Lecture 9: Numerical Partial Differential Equations(Part 1)

Finite Difference Method to Solve 2D Diffusion Equation

Consider to solve $\begin{cases} \dfrac{\partial u}{\partial t} = u_{xx} + u_{yy} + f(x, y) & in\ \Omega \\ u = 0 & on\ \ \partial\Omega \end{cases}$

by using an forward in time and backward in space (FTCS or explicit) finite difference scheme.

Here $\Omega = [0, a] \times [0, b], f(x, y) = xy$. a and b are constants and > 0.

Finite Differences

- Spatial Discretization: $0 = x_0 < \cdots < x_M = a$ with $x_i = \frac{i}{M} a$ and $0 = y_0 < \cdots < y_N = b$ with $y_j = \frac{j}{N} b$. Define $\Delta x = \frac{a}{M}$ and $\Delta y = \frac{b}{N}$.
- Differential quotient:

$$u_{xx}(x_i, y_j, t) \sim \frac{u(x_{i-1}, y_j, t) - 2u(x_i, y_j, t) + u(x_{i+1}, y_j, t)}{\Delta x^2}$$

$$u_{yy}(x_i, y_j, t) \sim \frac{u(x_i, y_{j-1}, t) - 2u(x_i, y_j, t) + u(x_i, y_{j+1}, t)}{\Delta y^2}$$

$$u_t(x_i, y_j, t_n) \sim \frac{u(x_i, y_j, t_{n+1}) - u(x_i, y_j, t_n)}{\Delta t}$$

Insert quotients into PDE yields:

$$\begin{aligned} v(x_i, y_j, t_{n+1}) &= v(x_i, y_j, t_n) \\ &+ \Delta t \left(\frac{v(x_{i-1}, y_j, t_n) - 2v(x_i, y_j, t_n) + v(x_{i+1}, y_j, t_n)}{\Delta x^2} \right. \\ &\left. + \frac{v(x_i, y_{j-1}, t_n) - 2v(x_i, y_j, t_n) + v(x_i, y_{j+1}, t_n)}{\Delta y^2} \right) + \Delta t f(x_i, y_j) \end{aligned}$$

Or in short notation

$$\begin{aligned} v_{i,j}^{n+1} = v_{i,j}^n + \Delta t \left(\frac{v_{i-1,j}^n - 2v_{i,j}^n + v_{i+1,j}^n}{\Delta x^2} + \frac{v_{i,j-1}^n - 2v_{i,j}^n + v_{i,j+1}^n}{\Delta y^2} \right) \\ + \Delta t f(x_i, y_j) \end{aligned}$$

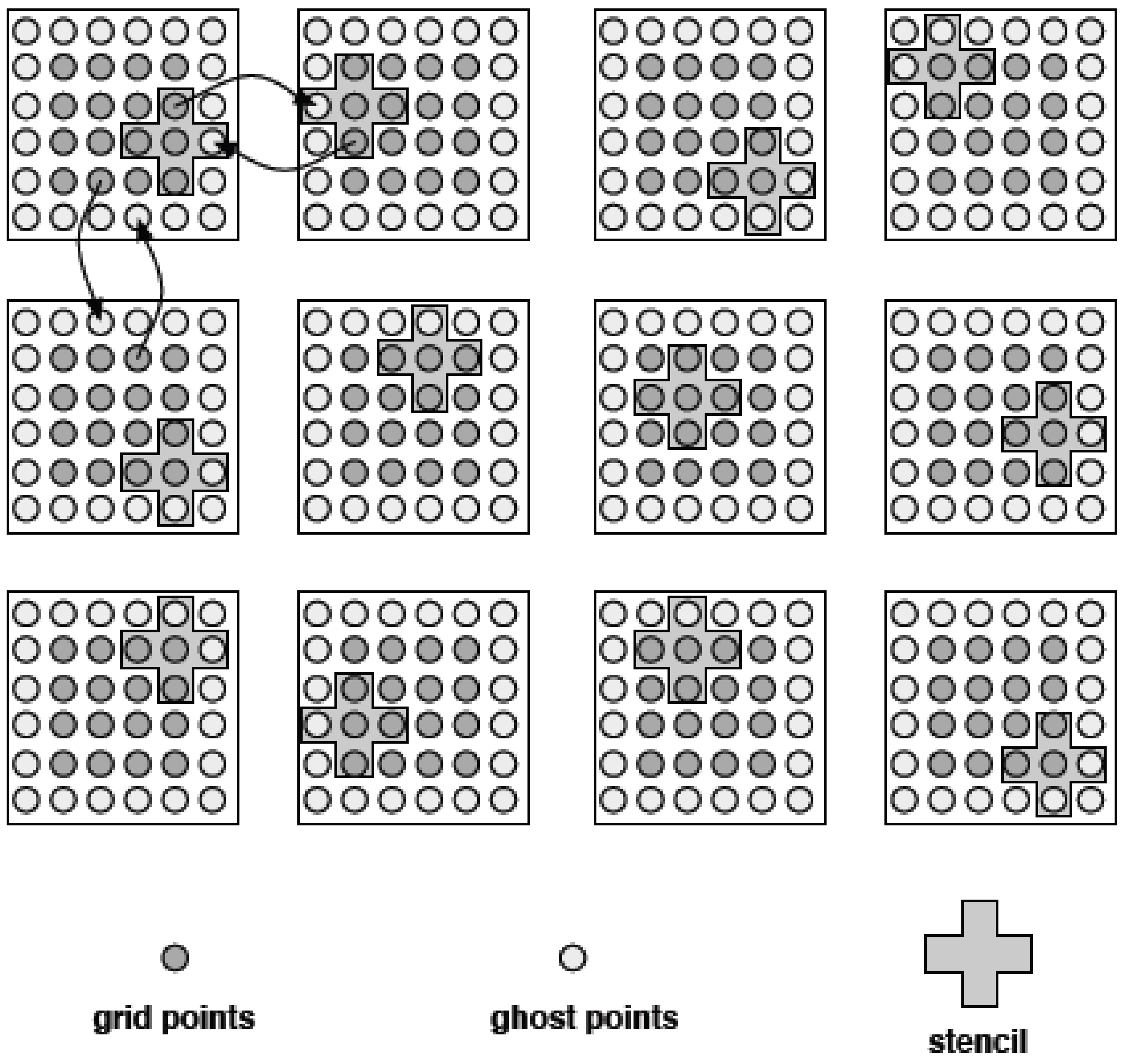
Boundary conditions:

