration moves through the mesh from top-left to bottom-right as a “front.”

- After the front corresponding to a certain iteration passes through a process, the process is free to perform subsequent iterations.

- Multiple fronts that correspond to different iterations are active simultaneously.
Parallel Gaussian Elimination: 2-D Mapping with Pipelining

- If each step (division, elimination, or communication) is assumed to take constant time, the front moves a single step in this time. The front takes $\Theta(n)$ time to reach $P_{n-1,n-1}$.

- Once the front has progressed past a diagonal processor, the next front can be initiated. In this way, the last front passes the bottom-right corner of the matrix $\Theta(n)$ steps after the first one.

- The parallel time is therefore $O(n)$, which is cost-optimal.
2-D Mapping with Pipelining

Pipelined Gaussian elimination for a $5 \times 5$ matrix with 25 processors.
Parallel Gaussian Elimination: 2-D Mapping with Pipelining and $p < n$

- In this case, a processor containing a completely active part of the matrix performs $n^2/p$ multiplications and subtractions, and communicates $n/\sqrt{p}$ words along its row and its column.

- The computation dominantes communication for $n >> p$.

- The total parallel run time of this algorithm is $(2n^2/p) \times n$, since there are $n$ iterations. This is equal to $2n^3/p$.

- This is three times the serial operation count!
## Parallel Gaussian Elimination: 2-D Mapping with Pipelining and $p < n$

The communication steps in the Gaussian elimination iteration corresponding to $k = 3$ for an $8 \times 8$ matrix on 16 processes of a two-dimensional mesh.
Parallel Gaussian Elimination: 2-D Mapping with Pipelining and \( p < n \)

(a) Block-checkerboard mapping

(b) Cyclic-checkerboard mapping

Computational load on different processes in block and cyclic 2-D mappings of an \( 8 \times 8 \) matrix onto 16 processes during the Gaussian elimination iteration corresponding to \( k = 3 \).
Parallel Gaussian Elimination: 2-D Cyclic Mapping

- The idling in the block mapping can be alleviated using a cyclic mapping.

- The maximum difference in computational load between any two processes in any iteration is that of one row and one column update.

- This contributes $\Theta(n\sqrt{p})$ to the overhead function. Since there are $n$ iterations, the total overhead is $\Theta(n^2 \sqrt{p})$. 

Gaussian Elimination with Partial Pivoting

- For numerical stability, one generally uses partial pivoting.

- In the $k$th iteration, we select a column $i$ (called the pivot column) such that $A[k, i]$ is the largest in magnitude among all $A[k, j]$ such that $k \leq j < n$.

- The $k$th and the $i$th columns are interchanged.

- Simple to implement with row-partitioning and does not add overhead since the division step takes the same time as computing the max.

- Column-partitioning, however, requires a global reduction, adding a $\log p$ term to the overhead.

- Pivoting precludes the use of pipelining.
Gaussian Elimination with Partial Pivoting: 2-D Partitioning

- Partial pivoting restricts use of pipelining, resulting in performance loss.

- This loss can be alleviated by restricting pivoting to specific columns.

- Alternately, we can use faster algorithms for broadcast.
Solving a Triangular System: Back-Substitution

- The upper triangular matrix $U$ undergoes back-substitution to determine the vector $x$.

    1. procedure BACK_SUBSTITUTION ($U$, $x$, $y$)
    2. begin
    3.    for $k := n - 1$ downto 0 do /* Main loop */
    4.        begin
    5.            $x[k] := y[k]$;
    6.            for $i := k - 1$ downto 0 do
    7.                $y[i] := y[i] - x[k] \times U[i, k]$;
    8.        endfor;
    9.    end BACK_SUBSTITUTION

A serial algorithm for back-substitution.
Solving a Triangular System: Back-Substitution

- The algorithm performs approximately $n^2/2$ multiplications and subtractions.

- Since complexity of this part is asymptotically lower, we should optimize the data distribution for the factorization part.

- Consider a rowwise block 1-D mapping of the $n \times n$ matrix $U$ with vector $y$ distributed uniformly.

- The value of the variable solved at a step can be pipelined back.

- Each step of a pipelined implementation requires a constant amount of time for communication and $\Theta(n/p)$ time for computation.

- The parallel run time of the entire algorithm is $\Theta(n^2/p)$. 
Solving a Triangular System: Back-Substitution

- If the matrix is partitioned by using 2-D partitioning on a $\sqrt{p} \times \sqrt{p}$ logical mesh of processes, and the elements of the vector are distributed along one of the columns of the process mesh, then only the $\sqrt{p}$ processes containing the vector perform any computation.

- Using pipelining to communicate the appropriate elements of $U$ to the process containing the corresponding elements of $y$ for the substitution step (line 7), the algorithm can be executed in $\Theta(n^2/\sqrt{p})$ time.

- While this is not cost optimal, since this does not dominate the overall computation, the cost optimality is determined by the factorization.