Matrix-Vector Multiplication

Multiplying a square matrix by a vector

Sequential algorithm

• Simply a series of dot products

- Inner loop requires n multiplications and n-1 additions
- Complexity of inner loop is $\Theta(n)$
- There are a total of m dot products
- Overall complexity: $\Theta(mn)$; $\Theta(n^2)$ for a square matrix

Data decomposition options

- Domain decomposition strategy
- Three options for decomposition
 - 1. Rowwise block striping
 - Divide matrix elements into group of rows (same as Floyd's algorithm)
 - Each process responsible for a contiguous group of either $\lfloor m/p \rfloor$ or $\lceil m/p \rceil$ rows
 - 2. Columnwise block striping
 - Divide matrix elements into group of columns
 - Each process responsible for a contiguous group of either $\lfloor n/p \rfloor$ or $\lceil n/p \rceil$ columns
 - 3. Checkerboard block decomposition
 - Form a virtual grid
 - Matrix is divided into 2D blocks aligning with the grid
 - Let the grid have r rows and c columns
 - Each process responsible for a block of matrix containing at most $\lceil m/r \rceil$ rows and $\lceil n/c \rceil$ columns
- Storing vectors vec and out
 - Divide vector elements among processes
 - * Each process is responsible for a contiguous group of either $\lfloor n/p \rfloor$ or $\lceil n/p \rceil$ elements
 - Replicate vector elements
 - * Vector replication acceptable because vectors have only n elements compared to n^2 elements in matrices
 - * A task storing a row or column of matrix and single element from either vector is responsible for $\Theta(n)$ elements
 - * And a task storing rows and columns of the matrix and all elements of the vectors is still responsible for $\Theta(n)$

• Six possible combinations: three ways to store matrices and two ways to store vectors

Rowwise block-striped decomposition

- Partitioning through domain decomposition
- · Primitive task associated with
 - Row of matrix
 - Entire vector
- Task i has row i of mat and the entire vector vec
- Each primitive task computes the inner product of an entire row with vec and assigns the result to one element of out
- Vector out replicated with an all-gather communication
- Mapping strategy decision tree
 - Agglomerate primitive tasks associated with contiguous groups of rows and assign each of these combined tasks to a single PE
 - Each PE computes a single element (or a block of elements in case of rowwise block striped matrix) of the result vector
- Assume m = n
 - Sequential matrix-vector multiplication time complexity is $\Theta(n^2)$
 - For parallel algorithm, each process multiplies its portion of the matrix by the vector
 - No process is responsible for more than $\lceil n/p \rceil$ rows
 - Complexity of multiplication portion is $\Theta(n^2/p)$
 - In an efficient all-gather communication, each PE sends $\lceil \log p \rceil$ messages, total number of elements passed is n(p-1)/p when p is a power of 2
 - Communication complexity: $\Theta(\log p + n)$
 - Overall complexity of parallel matrix-vector multiplication algorithm

$$\Theta(n^2/p + n + \log p)$$

- Isoefficiency of the parallel algorithm
 - * Time complexity of sequential algorithm: $\Theta(n^2)$
 - * Only overhead in parallel algorithm due to all-gather
 - * For reasonably large n, message transmission time is greater than message latency
 - * Simplify communication complexity to $\Theta(n)$
 - * Isoefficiency function given by

$$n^2 > Cpn \Rightarrow n > Cp$$

- * Memory utilization function: $M(n) = n^2$
- * Scalability function of parallel algorithm

$$\begin{array}{rcl} M(Cp)/p & = & C^2p^2/p \\ & = & C^2p \end{array}$$

- * Memory utilization must grow linearly with the number of PEs
- * Algorithm is not highly scalable

