Programming with Message Passing PART III: Examples

HPC Fall 2012

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Overview

- Parallel matrix multiplication
  - Parallel direct matrix multiplication with master and workers
  - Parallel blocked matrix multiplication with master and workers
  - Complexity lower bound of parallel matrix multiplication
  - Full recursive parallel blocked matrix multiplication
  - Cannon's algorithm
  - Systolic arrays
  - Fox' algorithm
- Iterative solver in MPI
- Heat distribution problem in MPI
- Further reading

Parallel Matrix Multiplication: Direct Implementation

- Basic algorithm, $n \times l$ matrix A, $l \times m$ matrix B, $n \times m$ matrix C

$$C = A \times B \qquad c_{i,j} = \sum_{k=0}^{l-1} a_{i,k} b_{k,j}$$

- Assume square matrices, thus $n = m = l$
- $P = n \times n$ worker processors with $c_{i,j}$ stored locally on $p_{i,j}$
- One master processor sends $2n$ elements $a_{i,k}$ and $b_{k,j}$ for $k = 0, \ldots, n\text{-}1$ to each worker $p_{i,j}$
- Workers compute and return $c_{i,j}$ to master processor
- Computation: $t_{comp} = 2n$
- Communication: $t_{comm} = \underbrace{n^2(t_{startup} + 2n\, t_{data})}_{master\ to\ workers} + \underbrace{n^2(t_{startup} + t_{data})}_{workers\ to\ master}$

Parallel Matrix Multiplication: Block Matrix Multiplication

- Block matrix multiplication algorithm, with $s \times s$ blocks of size $m \times m$ where $m = n/s$

```
for p = 0 to s-1
  for q = 0 to s-1
    C_p,q = 0
    for r = 0 to s-1
      C_p,q = C_p,q + A_p,r × B_r,q   // matrix +and × operations
```

- $P = s \times s$ worker processors with submatrices $C_{p,q}$ stored locally on $p_{p,q}$
- Master processor sends $2s$ blocks $A_{p,r}$ and $B_{r,q}$ of $m \times m$ for $r = 0, \ldots, s\text{-}1$ to each worker $p_{p,q}$
- Workers compute inner loop and return $C_{p,q}$ to master processor
- Computation: $t_{comp} = s(2m^3 + m^2) = O(sm^3) = O(nm^2)$
- Communication: $t_{comm} = \underbrace{2s^2\,(t_{startup} + nm\ t_{data})}_{\textit{master to workers}} + \underbrace{s^2\,(t_{startup} + m^2 t_{data})}_{\textit{workers to master}}$

Parallel Matrix Multiplication: Lower Bound on Complexity

- First assume we have $P = n \times n$ processors
- Each processor computes $c_{i,j}$ in parallel
- Assume zero communication overhead, so $a_{i,k}$ and $b_{k,j}$ for $k = 0, \ldots, n\text{-}1$ are directly available to all processors
- Now add another dimension of n processors ($P = n \times n \times n$) to compute

$$c_{i,j} = \sum_{k=0}^{n-1} a_{i,k} b_{k,j}$$

  using a parallel tree-reduction in $\log n$ steps
- Computation: $t_{comp} = 1 + \log n = O(\log n)$
- Not cost optimal: $O(P \log n) = O(n^3 \log n) \neq O(n^3)$

Parallel Matrix Multiplication: Recursive Implementation

- Block matrix multiplication in recursion by decomposing matrix in 2×2 submatrices and computing the submatrices recursively