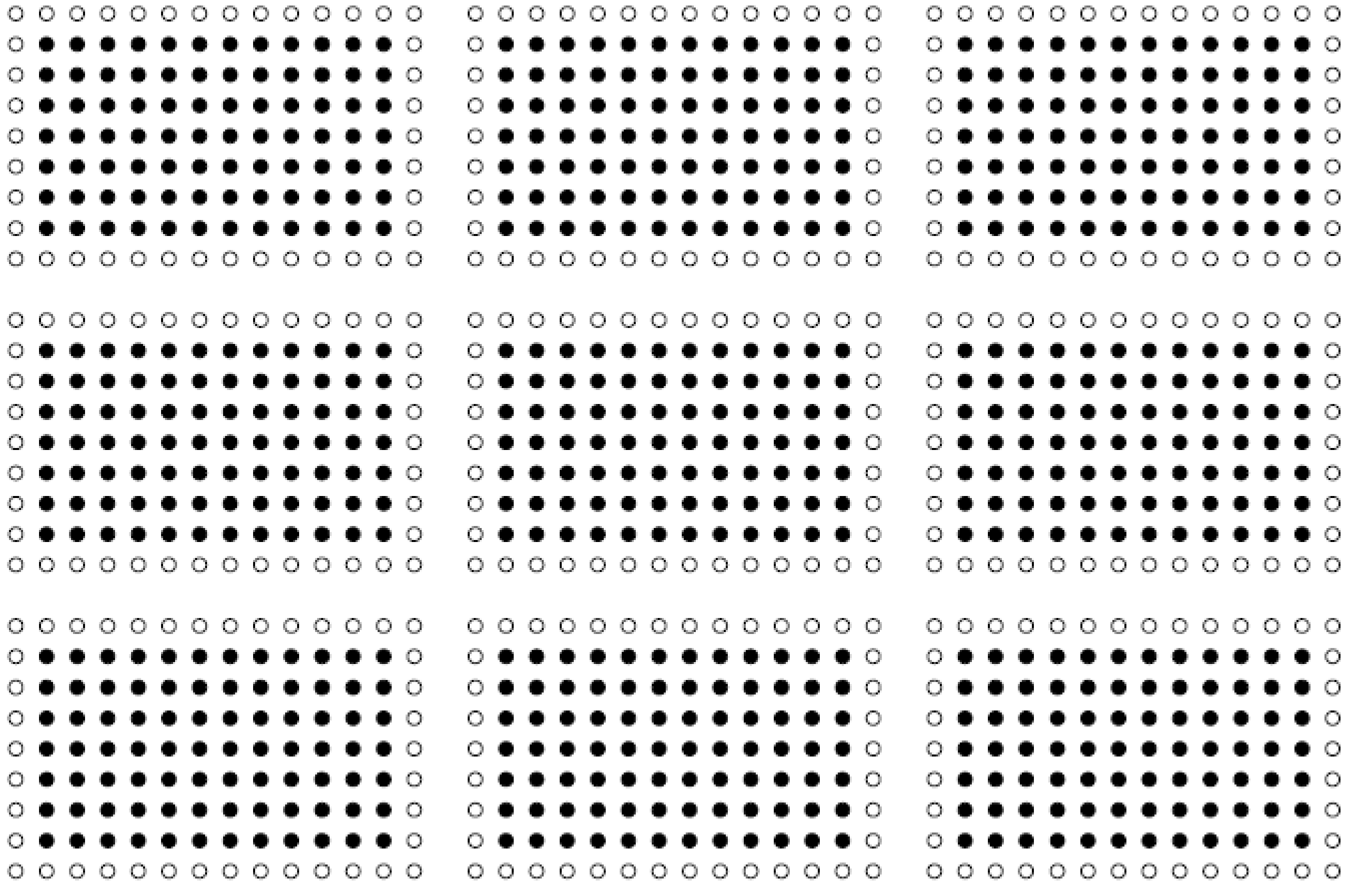
$v_{0,j}^{n+1} = 0; \quad v_{M,j}^{n+1} = 0; v_{i,0}^{n+1} = 0; v_{i,N}^{n+1} = 0.$