- Processes must concatenate their pieces of the vector into a complete vector
- Function MPI_Allgatherv
 - Gather data from all tasks and deliver the combined data to all tasks
 - If the number of items to be gathered from each process is the same, a simpler function MPI_Allgather may be used

```
int MPI_Allgatherv ( void * send_bufr, int send_count, MPI_Datatype send_type,
    void * recv_bufr, int * recv_count, int * recv_disp,
    MPI_Datatype recv_type, MPI_Comm comm );
```

send_bufr Starting address of send buffer

send_count Number of elements in send buffer

send_type Data type of send buffer elements

recv_buffr The only output parameter; Starting address of receive buffer to store the gathered elements

recv_count Integer array containing the number of elements to be received from each process

recv_disp Integer array to specify the displacement relative to recv_bufr at which to place the incoming data from processes

recv_type Data type of receive buffer elements

comm Communicator

- The block of data sent by ith process is received at every process and placed in the ith block of recv_bufr
- Replicated vector I/O
 - Assume binary file for input
 - Process p-1 opens the file to read; read n and transmits it to other processes
 - Each process allocates memory to store vector
 - Process p-1 reads the vector and broadcasts it to other processes
 - Replicated vector printed by a single process; each process has a copy of the vector
- Program code
- Benchmarking
 - Sequantial algorithm complexity: $\Theta(n^2)$
 - Time needed to compute a single iteration of the loop performing inner product given by χ
 - χ determined by dividing execution time of sequential algorithm by n^2
 - Expected time for computational portion of parallel program: $\chi n \lceil n/p \rceil$
 - All-gather reduction requires each process to send $\lceil \log p \rceil$ messages
 - * Latency of each message: λ
 - * Total number of vector elements transmitted: $n(2^{\lceil \log p \rceil} 1)/2^{\lceil \log p \rceil}$
 - * Each vector element a double occupying 8 bytes
 - * Expected execution time for all-gather step

$$\lambda \lceil \log p \rceil + 8n \frac{2^{\lceil \log p \rceil} - 1}{2^{\lceil \log p \rceil} \beta}$$

Columnwise block-striped decomposition

• Design and analysis

- Assume that each primitive task i has column i of matrix and element i of input and output vectors
- Each task i multiplies its matrix column by corresponding element of vector, giving a vector of partial results

$c_0 =$	$a_{0,0}b_0$ +	$a_{0,1}b_1$ +	$a_{0,2}b_2$ +	$a_{0,3}b_3$ +	$a_{0,4}b_4$
$c_1 =$	$a_{1,0}b_0$ +	$a_{1,1}b_1 +$	$a_{1,2}b_2$ +	$a_{1,3}b_3 +$	$a_{1,4}b_4$
$c_2 =$	$a_{2,0}b_0$ +	$a_{2,1}b_1 +$	$a_{2,2}b_2$ +	$a_{2,3}b_3 +$	$a_{2,4}b_4$
$c_3 =$	$a_{3,0}b_0$ +	$a_{3,1}b_1 +$	$a_{3,2}b_2$ +	$a_{3,3}b_3 +$	$a_{3,4}b_4$
$c_4 =$	$a_{4,0}b_0$ +	$a_{4,1}b_1$ +	$a_{4,2}b_2$ +	$a_{4,3}b_3 +$	$a_{4,4}b_4$
	Proc 0	Proc 1	Proc 2	Proc 3	Proc 4

- At the end of computation, each task needs only a single element of resultant vector c_i
- Need an all-to-all communication
 - * Every task has the n partial results needed to add to produce final result
 - * Partial result element j on task i must be transferred to task j
- Agglomeration and mapping
 - * Static number of tasks
 - * Regular communication pattern (all-to-all)
 - · Every primitive task has identical computation and communication requirements
 - · Agglomerating them into larger task with the same number of columns will help us balance the workload
 - * Computation time per task is constant
 - * Strategy
 - · Agglomerate groups of columns (primitive tasks) into metatasks
 - · Create one task per MPI process
- Complexity analysis
 - * Sequential algorithm complexity: $\Theta(n^2)$
 - * Assume square matrix (m = n)
 - * Each process multiplies its portion of matrix by its block of vector
 - · No process responsible for more than $\lceil n/p \rceil$ columns of matrix or elements of vector
 - · Time complexity of initial multiplication phase: $\Theta(n(n/p)) = \Theta(n^2/p)$
 - * p partial vectors, each of length at most $\lceil n/p \rceil$
 - * Time complexity to sum the partial vectors: $\Theta(n)$
 - * Overall computational complexity of parallel algorithm: $\Theta(n^2/p)$
 - * Number of steps for all-to-all exchange: $\lceil \log p \rceil$, using hypercube communication pattern
 - · In each step, a process sends n/2 values and receives n/2 values
 - · Total number of elements sent and received: $n \lceil \log p \rceil$
 - · Communication complexity of all-gather: $\Theta(n \log p)$
 - * Overall complexity: $\Theta(n^2/p + n \log p)$
- Isoefficiency analysis
 - * Sequential time complexity: $\Theta(n^2)$
 - * Parallel overhead limited to all-to-all operation
 - \cdot When n is large, message transmission time dominates message latency
 - · Use an approach where a process sends a message to each of the other p-1 processes
 - · Each message contains just the elements the destination is supposed to receive from the source
 - · Total number of messages is p-1 but each process passes $\leq n$ elements
 - · Parallel communication time: $\Theta(n)$
 - * Isoefficiency function: $n^2 \ge Cpn \implies n \ge Cp$
 - * Scalability function: C^2p