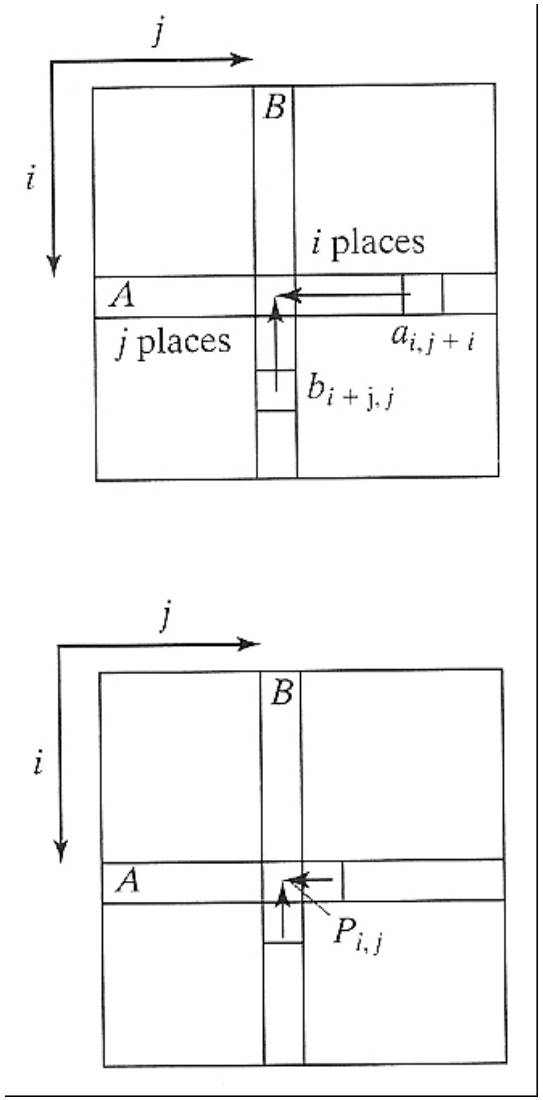
```
Mat matmul(Mat A, Mat B, int s)
{ if (s == 1)
    C = A * B;
  else
  { s = s/2;
    P0 = matmul(A_{p,p}, B_{p,p}, s);
    P1 = matmul(A_{p,q}, B_{q,p}, s);
    P2 = matmul(A_{p,p}, B_{p,q}, s);
    P3 = matmul(A_{p,q}, B_{q,q}, s);
    P4 = matmul(A_{q,p}, B_{p,p}, s);
    P5 = matmul(A_{q,q}, B_{q,p}, s);
    P6 = matmul(A_{q,p}, B_{p,q}, s);
    P7 = matmul(A_{q,q}, B_{q,q}, s);
    C_{p,p} = P0 + P1;
    C_{p,q} = P2 + P3;
    C_{q,p} = P4 + P5;
    C_{q,q} = P6 + P7;
  }
  return C;
}
```

P0…P7 *computed in parallel*

computed in parallel

- Level of parallelism increases with deepening recursion
- Suitable for shared memory systems
- Excessive message passing on distributed memory systems

Parallel Matrix Multiplication: Cannon's Algorithm



Rotate and compute:

```
send(a, p_{i,j-1})
recv(a, p_{i,j+1})
send(b, p_{i-1,j})
recv(b, p_{i+1,j})
c = c + a*b
```

