Distributed Parallel Programming with MPI - part 2

Ramses van Zon

PHY1610 Winter 2025

Communication patterns in MPI

Communication patterns in MPI

1. No communication between processes
   `MPI_Init`, `MPI_Comm_size`, `MPI_Comm_rank`, `MPI_Finalize`
2. Point-to-point
   `MPI_Ssend`, `MPI_Recv`, `MPI_Sendrecv`
3. Broadcast
   Send same data from one rank to all others
4. Reduction
   Combine results from all ranks (*e.g.* sum)
5. Scatter
   Send different data from one rank to all others
6. Gather
   Collect data from one rank to all others
7. All-to-all
   Everyone sends something to everyone

Recap: Send/Recv code

```
// fifthmessage.cpp
#include <iostream>
#include <string>
#include <mpi.h>
int main() {
    int rank, size, left, right;
    double msgsent, msgrcvd;
    MPI_Init(nullptr, nullptr);
    MPI_Comm_size(MPI_COMM_WORLD, &size);
    MPI_Comm_rank(MPI_COMM_WORLD, &rank);
    left = rank-1;
    if (left < 0) left = size-1;
    right = rank+1;
    if (right >= size) right = 0;
    msgsent = rank*rank;
    msgrcvd = -999.;
    MPI_Sendrecv(&msgsent, 1, MPI_DOUBLE, right, 749,
                 &msgrcvd, 1, MPI_DOUBLE, left, 749,
                 MPI_COMM_WORLD, MPI_STATUS_IGNORE);
    std::cout << std::to_string(rank) + ": Sent " + std::to_string(msgsent)
              + " and got " + std::to_string(msgrcvd) + "\n";
    MPI_Finalize();
}
```

By the way, about that string concatenation

To print a line of text from each process, the code does not have

```
std::cout << rank << ": Sent " << msgsent << " and got " << msgrcvd << "\n";
```

but instead uses string conversion and concatenation before streaming to the terminal

```
std::cout << std::to_string(rank) + ": Sent " + std::to_string(msgsent)
          + " and got " + std::to_string(msgrcvd) + "\n";
```

There's a good reason:

- In the first case, each "`<< SOMETHING`" is a request for output to the terminal.
- The requests are handled in (essentially) random order.
- This means the parts of the output lines are likely interleaved, and the lines don't make any sense.
- By concatenating everything on the same line to a string,
  each process has just one request to write a single line.
- While these can still be processed in any order, the lines stay intact.
- *Bonus: this will help in parallelization of output.*

3. MPI Broadcast

Broadcast

This involves one process sending data to all others.

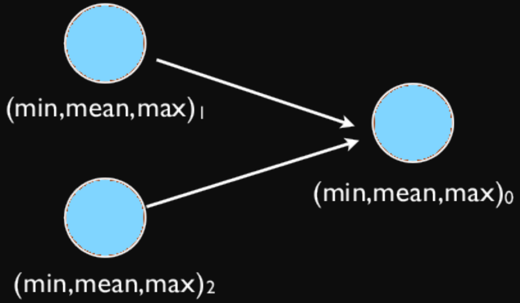
```
#include <mpi.h>
#include <string>
#include <iostream>
int main() {
    int rank, size, iorank = 0;
    std::string name;
    MPI_Init(nullptr, nullptr);
    MPI_Comm_rank(MPI_COMM_WORLD, &rank);
    if (rank == iorank) {
       std::cout << "What is your name? ";
       std::cin  >> name;
       size = name.size();
    }
    MPI_Bcast(&size, 1, MPI_INT,
              iorank, MPI_COMM_WORLD);
    name.resize(size);
    MPI_Bcast(&name[0], size, MPI_CHAR,
              iorank, MPI_COMM_WORLD);
    std::cout << "Rank " + std::to_string(rank)
                 + " knows " + name + "\n";
    MPI_Finalize();
}
```

```
$ mpicxx -o bcastex bcastex.cpp
$ mpirun -n 3 ./bcastex
What is your name? Ramses
Rank 0 knows Ramses
Rank 1 knows Ramses
Rank 2 knows Ramses
```

4. MPI Reductions

Reductions: Min, Mean, Max Example

- Calculate the min/mean/max of random numbers -1.0 . . . 1.0
- Should trend to -1/0/+1 for a large N.
- How to MPI it?
- Partial results on each node, collect all to node 0.