- · Not highly scalabale because in order to maintain a constant efficiency, memory used per processor must increase linearly with the number of processors
- Reading a columnwise block-striped matrix
 - Read a matrix stored in row-major order and distribute it among processes in columnwise block-striped fashion
 - Matrix elements not stored as a contiguous group in the file
 - * Each row of matrix must be scattered among all processes
 - Single process responsible for I/O
 - * Read a row of matrix into temporary buffer
 - * Scatter the elements of buffer among processes
- Function MPI Scatterv
 - Scatter a buffer in parts to all processes in a communicator

```
int MPI Scattery ( void * send bufr, int * send count, int * send disp,
                   MPI_Datatype send_type, void * recv_bufr, int recv_count,
                   MPI_Datatype recv_type, int root, MPI_COMM comm );
```

send_bufr Starting address of send buffer; significant only at root

send_count Number of elements in send buffer

send_disp Integer array to specify the displacement; relative to send_bufr from which to take the outgoing data; entry i in array corresponds to data going to process i

send_type Data type of send buffer elements

recv_bufr Starting address of receive buffer to store the process's portion of elements received

recv_count Integer array containing the number of elements to be received

recv_type Data type of receive buffer elements

root Rank of sending process

comm Communicator

- Collective communication function
 - * All processes in communicator participate in its execution
 - * Function requires each process to have previously initialized two arrays
 - 1. Array to indicate the number to send to each process
 - 2. Array to indicate displacement of block of elements being sent
- Printing a columnwise block-striped matrix
 - Data motion opposite to reading the matrix
 - Replace scatter with gather
 - Use MPI Gathery because different processes contribute different number of elements
- Function MPI Gatherv
 - Gathers into specific locations from all processes in a group

```
int MPI Gathery ( void * send bufr, int send count, MPI Datatype send type,
                  void * recv_bufr, int * recv_count, int * recv_disp,
                  MPI_Datatype recv_type, int root, MPI_COMM comm );
```

send_bufr Starting address of send buffer

send_count Number of elements in send buffer

send_type Data type of send buffer elements

recv_bufr Starting address of receive buffer; significant only at root

recv_count Integer array containing the number of elements to be received from each process; significant only at root

recv_disp Integer array to specify the displacement; relative to $recv_bufr$ at which to place the incoming data; entry i in array corresponds to data coming from process i

recv_type Data type of receive buffer elements

root Rank of sending process

comm Communicator

• Distributing partial results

- A series of m inner product operations create the m element result vector c

$$c_0 = a_{0,0}b_0 + a_{0,1}b_1 + \dots + a_{0,n-1}b_{n-1}$$

$$c_1 = a_{1,0}b_0 + a_{1,1}b_1 + \dots + a_{1,n-1}b_{n-1}$$

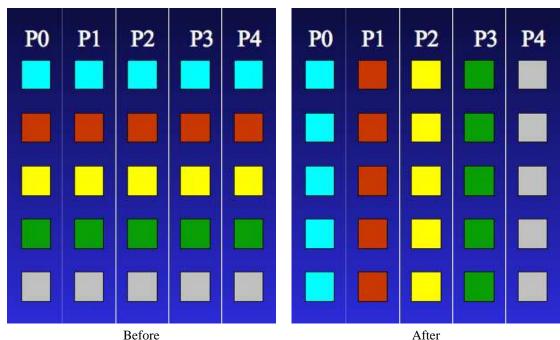
$$\vdots$$

$$c_{m-1} = a_{m-1,0}b_0 + a_{m-1,1}b_1 + \dots + a_{m-1,n-1}b_{n-1}$$

- Associate with each primitive task i column i of matrix A and element i of vector b
- Multiplying each element of column by b_i yields