Note: send-recv wrap around the processor grid

Note: subscripts are modulo n

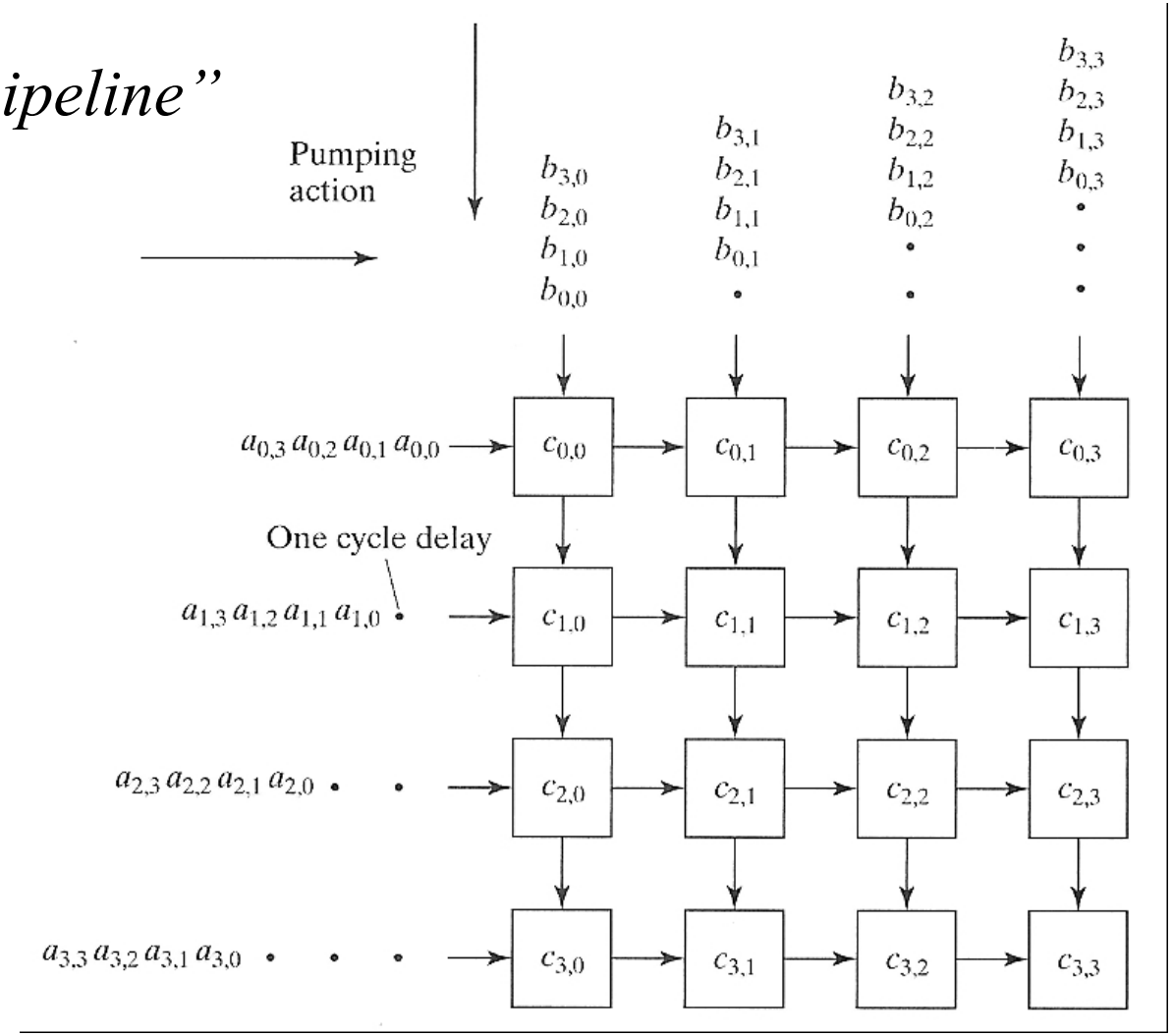
1. Initially each $p_{i,j}$ has $a_{i,j}$ and $b_{i,j}$
2. Align elements $a_{i,j}$ and $b_{i,j}$ by reordering them so that $a_{i,j+i}$ and $b_{i+j,j}$ are on $p_{i,j}$
3. Each $p_{i,j}$ computes $c_{i,j} = a_{i,j+i} * b_{i+j,j}$ ($a_{i,j+i}$ and $b_{i+j,j}$ are local on $p_{i,j}$)
4. For $k = 1$ to n-1 repeat 5-7:
5. Rotate A left by one column
6. Rotate B up by one row
7. Each $p_{i,j}$ computes $c_{i,j} = c_{i,j} + a_{i,j+i+k} * b_{i+j+k,j}$ ($a_{i,j+i+k}$ and $b_{i+j+k,j}$ are local on $p_{i,j}$ after k rotations)