Reductions: Min, Mean, Max Example (1/2)

```
// Computes the min,mean&max of random numbers
#include <mpi.h>
#include <iostream>
#include <algorithm>
#include <random>
#include <rarray>
int main()
{
  const long nx = 200'000'000;
  // find this process place
  int rank;
  int size;
  MPI_Init(nullptr, nullptr);
  MPI_Comm_size(MPI_COMM_WORLD, &size);
  MPI_Comm_rank(MPI_COMM_WORLD, &rank);
  // determine its subrange of data
  const long nxper=(nx+size-1)/size;
  const long nxstart=nxper*rank;
  const long nxown=(rank<size-1)?nxper
                 :(nx-nxper*(size-1));
  rvector<double> dat(nxown);
  std::uniform_real_distribution<double>
     uniform(-1.0,1.0);
  std::minstd_rand engine(14);
  // each process skip ahead to start
  std::engine.discard(nxstart);
  // compute local data
  for (long i=0;i<nxown;i++)
      dat[i] = uniform(engine);
  const long MIN=0, SUM=1, MAX=2;
  rvector<double> mmm(3);
  mmm = 1e+19, 0, -1e+19;
  for (long i=0;i<nxown;i++) {
      mmm[MIN] = min(dat[i], mmm[MIN]);
      mmm[MAX] = max(dat[i], mmm[MAX]);
      mmm[SUM] += dat[i];
  }
  // send results to a collecting rank
  const long collectorrank = 0;
  if (rank != collectorrank)
    MPI_Ssend(mmm.data(), 3,MPI_DOUBLE,
              collectorrank, 749,
              MPI_COMM_WORLD);
  else {
```

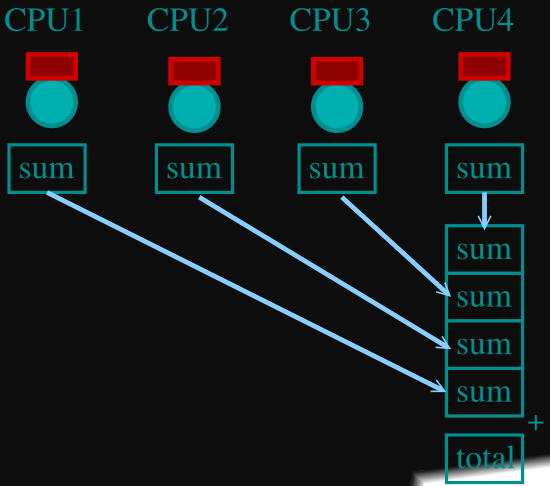
Reductions: Min, Mean, Max Example (1/2)

```
    rvector<double> recvmmm(3);
    for (long i = 1; i < size; i++) {
       MPI_Recv(recvmmm.data(), 3,
                MPI_DOUBLE,
                MPI_ANY_SOURCE, 749,
                MPI_COMM_WORLD,
                MPI_STATUS_IGNORE);
       mmm[MIN] = min(recvmmm[MIN],
                      mmm[MIN]);
       mmm[MAX] = max(recvmmm[MAX],
                      mmm[MAX]);
       mmm[SUM] += recvmmm[SUM];
    }
    // output
    std::cout << "Global Min/mean/max "
         << mmm[MIN] << " "
         << mmm[SUM]/nx <<" "
         << mmm[MAX] << "\n";
  }
  MPI_Finalize();
}
```

Efficiency?

- Requires (P-1) messages
- 2(P-1) if everyone then needs to get the answer.