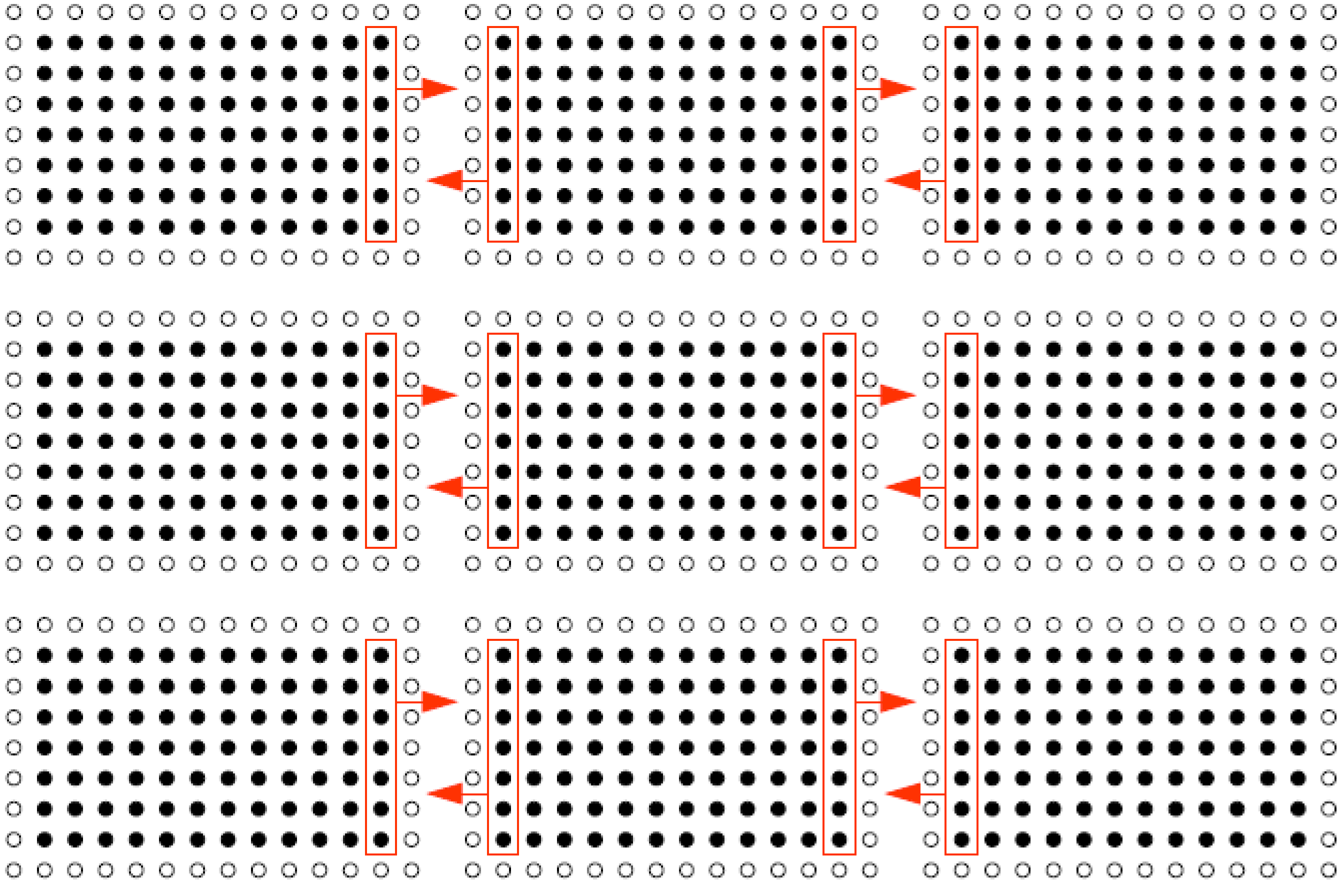
Parallel Computation with Grids

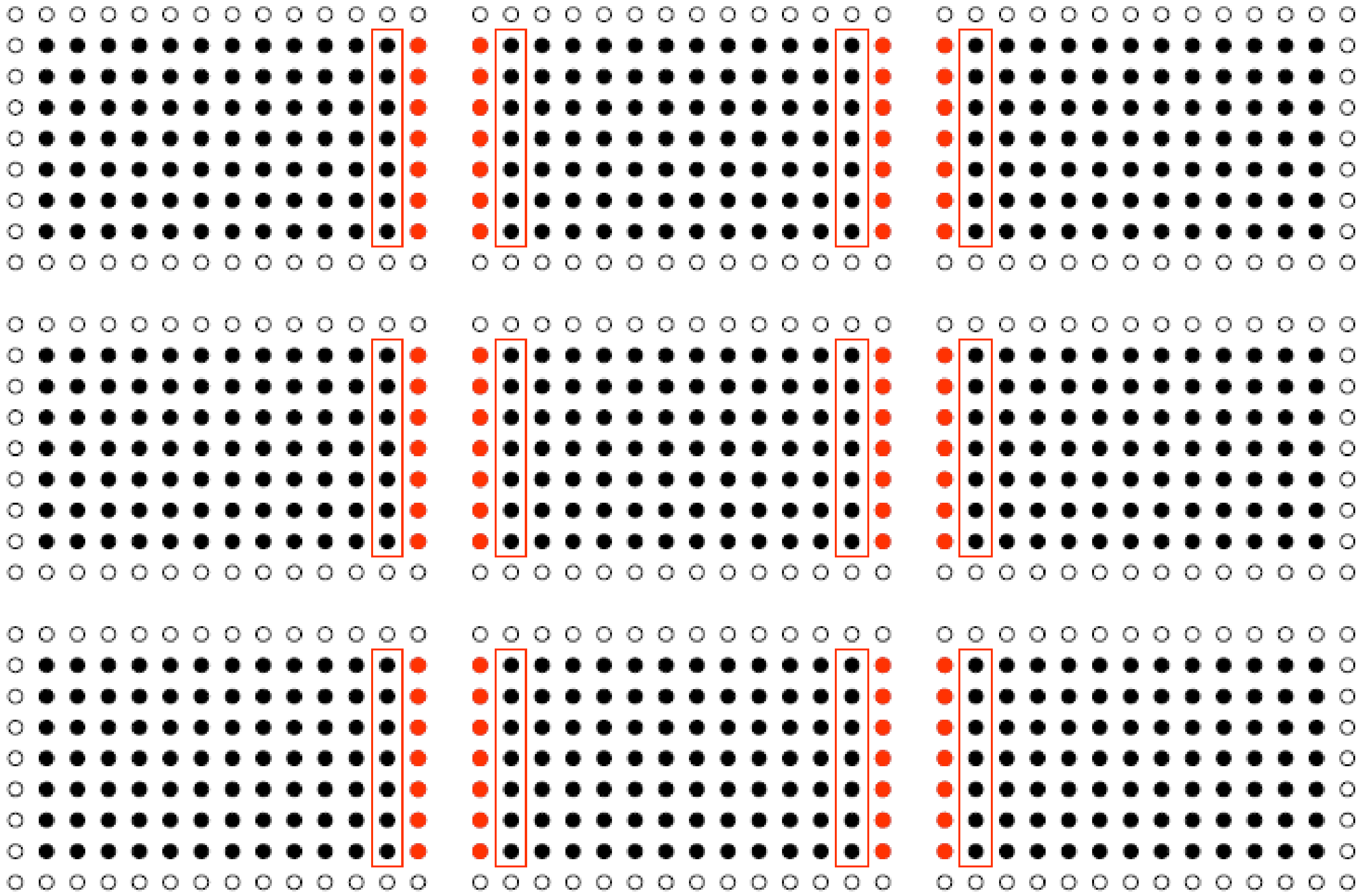
- Partition solution domain into subdomains.
- Distribute subdomains across processors
- Communication between processors is needed to provide interface between subdomains.
  - Communication is needed when stencil for given grid point includes points on another processor
  - For efficiency, ghost points are used for message passing at the end (or begin) of each iteration. Ghost points overlap between two subdomains, so as subgrids.