Parallel Matrix Multiplication: Analysis of Cannon's Algorithm

- Consider block matrix multiplication with Cannon's algorithm, with $s \times s$ blocks of size $m \times m$ where $m = n/s$
- Initial alignment requires s-1 rotations of A and B each moving $m \times m$ blocks in parallel
- Algorithm takes s steps
  - Each processor performs a local matrix multiply on its $m \times m$ block in $2m^3$ time and sums in m^2 time
  - Rotation of A and B on $m \times m$ blocks, where each processor sends and receives two $m \times m$ blocks (one per row and one per column)
- Computation: $t_{comp} = s(2m^3 + m^2) = O(m^2 n)$
- Communication: $t_{comm} = 4(s\text{-}1)(t_{startup} + m^2 t_{data}) = O(m^2 s)$

Parallel Matrix Multiplication: Systolic Array

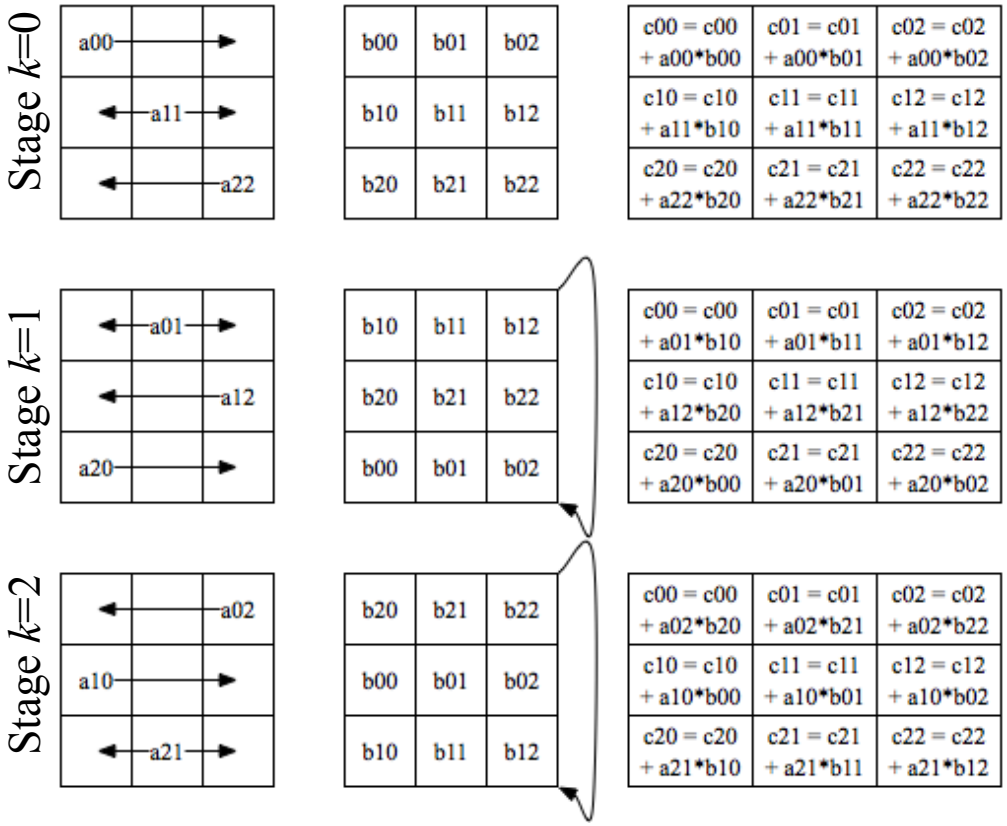
"Two-dimensional pipeline"



Each processor repeats a "recv-compute-send" stage n times:

```
recv(a, p_{i,j-1})
recv(b, p_{i-1,j})
c = c + a*b
send(a, p_{i,j+1})
send(b, p_{i+1,j})
```

Parallel Matrix Multiplication: Fox' Algorithm



- Similar to Cannon's algorithm
- No initial alignment
- Combines broadcast of A with rotation of B

1. For k=0 to n-1 repeat step 2-4:
2. For each row i, broadcast element $a_{i,i+k}$ along that row
3. Compute $c_{i,j} = c_{i,j} + a_{i,i+k} * b_{i+k,j}$ ($a_{i,i+k}$ and $b_{i+k,j}$ are local on $p_{i,j}$)
4. Rotate B up by one row

For this algorithm, what is t_{comp} and t_{comm}?