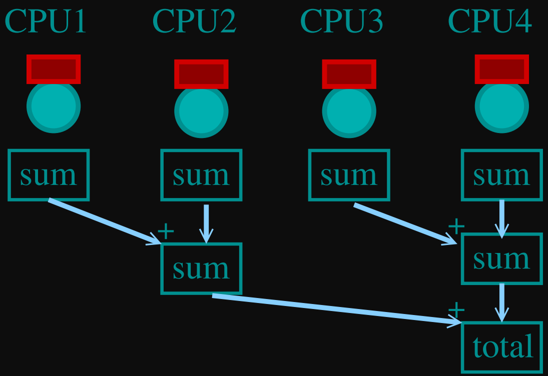
$$T_{comm} = PC_{comm}$$



Better Summing

- Pairs of processors; send partial sums
- Max messages received $\log_2(P)$
- Can repeat to send total back.

$$T_{comm} = 2\log_2(P)C_{comm}$$



Reduction: Works for a variety of operations (+,*,min,max)

MPI Collectives

```
MPI_Allreduce(sendptr, rcvptr, count, MPI_TYPE, MPI_Op, Communicator);

MPI_Reduce(sendbuf, recvbuf, count, MPI_TYPE, MPI_Op, root, Communicator);
```

- `sendptr/rcvptr`: pointers to buffers
- `count`: number of elements in ptrs
- `MPI_TYPE`: one of `MPI_DOUBLE`, `MPI_FLOAT`, `MPI_INT`, `MPI_CHAR`, etc.
- `MPI_Op`: one of `MPI_SUM`, `MPI_PROD`, `MPI_MIN`, `MPI_MAX`.
- `Communicator`: MPI_COMM_WORLD or user created.
- The "`All`" variant sends result back to all processes; non-`All` sends to process `root`.

Reductions: Min, Mean, Max with MPI Collectives

```
rvector<double> globalmmm(3);
MPI_Allreduce(&mmm[MIN], &globalmmm[MIN], 1, MPI_DOUBLE, MPI_MIN, MPI_COMM_WORLD);
MPI_Allreduce(&mmm[MAX], &globalmmm[MAX], 1, MPI_DOUBLE, MPI_MAX, MPI_COMM_WORLD);
MPI_Allreduce(&mmm[SUM], &globalmmm[SUM], 1, MPI_DOUBLE, MPI_SUM, MPI_COMM_WORLD);
if (rank==0)
   std::cout << "Global Min/mean/max "
             << mmm[MIN] << " "
             << mmm[SUM]/nx << " "
             << mmm[MAX] << endl;
```

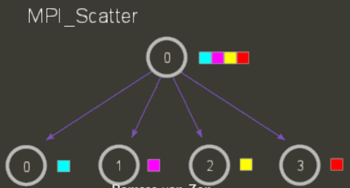
More Collective Operations

Collective

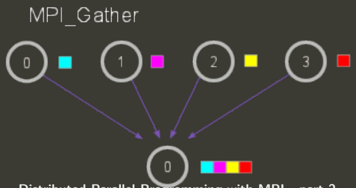
- Reductions are an example of a ***collective*** operation.
- As opposed to the pairwise messages we've seen before
- All processes in the communicator must participate.
- Cannot proceed until all have participated.
- Don't necessarity know what's "under the hood".

Other MPI Collectives

5. Scatter



6. Gather



7. Even more:

- All-to-all . . .
- File I/O
- Barriers (avoid!)

MPI Domain decomposition

Solving the diffusion equation with MPI

Consider a diffusion equation with an explicit **finite-difference**, **time-marching** method.

Imagine the problem is too large to fit in the memory of one node, so we need to do **domain decomposition**, and use **MPI**.

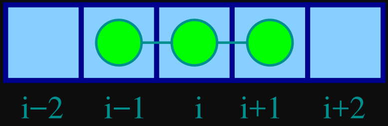
Discretizing Derivatives

- Partial Differential Equations like the diffusion equation

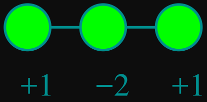
$$\frac{\partial T}{\partial t} = D\frac{\partial^2 T}{\partial x^2}$$

are usually numerically solved by finite differencing the discretized values.

$$\frac{\partial^2 T}{\partial x^2} \approx \frac{T_{i+1} - 2T_i + T_{i-1}}{\Delta x^2}$$



- Implicitly or explicitly involves interpolating data and taking the derivative of the interpolant.



- Larger “stencils” → More accuracy.