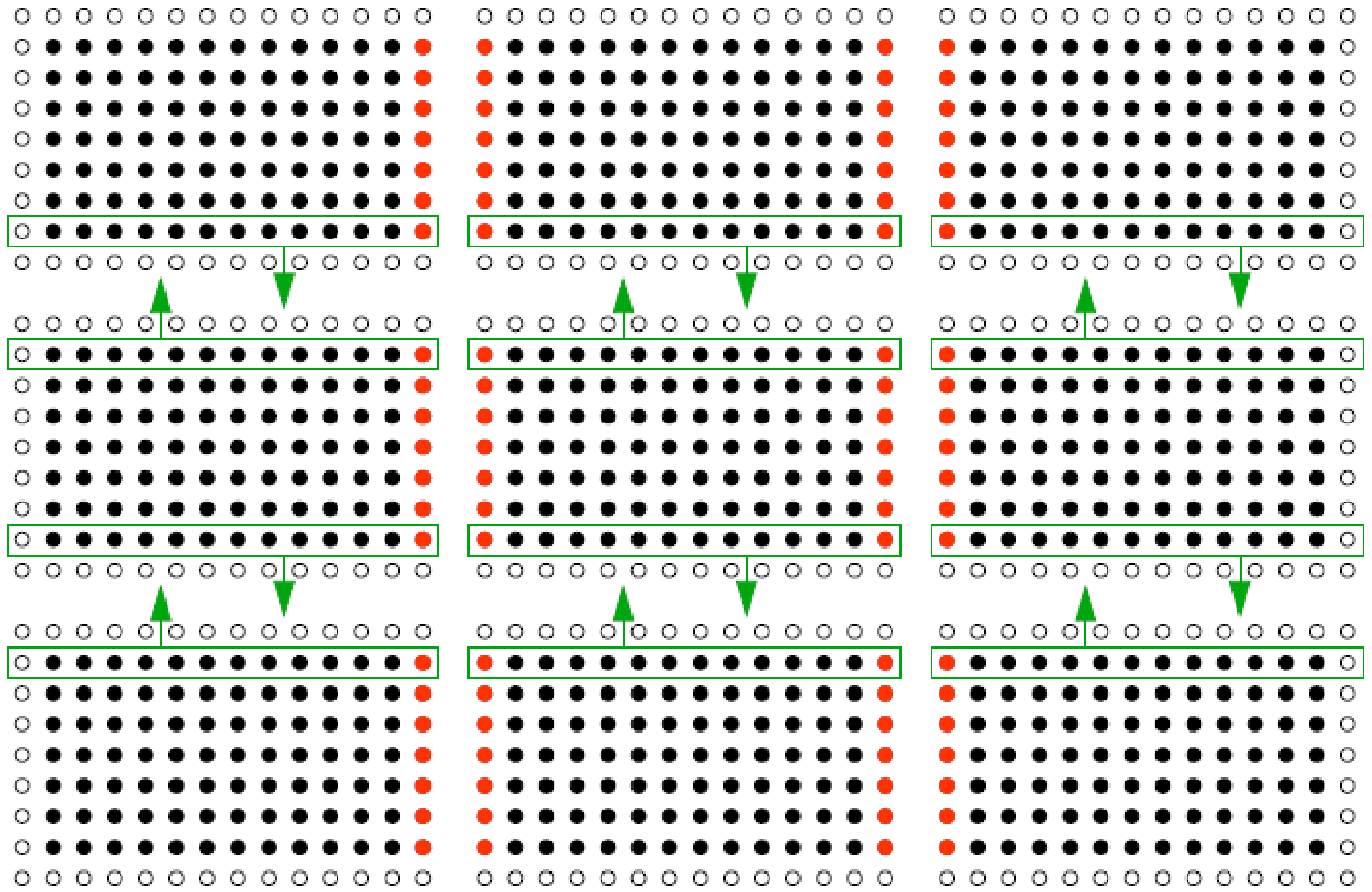
Ghost Points

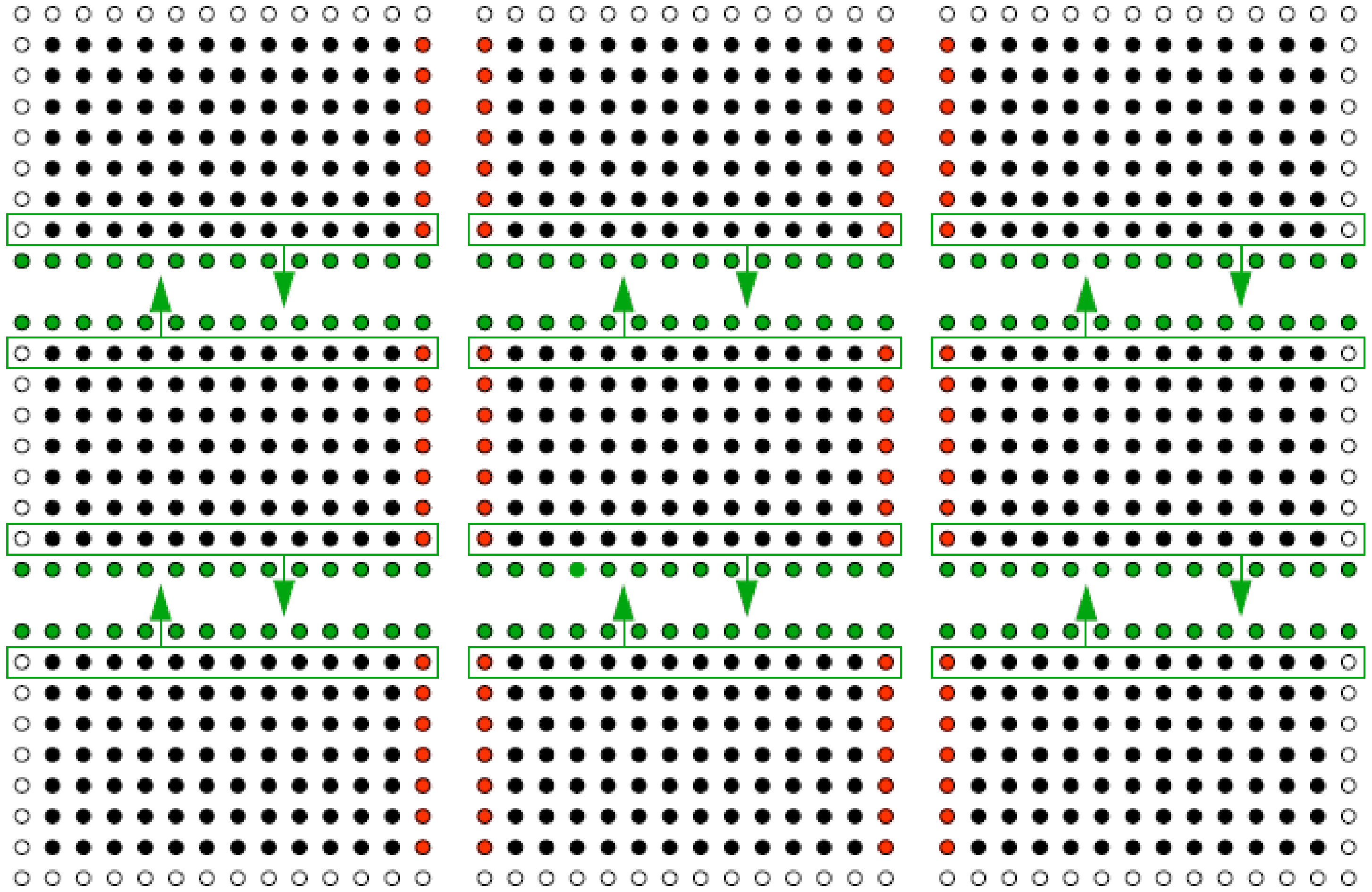












Grid Structure

```
struct _RECT_GRID {
        double L[3];       /* Lower corner of rectangle containing grid */
        double U[3];       /* Upper corner of rectangle containing grid */
        double h[3];       /* Average grid spacings in the grid         */
        int   gmax[3];    /* Number of grid blocks                      */
        int   dim;        /* Dimension of Grid */

                /* Specifications for virtual domains and variable grids */

        double GL[3];      /* Lower corner of global grid */
        double GU[3];      /* Upper corner of global grid */
        double VL[3];      /* Lower corner of virtual domain */
        double VU[3];      /* Upper corner of virtual domain */
        int   lbuf[3];    /* Lower buffer zone width */
        int   ubuf[3];    /* Upper buffer zone width */
};
typedef struct _RECT_GRID RECT_GRID;
```

Solution Storage

```
#define  soln(u, ic, gr)     (u[n_indx((ic), (gr))])
#define  n_indx(ic, gr)     ((ic)[1]*((gr)->gmax[0]+(gr)->lbuf[0]+(gr)->ubuf[0]) + (ic)[0])


double  *u_store, *u;
int          x_size, y_size, i, ic[2];
RECT_GRID *gr;
….
// properly initialize gr.
….
x_size = gr->gmax[0]+gr->lbuf[0]+gr->ubuf[0];
y_size = gr->gmax[1]+gr->lbuf[1]+gr->ubuf[1];

u_store = new double [x-size*y-size];
u = u_store + gr->lbuf[1]*x_size + gr->lbuf[0];


// show state at the first row of the grid
ic[1] = 0;
for(i = -gr->lbuf[0]; i < gr->lbuf[0]+gr->ubuf[0]; i++)
{
   ic[0] = i;
   cout << “state = “ << soln(u,ic,gr) <<endl;
}
```