Parallel Matrix Multiplication: Fox' Blocked Algorithm

```
dn = proc[(p+1) mod s), q];
up = proc[(p-1) mod s), q];
B′ = B_{p,q};
for (k = 0; k < s; k++)
{
  r = (p+k) mod s;
  bcast A_{p,r} to A′ across row p
  C_{p,q} = C_{p,q} + A′ * B′;
  send B′ to up;
  recv B′ from dn;
}
```

- Fox' block matrix multiply with $s \times s$ blocks of size $m \times m$ where $m = n/s$

1. For k=0 to s-1 repeat 2-4:
2. For each processor row p, broadcast submatrix $A_{p,q+k}$ along processor row p
3. Compute $C_{p,q} = C_{p,q} + A_{p,q+k} * B_{p+k,q}$ ($A_{p,q+k}$ & $B_{p+k,q}$ are local on $p_{p,q}$)
4. Rotate B up by one processor row

Parallel Matrix Multiplication: Fox' Algorithm in MPI

```
void Fox(GridInfo *grid, Matrix *Apq, Matrix *Bpq, Matrix *Cpq, int M)
{
  int k, r;
  int dn = (grid->p + 1) % grid->s;
  int up = (grid->p + grid->s - 1) % grid->s;
  MPI_Status stat;
  Matrix Atmp[M*M];

  setzero(C);
  for (k = 0; k < grid->s; k++)
  {
    r = (grid->p + k) % grid->s;
    if (r == grid->q)
    { MPI_Bcast(Apq, M*M, MPI_DOUBLE, r, grid->row);
      matmul(Apq, Bpq, Cpq, M);
    }
    else
    { MPI_Bcast(Atmp, M*M, MPI_DOUBLE, r, grid->row);
      matmul(Atmp, Bpq, Cpq, M);
    }
    MPI_Sendrecv_replace(Bpq, M*M, MPI_DOUBLE, up, 0, dn, 0, grid->col, &stat);
  }
}
```

The "below" and "above" processes

Row and column communicators (these are relative to each process)

Parallel Matrix Multiplication: Fox' Algorithm in MPI (cont'd)

```
typedef struct GridInfo
{
  int s;
  int p, q;
  MPI_Comm row, col;
} GridInfo;
```

The s×s processor grid

Position (p,q) of the process on the grid

Row and column communicators

```
void setup(GridInfo *grid)
{
  MPI_Comm comm;
  int numproc, rank, dim[2], wrap[2], coord[2], freecoord[2];

  MPI_Comm_size(MPI_COMM_WORLD, &numproc);
  grid->s = (int)sqrt(numproc);

  dim[0] = dim[1] = grid->s;
  wrap[0] = wrap[1] = 1;
  MPI_Cart_create(MPI_COMM_WORLD, 2, dim, wrap, 1, &comm);
  MPI_Comm_rank(comm, &rank);
  MPI_Cart_coords(comm, rank, 2, coord);
  grid->p = coord[0];
  grid->q = coord[1];
  …
```

Number of processes should be perfect square

Setup 2 by 2 Cartesian grid

Find process' location on the grid

Parallel Matrix Multiplication: Fox' Algorithm in MPI (cont'd)

```
typedef struct GridInfo
{
  int s;
  int p, q;
  MPI_Comm row, col;
} GridInfo;
```

The s×s processor grid

Position (p,q) of the process on the grid

Row and column communicators

Setup row communicator

Setup column communicator

```
void setup(GridInfo *grid)
{
  …
  freecoord[0] = 0;
  freecoord[1] = 1;
  MPI_Cart_sub(comm, freecoord, &grid->row);

  freecoord[0] = 1;
  freecoord[1] = 0;
  MPI_Cart_sub(comm, freecoord, &grid->col);
}
```