Diffusion equation in higher dimensions

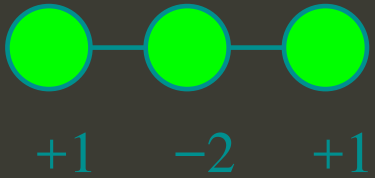
Spatial grid separation: Δx. Time step Δt.

Grid indices: i, j. Time step index: (n)

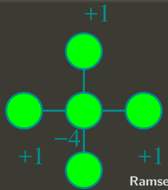
1D

$$\left.\frac{\partial T}{\partial t}\right|_i \approx \frac{T_i^{(n)} - T_i^{(n-1)}}{\Delta t}$$

$$\left.\frac{\partial^2 T}{\partial x^2}\right|_i \approx \frac{T_{i-1}^{(n)} - 2T_i^{(n)} + T_{i+1}^{(n)}}{\Delta x^2}$$



2D



$$\left.\frac{\partial T}{\partial t}\right|_{i,j} \approx \frac{T_{i,j}^{(n)} - T_{i,j}^{(n-1)}}{\Delta t}$$

$$\left.\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right)\right|_{i,j} \approx \frac{T_{i-1,j}^{(n)} + T_{i,j-1}^{(n)} - 4T_{i,j}^{(n)} + T_{i+1,j}^{(n)} + T_{i,j+1}^{(n)}}{\Delta x^2}$$

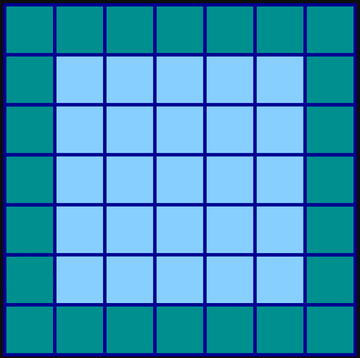
Stencils and Boundaries

- How do you deal with boundaries?
- The stencil juts out, you need info on cells beyond those you're updating.
- Common solution: ***Guard cells***:
  - Pad domain with these guard celss so that stencil works even for the first point in domain.
  - Fill guard cells with values such that the required boundary conditions are met.

1D

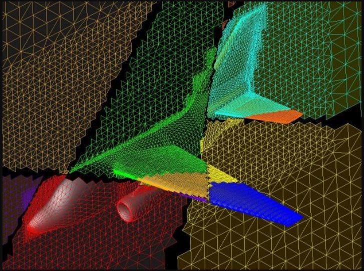
- Number of guard cells $n_g = 1$
- Loop from $i = n_g..N - 2n_g$.

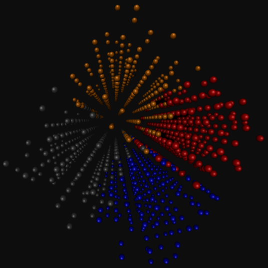
2D

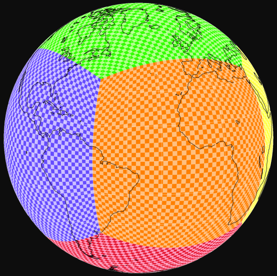


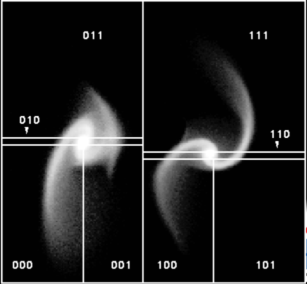
Domain decomposition

- A very common approach to parallelizing on distributed memory computers.
- Subdivide the domain into contiguous subdomains.
- Give each subdomain to a different MPI process.
- No process contains the full data!
- Maintains locality.
- Need mostly local data, ie., only data at the boundary of each subdomain will need to be sent between processes.



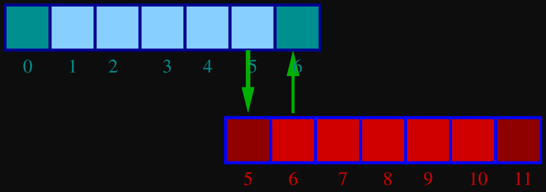






Guard cell exchange

- In the domain decomposition, the stencils will jut out into a neighbouring subdomain.
- Much like the boundary condition.
- One uses guard cells for domain decomposition too.
- If we managed to fill the guard cell with values from neighbouring domains, we can treat each coupled subdomain as an isolated domain with changing boundary conditions.