$$(a_{0,i}b_i), (a_{1,i}b_i), \ldots, (a_{m-1,i}b_i)$$

- Product $a_{i,j}b_i$ is the *i*th term of the inner product for c_j , $0 \le j < n$
- After multiplication, each task needs to distribute n-1 result terms to other processors and collect n-1 terms from them
- all-to-all exchange
- After the exchange, add the m elements to produce c_i
- Function MPI_Alltoallv
 - Send data from all to all processors



- Each process may send different amount of data and provide displacements for the input and output data

send_bufr Starting address of send buffer

send_count Number of elements in send buffer

send_disp Integer array to specify the displacement; relative to send_bufr from which to take the outgoing data; entry *i* in array corresponds to data going to process *i*

send_type Data type of send buffer elements

recv_bufr Starting address of receive buffer; significant only at root

recv_count Integer array containing the number of elements to be received from each process; significant only at root

recv_disp Integer array to specify the displacement; relative to $recv_bufr$ at which to place the incoming data; entry i in array corresponds to data coming from process i

recv_type Data type of receive buffer elements

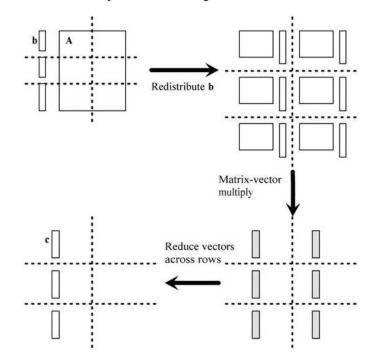
root Rank of sending process

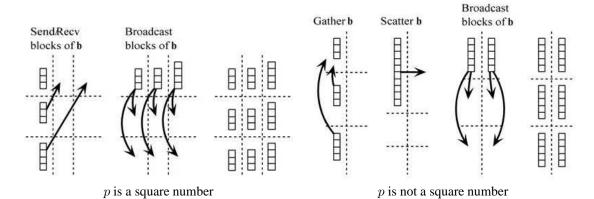
comm Communicator

- Requires two pairs of count/displacement arrays
 - 1. First pair for values being sent
 - * send_count: Number of elements
 - * send_disp: Index of first element in the array
 - 2. Second pair for values being received
 - * recv count: Number of elements
 - * recv_disp: Index of first element in the array
- The code
- Benchmarking
 - Time needed to compute a single iteration of the loop performing inner product given by χ
 - Expected time for computational portion of parallel program: $\chi n \lceil n/p \rceil$
 - Algorithm performs all-to-all exchange of partially computed portions of vector
 - Two methods to perform all-to-all exchange
 - 1. Each process sends $\lceil \log p \rceil$ messages of length n/2
 - * Total data elements transmitted: $\lceil \log p \rceil n/2$
 - 2. Each process sends directly to each of the other processes the elements meant for the process
 - * Each process sends p-1 messages
 - * Total data elements transmitted: n(p-1)/p
 - For large n, transmission time dominates latency; second approach will be better
 - * Time needed for transmission of single byte: $1/\beta$
 - * Time to perform all-gather of doubles: $(p-1)/(\lambda + 8n/(p\beta))$
 - Total execution time

$$\chi n \left\lceil \frac{n}{p} \right\rceil + (p-1) \left(\lambda + \frac{8n}{p\beta} \right)$$

- Design and analysis
 - Associate a primitive task with each element of matrix
 - Each primitive task performs one multiply: $d_{ij} = a_{ij} \times b_j$
 - Each element of the resulting vector $c_i = \sum_{j=0}^{n-1} d_{ij}$
 - st For each row i, add all the d_{ij} terms to produce c_i
 - Agglomerate primitive tasks into rectangular blocks
 - * Associate a task with each block
 - * Processes form a 2D grid
 - * Vector distributed by blocks among processes in first column of grid
 - Three principal tasks of parallel algorithm
 - 1. Redistribute vector so that each task has its correct portion
 - * Move vector from processes in first row to processes in first column
 - (a) p is a square
 - · First column/first row processes send/receive portions of vector
 - (b) p is not a square
 - · Gather vector on process (0,0)
 - · Process (0,0) broadcasts to processes in first row
 - * First row processes scatter vector within columns
 - 2. Perform matrix-vector multiplication with the portion assigned to task
 - 3. Perform sum-reduction on the task's portion of resulting vector