Communication of Rectangular Lattice States

```
*     i = 0
*
*                l[0]+lbuf[0]     u[0]-ubuf[0]
*                    |               |
*                   \|/             \|/
*      l[1] |------|-----------------------------|------|
*           |      |      |          |      |      |
*           |  R   |      |          |      |  R   |
*           |  E   |      |          |      |  E   |
*           |  C   |  S   |          |  S   |  C   |
*           |  E   |  E   |          |  E   |  E   |
*           |  I   |  N   |          |  N   |  I   |
*           |  V   |  D   |          |  D   |  V   |
*           |  E   |      |          |      |  E   |
*           |      |      |          |      |      |
*           |      |      |          |      |      |
*           |      |      |          |      |      |
*      l[1]|------|-----------------------------|------|
*      Vl[0]     l[0]                     u[0]  Vu[0]
*    i = 1
*
*     Vu[1]--------------------------------------------
*         |                                           |
*         |          RECEIVE                          |
*     l[1] |------------------------------------------|
*         |                                           |
*         |            SEND                           |
*         |------------------------------------------|
*         |                                           |
*         |                                           |
*         |                                           |
*         |                                           |
*         |                                           |
*         |                                           |
*         |------------------------------------------|
*         |                                           |
*         |            SEND                           |
*      l[1]|------------------------------------------|
*         |                                           |
*         |          RECEIVE                          |
*     Vl[1]--------------------------------------------
*     Vl[0]                                  Vu[0]
```

```
// Assume we have created a Cartesian grid topology with communicator
// grid_comm

void scatter_states(
double       *u,
RECT_GRID *gr)
{
    int     my_id, side, dim = 2, i;
    int     me[2];

    MPI_Comm_rank(grid_comm , &my_id);
    MPI_Cart_coords(grid_comm, my_id, 2, me);
    for(i = 0; i < dim;  i++)
    {
        for(side = 0; side < 2; side++)
        {
            MPI_Barrier(MPI_Comm);
            pp_send_interior_states(me, i, side, u);
            pp_receive_interior_states(me, i, (side+1)%2, u);
        }
    }
}
```

```
// Assume G[2] stores orders of process grid
void pp_send_interior_states(
int  *me,
int   dir,
int   side,
double *u)
{
    int   him[2], i, dim = 2;
    int   dst_id;
    int   L[3], U[3];
    double     *storage;

    for (i = 0; i < dim; i++)
          him[i] = me[i];
     him[dir] = (me[dir] + 2*side - 1);
     if (him[dir] < 0)
          him[dir] = G[dir] - 1;
      if (him[dir] >= G[dir])
          him[dir] = 0;
      MPI_Cart_rank(grid_comm, him, &dst_id);

      /// figure out region in which the data need to be sent
      set_send_domain(L,U,dir,side,gr);

      storage = new double [(U[0]-L[0])*(U[1]-L[1])];
      // collect data and put into storage
       …
     //
     MPI_Bsend(storage, (U[0]-L[0])*(U[1]-L[1]), MPI_DOUBLE, dst_id, 100, MPI_COMM);
}
```

```
set_send_domain(int *L, int *U,int dir, int side,RECT_GRID *gr)
{
      int           dim = gr->dim;
      int           *lbuf = gr->lbuf;
      int           *ubuf = gr->ubuf;
      int           *gmax = gr->gmax;
      int           j;
      for (j = 0; j < dir; ++j)
      {
         L[j] = -lbuf[j];
         U[j] = gmax[j] + ubuf[j];
      }
      if (side == 0)
      {
         L[dir] =  0;
         U[dir]] = lbuf[dir];
      }
      else
      {
         L[dir] = gmax[dir] - ubuf[dir];
         U[dir]] = gmax[dir];
      }
      for (j = dir+1; j < dim; ++j)
      {
         L[j] = -lbuf[j];
         U[j] = gmax[j] + ubuf[j];
      }
}
```

```
void pp_receive_interior_states(
int  *me,
int   dir,
int   side,
double *u)
{
    int   him[2], i, dim = 2;
    int   src_id;
    int   L[3], U[3];
    double     *storage;
     MPI_Status   *status;

    for (i = 0; i < dim; i++)
          him[i] = me[i];
     him[dir] = (me[dir] + 2*side - 1);
     if (him[dir] < 0)
          him[dir] = G[dir] - 1;
      if (him[dir] >= G[dir])
          him[dir] = 0;
      MPI_Cart_rank(grid_comm, him, &src_id);

      /// figure out region in which the data need to be sent
      set_receive_domain(L,U,dir,side,gr);

      storage = new double [(U[0]-L[0])*(U[1]-L[1])];

      MPI_Recv(storage, (U[0]-L[0])*(U[1]-L[1]), MPI_DOUBLE, src_id, 100, MPI_COMM,&status);
     // Put received data into proper places of u
}
```

```
set_receive_domain(int  *L,int *U,int dir,int side, RECT_GRID *gr)
{
        int             dim = gr->dim;
        int             *lbuf = gr->lbuf;
        int             *ubuf = gr->ubuf;
        int             *gmax = gr->gmax;
        int             j;
        for (j = 0; j < dir; ++j)
        {
            L[j] = -lbuf[j];
            U[j] = gmax[j] + ubuf[j];
        }
        if (side == 0)
        {
            L[dir] = -lbuf[dir];
            U[dir] = 0;
        }
        else
        {
            L[dir] = gmax[dir];
            U[dir] = gmax[dir] + ubuf[dir];
        }
        for (j = dir+1; j < dim; ++j)
        {
            L[j] = -lbuf[j];
            U[j] = gmax[j] + ubuf[j];
        }
}
```

Putting Together

```
int main()
{
    int      i, j, k, Max_steps = 10000, ic[2];
    RECT_GRID     *gr;
    double            *u, *u_prev, *tmp;

    // initialize lattice grid: gr
    // initialize storage: *u;
    // initialize state
    // computation
    for(i = 0; i < Max_steps; i++)
    {
       /// time stepping
       for(j = 0; j < gr->gmax[0]; j++)
       {
           ic[0] = j;
           for(k = 0; k < gr->gmax[1]; k++)
           {
               ic[1] = k;
                // update soln:  soln(u, ic, gr) = soln(u_prev, ic, gr) + … ;
            }
       }
       // communication to update ghost points
       scatter_states( u, gr);

       // swap storage for next step
       tmp = u;          u = u_prev;
       u_prev = tmp;
    }
}
```

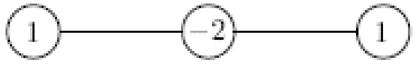
Lecture 9: Numerical Partial Differential Equations(Part 2)

Finite Difference Method to Solve Poisson's Equation

- Poisson's equation in 1D:

$$\begin{cases} -\frac{d^2u}{dx^2} = f(x),\ x \in (0,1) \\ u(0) = u(1) = 0 \end{cases}.$$

- Spatial Discretization: $0 = x_0 < \cdots < x_M = 1$. Define $\Delta x = \frac{1}{M}$. Then $x_i = i\Delta x$.
- $\frac{d^2u(x_i)}{dx^2} \sim \frac{u(x_{i-1}) - 2u(x_i) + u(x_{i+1})}{\Delta x^2}$
- Stencil of finite difference approximation



- Finite difference equations: for $i = 1, \dots, M-1$

$$-u_{i-1} + 2u_i - u_{i+1} = \Delta x^2 f_i$$
$$u_0 = 0$$
$$u_M = 0$$

with $f_i = f(x_i)$

- Put into matrix equation format:

  Let $\boldsymbol{u} = (u_1, u_2, \dots, u_{M-1})^T$, $\boldsymbol{f} = (f_1, f_2, \dots, f_{M-1})^T$

$$A\boldsymbol{u} = \Delta x^2 \boldsymbol{f}$$

$$A = \begin{bmatrix} 2 & -1 & & & & & \\ -1 & 2 & -1 & & & & \\ & -1 & 2 & -1 & & & \\ & & \ddots & \ddots & \ddots & & \\ & & -1 & 2 & -1 & & \\ & & & -1 & 2 & -1 \\ & & & & -1 & 2 \end{bmatrix}$$

2D Poisson's Equation

Consider to solve

$$\begin{cases} -(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}) = f(x,y), \ (x,y) \in \Omega \\ \qquad u(x,y) = 0 \quad on \quad \partial\Omega \end{cases}$$

with Ω is rectangle $(0,1) \times (0,1)$ and $\partial\Omega$ is its boundary.

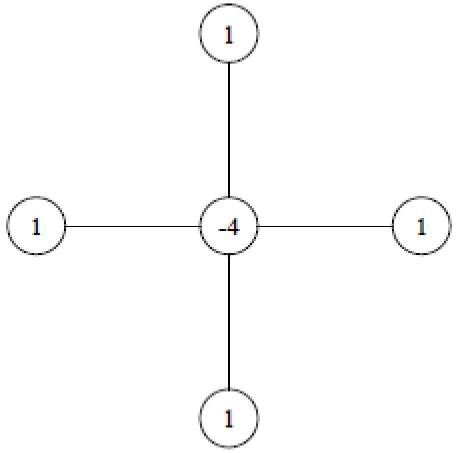
- Define $h = \frac{1}{M}$.
- Spatial Discretization: $0 = x_0 < \cdots < x_M = a$ with $x_i = ih$ and $0 = y_0 < \cdots < y_M = 1$ with $y_j = jh$.