Parallel Iterative Solver: Jacobi Method

$$x_i^k = \frac{1}{a_{i,i}}\left[b_i - \sum_{j \neq i} a_{i,j} x_j^{k-1}\right]$$

```
for (i = 0; i < m; i++)
  xp[i] = bp[i];
do
{
  allGather xp[0…m-1] into xold[0…n-1];
  for (i = 0; i < m; i++)
  {
    xp[i] = bp[i];
    for (j = 0; j < n; j++)
      if (j != p*m+i)
        xp[i] = xp[i] - Ap[i,j]*xold[j];
    xp[i] = xp[i]/Ap[i,i];
  }
} while (…);
```

1. Distribute $n \times n$ matrix A by rows and vector b in blocks of size $m = n/P$ over P processors into local A_p and b_p
2. Assign $x_p = b_p$
3. Repeat 4-6 until convergence or max iterations reached:
4. Gather x_p into $xold$ } allGather
5. Broadcast $xold$
6. Compute new x_p using A_p, b_p, $xold$

Parallel Iterative Solver: Jacobi Method in MPI – v1

```
void Jacobi(Matrix *Ap, Vector *bp, Vector *xp, int N, int M)
{
  Vector xold[N];
  int i, j, p;

  MPI_Comm_rank(MPI_COMM_WORLD, &p);
  for (i = 0; i < M; i++)
    xp[i] = bp[i];
  do
  {
    MPI_Allgather(xp, M, MPI_DOUBLE, xold, M, MPI_DOUBLE, MPI_COMM_WORLD);
    for (i = 0; i < M; i++)
    {
      xp[i] = bp[i];
      for (j = 0; j < p*M+i; j++)
        xp[i] = xp[i] - Ap[i][j]*xold[j];
      for (j = p*M+i+1; j < N; j++)
        xp[i] = xp[i] - Ap[i][j]*xold[j];
      xp[i] = xp[i]/Ap[i][i];
    }
  } while (…);
}
```

The global row index I = pm+i

Parallel Iterative Solver: Jacobi Method in MPI - v2

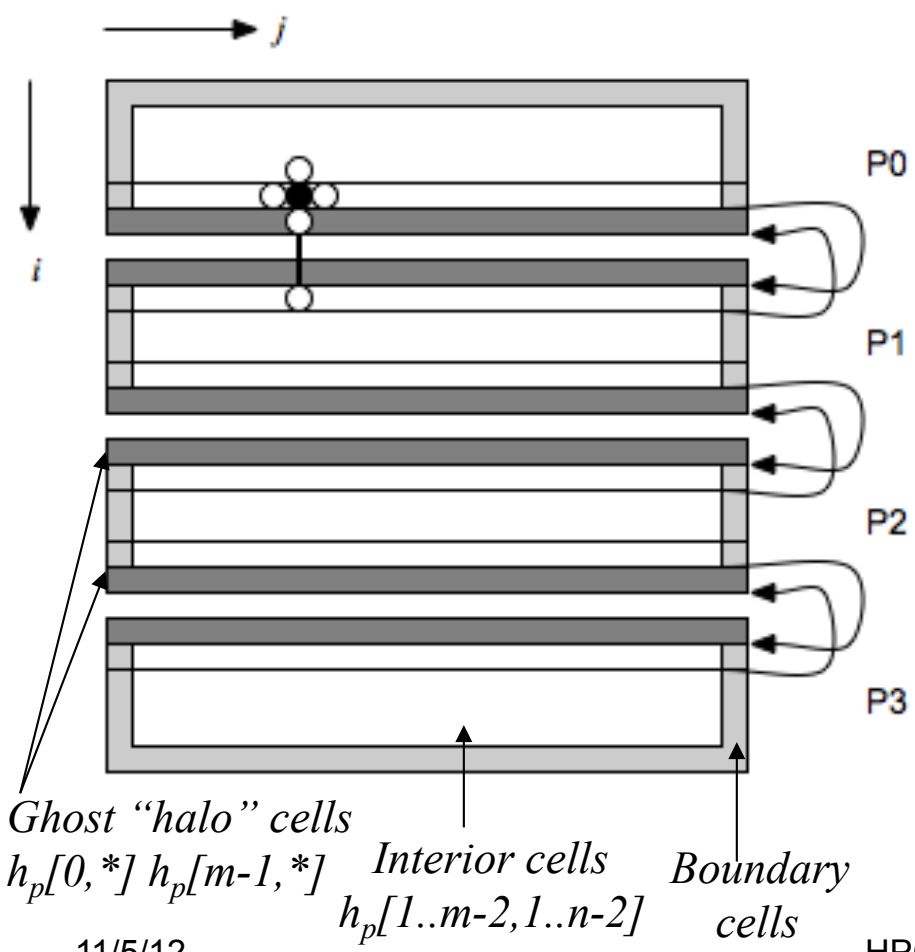
```
void Jacobi(Matrix *Ap, Vector *bp, Vector *xp, int N, int M)
{
  Vector xold[N];
  int i, j, p;

  MPI_Comm_rank(MPI_COMM_WORLD, &p);
  for (i = 0; i < M; i++)
    xp[i] = bp[i];
  do
  {
    MPI_Allgather(xp, M, MPI_DOUBLE, xold, M, MPI_DOUBLE, MPI_COMM_WORLD);
    for (i = 0; i < M; i++)
    {
      xp[i] = bp[i] + Ap[i][p*M+i]*xold[p*M+i];
      for (j = 0; j < n; j++)
        xp[i] = xp[i] - Ap[i][j]*xold[j];
      xp[i] = xp[i]/Ap[i][i];
    }
  } while (…);
}
```