- Analyzing complexity
 - * p is a square number
 - · If grid is $1 \times p$, columnwise block-striped
 - · If grid is $p \times 1$, rowwise block-striped
 - * Each process does its share of computation: block of size $\lceil n/\sqrt{p} \rceil \times \lceil n/\sqrt{p} \rceil \Rightarrow \Theta(n^2p)$
 - * Redistribute vectors: $\Theta(n/\sqrt{p} + (\log p)(n/\sqrt{p})) = \Theta(n \log p/\sqrt{p})$
 - * Reduction of partial results vectors: $\Theta(n \log p / \sqrt{p})$
 - * Overall parallel complexity

$$\Theta(n^2/p + n \log p/\sqrt{p})$$

- Isoefficiency analysis
 - * Sequential complexity: $\Theta(n^2)$
 - * Parallel communication complexity: $\Theta(n \log p / \sqrt{p})$
 - * Isoefficiency function

$$n^2 \geq C n \sqrt{p} \log p \Rightarrow n \geq C \sqrt{p} \log p$$

* Since $M(n) = n^2$, scalability function is:

$$\frac{M(C\sqrt{p}\log p)}{p} = \frac{C^2p\log^2 p}{p}$$
$$= C^2\log^2 p$$

- * Checkerboard is more scalable than the other two implementations
- Creating communicators
 - Communicator provides the environment for message-passing among processes
 - * Default communicator is MPI_COMM_WORLD
 - Four collective communication operations involving subsets of processes in matrix-vector multiplication with checkerboard block decomposition
 - 1. Processes in first column of grid gather vector b when p is not square
 - 2. Processes in first row of grid scatter vector b when p is not square
 - 3. Each first row process broadcasts its block of vector b to other processes in the same column of grid
 - 4. Each row of processes in grid performs an independent sum-reduction, yielding result vector in the first column
 - Want processes in a virtual 2D grid
 - * Create a custom communicator
 - * Collective communications involve all processes in a communicator
 - * Need to do broadcasts and reductions among subsets of processes

- * Create communicators for processes in the same row or same column
- Communicator contains
 - * Process group
 - * Context
 - * Attributes
 - · Topology allows us to address processes in another way compared to the rank
 - · MPI supports two topologies Cartesian/grid and graph
- Function MPI_Dims_create
 - Create a division of processors in a Cartesian grid
 - Prefer to create a virtual mesh of processes that is as close to square as possible for scalability

```
int MPI_Dims_create ( int num_nodes, int num_dims, int * dims );
```

- IN num_nodes Number of nodes/processes in the grid
- IN num_dims Number of Cartesian dimensions

INOUT dims Integer array of size num_dims specifying the number of nodes in each dimension; a value of 0 indicates that the function should fill in a suitable value

- Usage example

```
int p;
int sz[2];
...
MPI_Comm_size ( MPI_COMM_WORLD, &p );
...
sz[0] = sz[1] = 0;
MPI_Dims_create ( p, 2, sz );
```

- Function MPI_Cart_create
 - Make a new communicator to which topology information has been attached
 - Done after determining the size of each dimension of virtual grid of processes

- IN comm_old Input communicator
- IN num_dims Number of Cartesian dimensions
- IN dims Integer array of size num_dims specifying the number of processes in each dimension
- IN periods Logical array of size num_dims specifying whether the grid is periodic (true) or not (false) in each dimension
 - * Grid is periodic if communication wraps around the edges

IN reorder Ranking may be reordered (true) or not (false); currently being ignored by MPI functions