Finite difference equation at grid point (i, j):

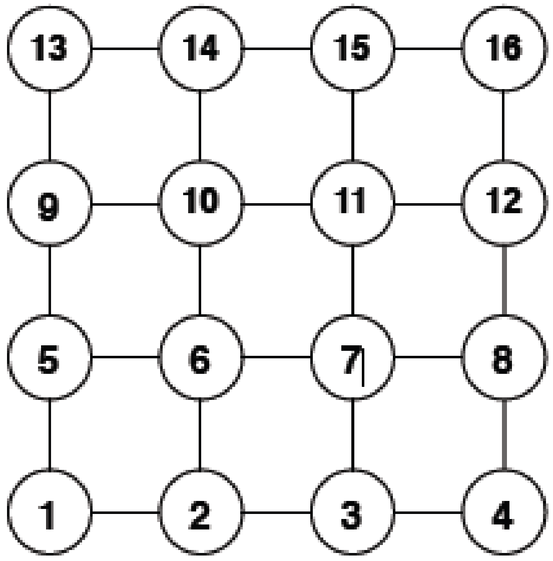
$$-\left(\frac{u_{i-1,j}-2u_{i,j}+u_{i+1,j}}{h^2}+\frac{u_{i,j-1}-2u_{i,j}+u_{i,j+1}}{h^2}\right)=f(x_i,y_j) \text{ or}$$

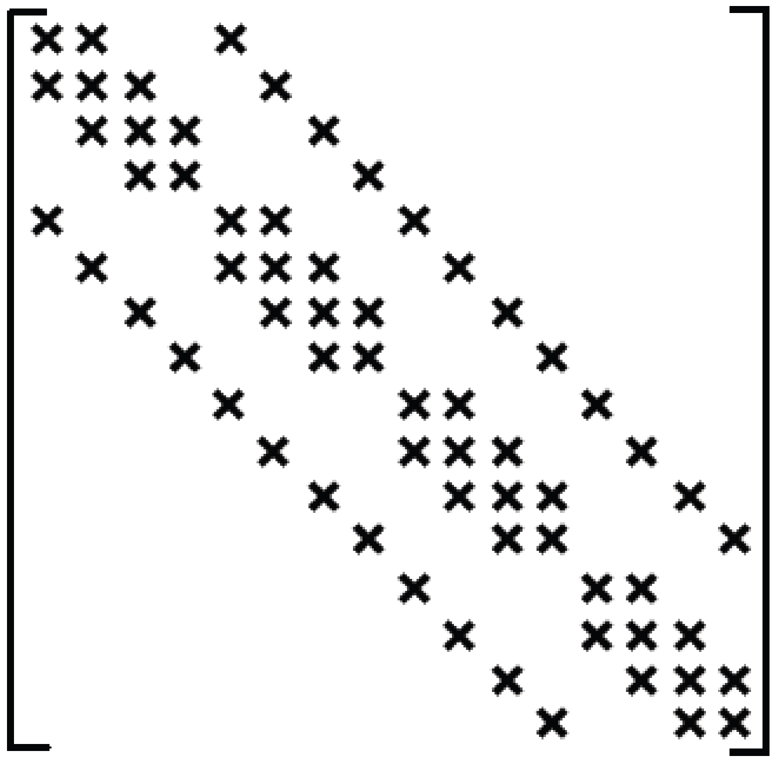
$$-u_{i,j-1}-u_{i-1,j}+4u_{i,j}-u_{i+1,j}-u_{i,j+1}=h^2 f(x_i,y_j)$$

- Five-point stencil of the finite difference approximation



Natural Row-Wise Ordering



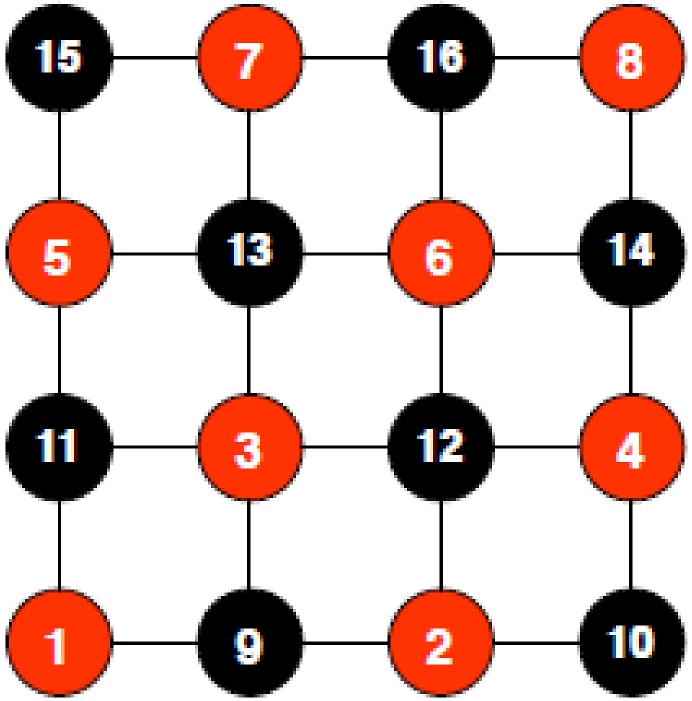


$$u_{ij}^{(k+1)} = (1-w)u_{ij}^{(k)} \\ + w/4\left(h^2 f_{ij} + u_{i-1,j}^{(k+1)} + u_{i,j-1}^{(k+1)} + u_{i+1,j}^{(k)} + u_{i,j+1}^{(k)}\right)$$

This is completely sequential.

Red-Black Ordering

- Color the alternate grid points in each dimension red or black



R/B SOR

- First iterates on red points by

$$u_{ij}^{(k+1)} = (1-w)u_{ij}^{(k)} + w/4\left(h^2 f_{ij} + u_{i-1,j}^{(k)} + u_{i,j-1}^{(k)} + u_{i+1,j}^{(k)} + u_{i,j+1}^{(k)}\right)$$

- Then iterates on black points by

$$u_{ij}^{(k+1)} = (1-w)u_{ij}^{(k)} + w/4\left(h^2 f_{ij} + u_{i-1,j}^{(k+1)} + u_{i,j-1}^{(k+1)} + u_{i+1,j}^{(k+1)} + u_{i,j+1}^{(k+1)}\right)$$

- R/B SOR can be implemented in parallel on the same color grid points.
- The renumbering of the matrix A changes the iteration formula.

For the example just shown:

$$A = \begin{bmatrix} D_r & -C \\ -C^T & D_b \end{bmatrix}$$

Diagonal matrices $D_r = D_b = 4I_8$.

$$C = \begin{pmatrix} 1 & & 1 & & & & & \\ 1 & 1 & & 1 & & & & \\ 1 & & 1 & & 1 & 1 & & \\ & 1 & & 1 & & 1 & & \\ & & 1 & & 1 & & 1 & \\ & & & 1 & 1 & 1 & & 1 \\ & & & & 1 & & 1 & 1 \\ & & & & & 1 & & 1 \end{pmatrix}$$

$$\begin{bmatrix} \times & & & & & & & & \times & & \times & & & & & \\ & \times & & & & & & & \times & \times & & \times & & & & \\ & & \times & & & & & & \times & & \times & \times & \times & & & \\ & & & \times & & & & & & \times & & \times & & \times & & \\ & & & & \times & & & & & & \times & & \times & & \times & \\ & & & & & \times & & & & & & \times & \times & \times & & \times \\ & & & & & & \times & & & & & & \times & & \times & \times \\ & & & & & & & \times & & & & & & \times & & \times \\ \times & \times & \times & & & & & & \times & & & & & & & \\ & \times & & \times & & & & & & \times & & & & & & \\ \times & & \times & & \times & & & & & & \times & & & & & \\ & \times & \times & \times & & \times & & & & & & \times & & & & \\ & & \times & & \times & \times & \times & & & & & & \times & & & \\ & & & \times & & \times & & \times & & & & & & \times & & \\ & & & & \times & & \times & & & & & & & & \times & \\ & & & & & \times & \times & \times & & & & & & & & \times \end{bmatrix}$$