more efficient

Heat Distribution Problem: Parallel Jacobi Iteration

$$h_{i,j} = \frac{h_{i-1,j} + h_{i+1,j} + h_{i,j-1} + h_{i,j+1}}{4}$$



1. Distribute $n \times n$ matrix h block-wise by rows into local h_p
2. Extend local h_p with additional top and bottom rows to form "halos" (ghost cells), each block has size $m \times n$, where $m=(n-2)/P+2$
3. Repeat 4-5 until convergence:
4. Exchange rows with neighbor processors to update halo rows
5. Compute $hnew_p$
6. Assign $hnew_p$ to h_p

Heat Distribution Problem in MPI – v1

dest /src *tag*

"even" processor exchanges bottom rows with "odd" processor top rows

"odd" processor exchanges bottom rows with "even" processor top rows

```
void HDStep(Matrix *hp, int N, int M)
{
  int i, j;
  Matrix hnew[M*N];
  MPI_Status s;
  if (p % 2 == 0 && p < P-1)
    MPI_Sendrecv(hp[M-2], N, MPI_FLOAT, p+1, 0,
                 hp[M-1], N, MPI_FLOAT, p+1, 1, MPI_COMM_WORLD, &s);
  else
    MPI_Sendrecv(hp[1], N, MPI_FLOAT, p-1, 1,
                 hp[0], N, MPI_FLOAT, p-1, 0, MPI_COMM_WORLD, &s);
  if (p % 2 == 1 && p < P-1)
    MPI_Sendrecv(hp[M-2], N, MPI_FLOAT, p+1, 2,
                 hp[M-1], N, MPI_FLOAT, p+1, 3, MPI_COMM_WORLD, &s);
  else if (p > 0)
    MPI_Sendrecv(hp[1], N, MPI_FLOAT, p-1, 3,
                 hp[0], N, MPI_FLOAT, p-1, 2, MPI_COMM_WORLD, &s);
  for (i = 1; i < M-1; i++)
    for (j = 1; j < N-1; j++)
      hnew[i][j] = 0.25*(hp[i-1][j]+hp[i+1][j]+hp[i][j-1]+hp[i][j+1]);
  for (i = 1; i < M-1; i++)
    for (j = 1; j < N-1; j++)
      hp[i][j] = hnew[i][j];
}
```