OUT comm_cart Communicator with new Cartesian topology

- Usage example
 - * Making new communicator from MPI_COMM_WORLD

- Reading a checkerboard matrix
 - Single process (process 0) responsible to read the matrix and distribute contents to appropriate processes
 - Distribution pattern similar to the method for columnwise striping
 - Each row scattered among a subset of processes, within the same row of virtual grid
 - Matrix read by process 0
 - * Each time a row is read, send it to appropriate process in the appropriate row of process grid
 - * Receiving process gets the matrix row, and scatters it among the processes in its row of the process grid
 - * Achieved by MPI_Cart_rank, MPI_Cart_coords, and MPI_Comm_split
- Function MPI_Cart_rank
 - Process 0 needs to know its rank to send a matrix row to the first process in appropriate row in the process grid
 - Determine process rank in communicator given Cartesian location

coords Integer arrays of size num_dims of Cartesian topology associated with comm specifying the Cartesian coordinates of the process

- Usage example
 - * Assume r rows in virtual process grid and m rows in matrix
 - * Row i of the input matrix mapped to row of process grid specified by BLOCK OWNER(i, r, m) int // Rank of process receiving row int dest_rank; // Rank of process in virtual grid int grid_rank; int i; for (i = 0; i < m; i++)dest_coord[0] = BLOCK_OWNER(i, r, m); dest_coord[1] = 0; MPI_Cart_rank (grid_comm, dest_coord, &dest_rank); if (grid_rank == 0) // Read matrix row i // Send matrix row i to process dest rank } else if (grid-rank == dest_rank) { // Receive matrix row i from process 0 in virtual grid }
- Function MPI_Cart_coords
 - Determine process coordinates in Cartesian topology given its rank in the group

- Allows process to allocate correct amount of memory for its portion of matrix and vector
- Allows process 0 (the one reading the matrix) to find out its coordinates
 - * Knowing its coordinates enables process 0 to avoid sending itself a message if it happens to be the first process in a row of process grid

max_dims Length of vector coords in the calling program

coords Integer array of size max_dims to return the Cartesian coordinates of specified process

Usage example

```
int     grid_id;
MPI_Comm grid_comm;
int grid_coords[2];
...
MPI_Cart_coords ( grid_comm, grid_id, 2, grid_coords );
```

- Function MPI_Comm_split
 - Partitions the processes of a communicator into one or more subgroups
 - * Scatter is a collective operation
 - * The input row is scattered amond only the processes in a single row of the process grid by dividing the Cartesian communicator into separate communicators for every row in process grid
 - Constructs a communicator for each subgroup, based on colors and keys
 - Allows processes in each subgroup to perform their own collective communications
 - Needed for columnwise scatter and rowwise reduce

color Control of subset assignment as a nonnegative integer; processes with the same color are in the same new communicator

key Ranking order of processes in new communicator

new_comm New communicator shared by processes in same partition

- We determined the process coordinates by using MPI_Cart_coords
- Usage example
 - * Group together processes in the same row by using the value of grid_coords[0] as color
 - * Rank processes according to their column by using grid_coords[1] as ranking order determinant

 This function can also be used to divide the Cartesian communicator into separate communicators for every column of the grid

Benchmarking

- \bullet Analytical model, considering p as a square number
- Time to perform a single iteration of the loop to compute inner product: χ
- Each process responsible for a block of matrix with size $\left\lceil \frac{n}{\sqrt{p}} \right\rceil \times \left\lceil \frac{n}{\sqrt{p}} \right\rceil$
- Estimated computation time of parallel program: $\chi\left\lceil\frac{n}{\sqrt{p}}\right\rceil \times \left\lceil\frac{n}{\sqrt{p}}\right\rceil$
- Redistribute vector b
 - Processes in first column of grid pass their blocks of vector to processes in the first row of grid
 - Each process responsible for at most $\left\lceil \frac{n}{\sqrt{p}} \right\rceil$ elements of vector
 - Time to send/receive: $\lambda + 8 \left[\frac{n}{\sqrt{p}} \right] / \beta$
 - Each process then broadcasts its block to other processes in the column
 - Time to broadcast: $\log \sqrt{p} \left(\lambda + 8 \left\lceil \frac{n}{\sqrt{p}} \right\rceil / \beta \right)$
- Reduce partial results
 - Ignore the time for addition as the communications time dominates
 - Communications time same as that needed for broadcast: $\log \sqrt{p} \left(\lambda + 8 \left\lceil \frac{n}{\sqrt{p}} \right\rceil / \beta \right)$