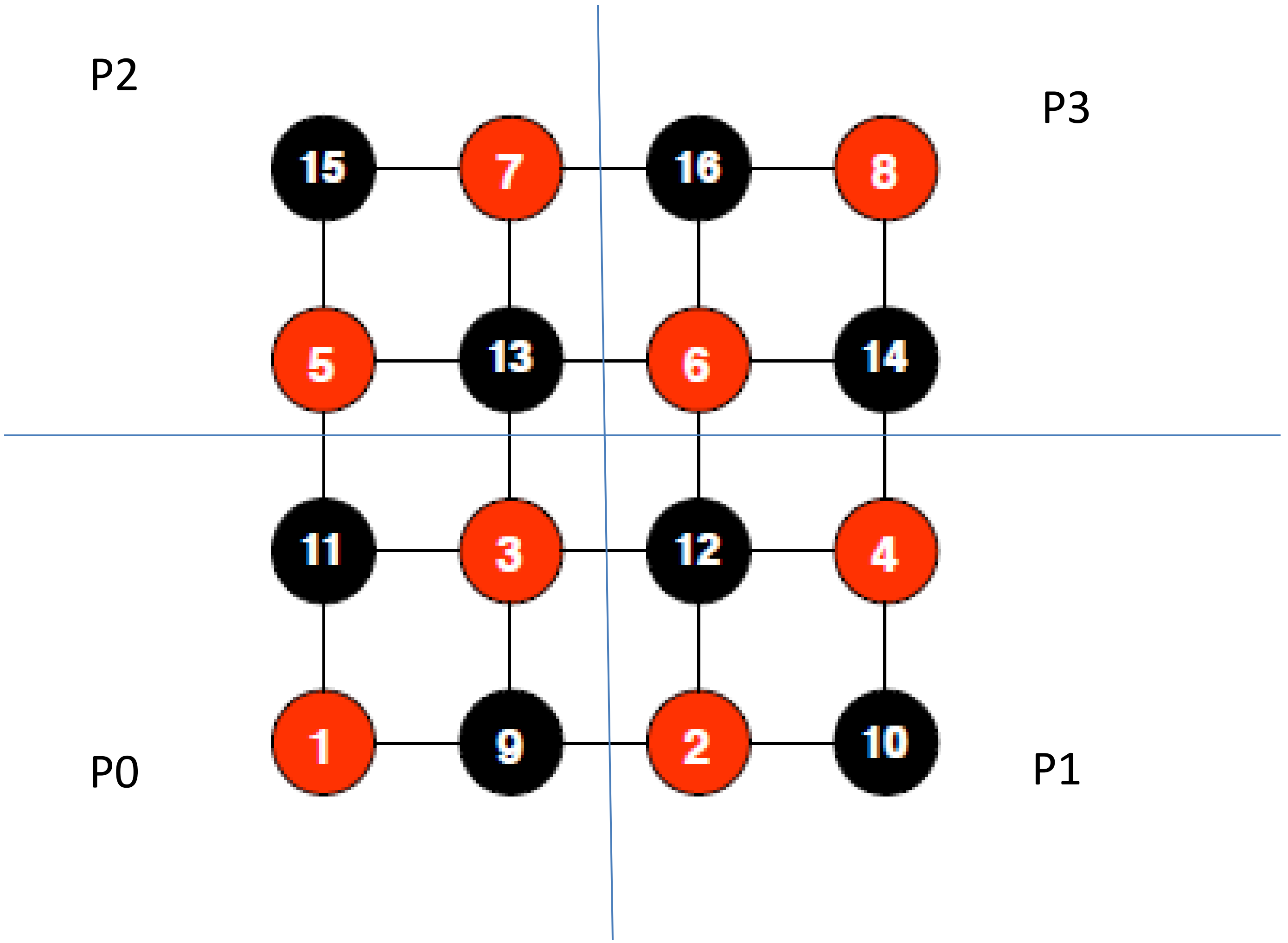
- Using GS:

$$\begin{bmatrix} D_r & 0 \\ -C^T & D_b \end{bmatrix} \begin{bmatrix} \boldsymbol{u}_r^{(k+1)} \\ \boldsymbol{u}_b^{(k+1)} \end{bmatrix} = \begin{bmatrix} 0 & C \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{u}_r^{(k)} \\ \boldsymbol{u}_b^{(k)} \end{bmatrix} + h^2 \boldsymbol{f}$$

Here $\boldsymbol{u}_r = (u_1, u_2, u_3, u_4, \ldots, u_8)^T$

$$\boldsymbol{u}_b = (u_9, u_{10}, u_{11}, u_{12}, \ldots, u_{16})^T$$

Parallel R/B SOR



Algorithm

```
While error > TOL, do:
    – Compute all red-points
    – Send/Recv values of the red-points at the boarder of
      the subdomain to neighboring processes
    – Compute all black-points
    – Send/Recv values of the black-points at the boarder of
      the subdomain to neighboring processes
    Compute residual error
Endwhile
```

References

- L. Adams and J.M. Ortega. A Multi-Color SOR Method for Parallel Computation. ICASE 82-9. 1982.
- L. Adams and H.F. Jordan. Is SOR Color-Blind? *SIAM J. Sci. Stat. Comput.* 7(2):490-506, 1986
- D. Xie and L. Adams. New Parallel SOR Method by Domain Partitioning. *SIAM J. Sci. Comput.* 20(6), 1999.

Lecture 9: Numerical Partial Differential Equations(Part 3) – MPI user-defined Datatype

From SOR.c

```
ierr = MPI_Sendrecv(&Phi[(i_send*ColNumber)+j_send], 1, MPI_InteriorPointsCol,
mynode.west,tag, &Phi[(i_recv*ColNumber)+j_recv],
1,MPI_InteriorPointsCol,mynode.east,tag, MPI_COMM_WORLD, &status);
```

Derived Datatypes

- Techniques for describing non-contiguous and heterogeneous (structure) data
  - Data are not contiguous in memory
- MPI uses *derived datatypes* for this purpose.

MPI type-definition functions

- *MPI_Type_Contiguous*: a replication of datataype into contiguous locations
- *MPI_Type_vector*: replication of datatype into locations that consist of equally spaced blocks
- *MPI_Type_commit:* commit user defined derived datatype
- *MPI_Type_free:* free the derived datatype
- *MPI_Type_create_hvector:* like vector, but successive blocks are not multiple of base type extent
- *MPI_Type_indexed:* non-contiguous data layout where displacements between successive blocks need not be equal
- *MPI_Type_create_struct:* most general – each block may consist of replications of different datatypes

- *MPI_Type_contiguous* (int count, MPI_Datatype oldtype, MPI_Datatype *newtype)
  - IN count (replication count)
  - IN oldtype (base data type)
  - OUT newtype (handle to new data type)

- Creates a new type which is simply a replication of oldtype into contiguous locations

Example 1:

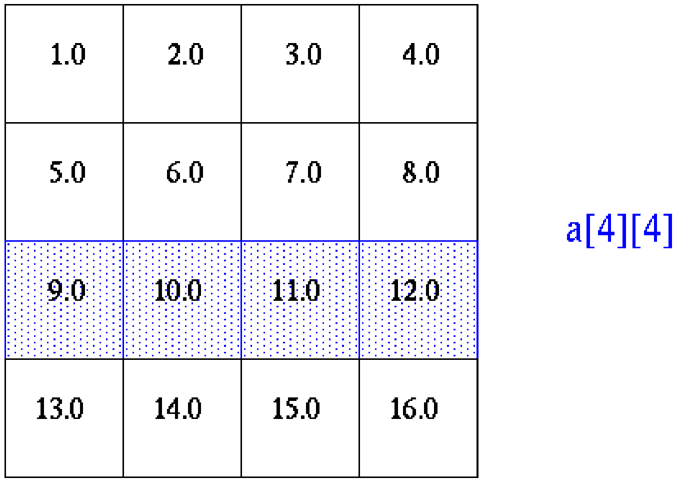
```
/* create a type which describes a line of ghost cells */
/* buf[0], buf1],...,buf[nxl-1] set to ghost cells */
        int nxl;
       MPI_Datatype ghosts;

       MPI_Type_contiguous (nxl, MPI_DOUBLE, &ghosts);
       MPI_Type_commit(&ghosts)
       MPI_Send (buf, 1, ghosts, dest,  tag, MPI_COMM_WORLD);
       ..
       ..
       MPI_Type_free(&ghosts);
```