Heat Distribution Problem in MPI – v2

dest /src *tag*

Send bottom interior row, receive top halo row

Send top interior row, receive bottom halo row

Send bottom interior row, receive bottom halo row

Send top interior row, receive top halo row

```
void HDStep(Matrix *hp, int N, int M)
{
  int i, j;
  Matrix hnew[M*N];
  MPI_Status s;
  if (p > 0 && p < P-1)
  { MPI_Sendrecv(hp[M-2], N, MPI_FLOAT, p+1, 0,
                 hp[0],   N, MPI_FLOAT, p-1, 0, MPI_COMM_WORLD, &s);
    MPI_Sendrecv(hp[1],   N, MPI_FLOAT, p-1, 1,
                 hp[M-1], N, MPI_FLOAT, p+1, 1, MPI_COMM_WORLD, &s);
  }
  else if (p == 0)
    MPI_Sendrecv(hp[M-2], N, MPI_FLOAT, p+1, 0,
                 hp[M-1], N, MPI_FLOAT, p+1, 1, MPI_COMM_WORLD, &s);
  else
    MPI_Sendrecv(hp[1],   N, MPI_FLOAT, p-1, 1,
                 hp[0],   N, MPI_FLOAT, p-1, 0, MPI_COMM_WORLD, &s);
  for (i = 1; i < M-1; i++)
    for (j = 1; j < N-1; j++)
      hnew[i][j] = 0.25*(hp[i-1][j]+hp[i+1][j]+hp[i][j-1]+hp[i][j+1]);
  for (i = 1; i < M-1; i++)
    for (j = 1; j < N-1; j++)
      hp[i][j] = hnew[i][j];
}
```

Heat Distribution Problem in MPI – v3

```
void HDStep(Matrix *hp, int N, int M, int step)
{
  int i, j;
  int dntag = 2*step;
  int uptag = 2*step + 1;
  Matrix hnew[M*N];
  MPI_Request sndreq[2], rcvreq[2];
  MPI_Status stat[2];

  if (p < P-1)
  { MPI_Isend(hp[M-2], N, MPI_FLOAT, p+1, dntag, MPI_COMM_WORLD, &sndreq[0]);
    MPI_Irecv(hp[M-1], N, MPI_FLOAT, p+1, uptag, MPI_COMM_WORLD, &rcvreq[0]);
  }
  if (p > 0)
  { MPI_Isend(hp[1],   N, MPI_FLOAT, p-1, uptag, MPI_COMM_WORLD, &sndreq[1]);
    MPI_Irecv(hp[0],   N, MPI_FLOAT, p-1, dntag, MPI_COMM_WORLD, &rcvreq[1]);
  }

  for (i = 2; i < M-2; i++)
    for (j = 1; j < N-1; j++)
      hnew[i][j] = 0.25*(hp[i-1][j]+hp[i+1][j]+hp[i][j-1]+hp[i][j+1]);
  …
```

Tag for "down" sends

Tag for "up" sends

Send interior bottom row

Receive halo bottom row

Send interior top row

Receive halo top row

Compute only interior points not on interior top row and not on interior bottom row

Heat Distribution Problem in MPI – v3 (cont'd)

```
void HDStep(Matrix *hp, int N, int M, int step)
{
  …
  if (p == 0)
    MPI_Wait(&rcvreq[0], stat);
  else if (p == P-1)
    MPI_Wait(&rcvreq[1], stat);
  else
    MPI_Waitall(2, rcvreq, stat);
  for (j = 1; j < N-1; j++)
  { hnew[1][j]   = 0.25*(hp[0][j]  +hp[2][j]  +hp[1][j-1]  +hp[1][j+1]);
    hnew[M-2][j] = 0.25*(hp[M-3][j]+hp[M-1][j]+hp[M-2][j-1]+hp[M-2][j+1]);
  }
  if (p == 0)
    MPI_Wait(&sndreq[0], stat);
  else if (p == P-1)
    MPI_Wait(&sndreq[1], stat);
  else
    MPI_Waitall(2, sndreq, stat);
  for (i = 1; i < M-1; i++)
    for (j = 1; j < N-1; j++)
      hp[i][j] = hnew[i][j];
}
```

Wait for completion of receives, then compute interior points on interior top and bottom rows

Wait for completion of sends to ensure **hp** *can be written again, then assign updated* **hp** *values*

Further Reading

- [PP2] pages 340-365