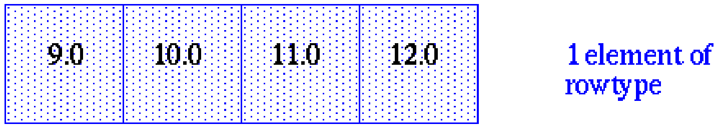
From red_black_SOR.c

```
ierr   =  MPI_Type_contiguous(BlockLenH,MPI_DOUBLE,&MPI_InteriorPointsRow);
```

```
count = 4;
MPI_Type_contiguous(count, MPI_FLOAT, &rowtype);
```



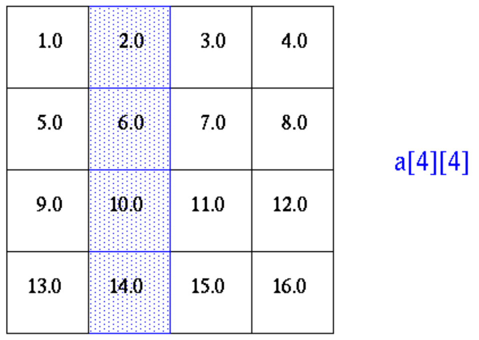
```
MPI_Send(&a[2][0], 1, rowtype, dest, tag, comm);
```



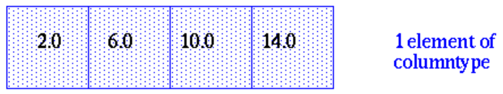
- *MPI_Type_vector* (int count, int blocklength, int stride, MPI_Datatype oldtype, MPI_Datatype *newtype);
  - IN count (number of blocks)
  - IN blocklength (number of elements per block)
  - IN stride (spacing between start of each block, measured in # elements)
  - IN oldtype (base datatype)
  - OUT newtype (handle to new type)

  - Allows replication of old type into locations of equally spaced blocks. Each block consists of same number of copies of oldtype with a stride that is multiple of extent of old type.

```
count = 4;   blocklength = 1;   stride = 4;
MPI_Type_vector(count, blocklength, stride, MPI_FLOAT,
                &columntype);
```



```
MPI_Send(&a[0][1], 1, columntype, dest, tag, comm);
```



Example 1. Use MPI_Type_vector to send a submatrix: Suppose There is a 4x4 matrix and we want to send the middle four elements.

Type_vector.c

Example 2. red_black_SOR.c

```
ierr  |=  MPI_Type_vector(BlockLenV,1,ColNumber,MPI_DOUBLE,
                         &MPI_InteriorPointsCol);
```

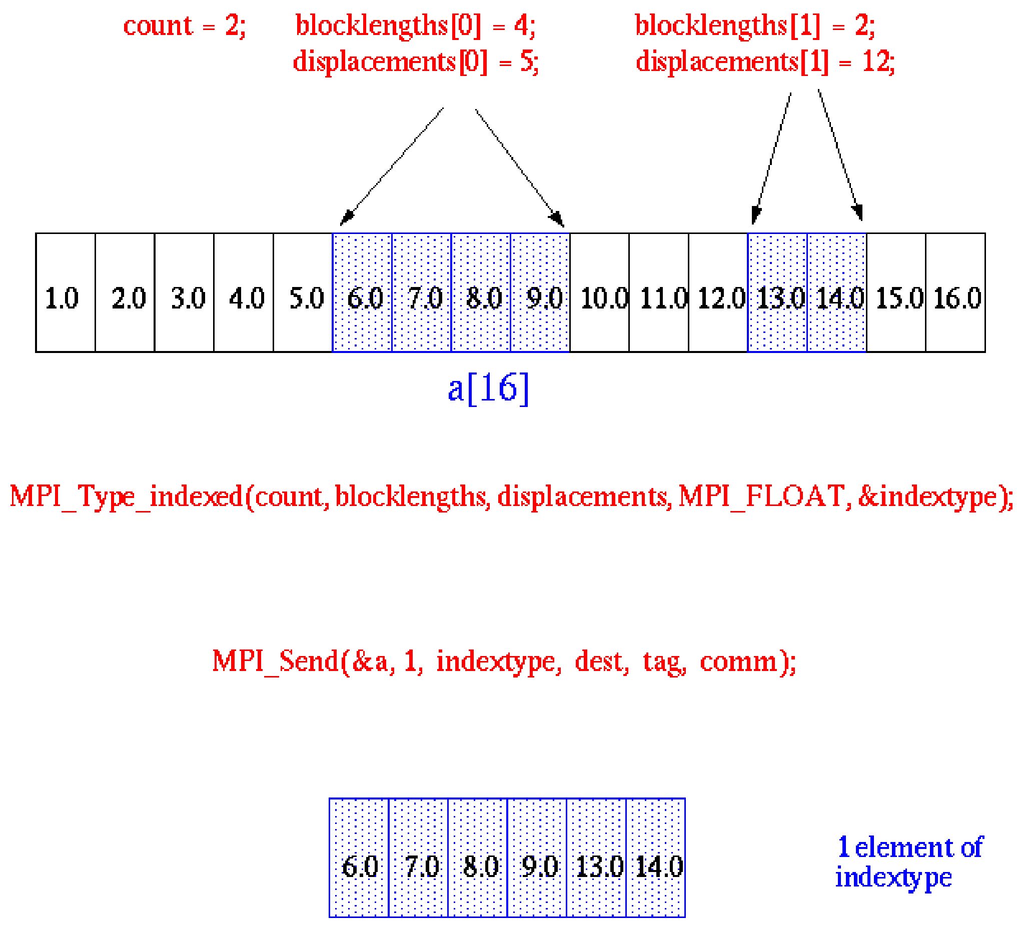
- *MPI_Type_create_hvector* (int count, int blocklength, MPI_Aint stride, MPI_Datatype old, MPI_Datatype *new)
  - IN count (number of blocks)
  - IN blocklength (number of elements/block)
  - IN stride (number of bytes between start of each block)
  - IN old (old datatype)
  - OUT new (new datatype)
- Same as MPI_Type_vector, except that stride is given in bytes rather than in elements (‘h’ stands for ‘heterogeneous).

- *MPI_Type_indexed* (int count, int *array_of_blocklengths, int *array_of_displacements, MPI_Datatype oldtype, MPI_Datatype *newtype);
  - IN count (number of blocks)
  - IN array_of_blocklengths (number of elements/block)
  - IN array_of_displacements (displacement for each block, measured as number of elements)
  - IN oldtype
  - OUT newtype

- Displacements between successive blocks need not be equal. This allows gathering of arbitrary entries from an array and sending them in a single message.

- The high level view of MPI_Type_indexed is that you create a type to represent a particular part of a matrix. And then you commit that type using MPI_Type_commit. So, You specify an arbitrary number of blocks(i.e. continuous elements) of arbitrary lengths within the matrix. *Count* is the total number of elements that you are sending of *old_type*, *array_of_blocklengths* is an array the length of each block you will send, and *array_of_displacements* is an array of where each block begins (i.e. displacement from the beginning of the array.

- **Example.** Use MPI_Type_indexed to send a subarray: sample_Type_index.c


count = 2;
blocklengths[0] = 4;
displacements[0] = 5;
blocklengths[1] = 2;
displacements[1] = 12;
1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 15.0 16.0
a[16]
MPI_Type_indexed(count, blocklengths, displacements, MPI_FLOAT, &indextype);
MPI_Send(&a, 1, indextype, dest, tag, comm);
6.0 7.0 8.0 9.0 13.0 14.0
1 element of indextype