- Could use even/odd trick, or sendrecv.

1D diffusion with MPI

Before MPI

```
a = 0.25*dt/pow(dx,2);
guardleft = 0;
guardright = n+1;
for (int t=0;t<maxt;t++) {
 T[guardleft] = 0.0;
 T[guardright] = 0.0;
 for (int i=1; i<=n; i++)
   newT[i] = T[i] + a*(T[i+1]+T[i-1]-2*T[i]);
 for (int i=1; i<=n; i++)
   T[i] = newT[i];
}
```

After MPI

```
MPI_Init(&argc,&argv);
MPI_Comm_rank(MPI_COMM_WORLD,&rank);
MPI_Comm_size(MPI_COMM_WORLD,&size);
left  = rank-1; if(left<0)left=MPI_PROC_NULL;
right = rank+1; if(right>=size)right=MPI_PROC_NULL;
localn = n/size;
a = 0.25*dt/pow(dx,2);
guardleft = 0;
guardright = localn+1;
for (int t=0;t<maxt;t++) {
 MPI_Sendrecv(&T[1],          1,MPI_DOUBLE,left, 11,
              &T[guardright],1,MPI_DOUBLE,right,11,
              MPI_COMM_WORLD,MPI_STATUS_IGNORE);
 MPI_Sendrecv(&T[nlocal],     1,MPI_DOUBLE,right,11,
              &T[guardleft], 1,MPI_DOUBLE,left, 11,
              MPI_COMM_WORLD,MPI_STATUS_IGNORE);
 if (rank==0) T[guardleft] = 0.0;
 if (rank==size-1) T[guardright] = 0.0;
 for (int i=1; i<=localn; i++)
   newT[i] = T[i] + a*(T[i+1]+T[i-1]-2*T[i]);
 for (int i=1; i<=n; i++)
   T[i] = newT[i];
}
```

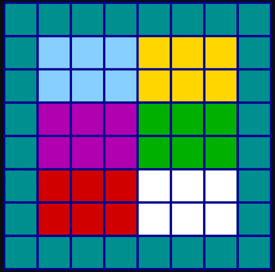
Note:

- the for-loop over i could also have been a call to dgemv for a submatrix.
- the for-loop over i could also easily be parallelized with OpenMP

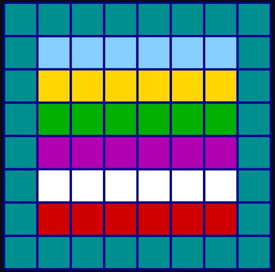
(→ hybrid MPI-OpenMP code)

2D diffusion with MPI

How to divide the work in 2d?



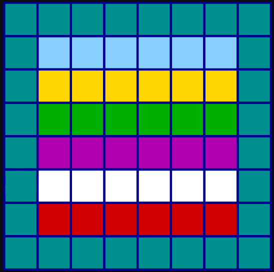
- Less communication (18 edges).
- Harder to program, non-contiguous data to send, left, right, up and down.



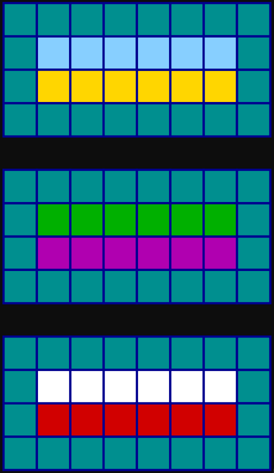
- Easier to code, similar to 1d, but with contiguous guard cells to send up and down.
- More communication (30 edges).

Let's look at the easiest domain decomposition.

***Serial*:**



Parallel* ($P = 3$)*:



Communication pattern:

- Copy upper stripe to upper neighbour bottom guard cell.
- Copy lower stripe to lower neighbout top guard cell.
- Contiguous cells: can use `count` in `MPI_Sendrecv`.
- Similar to 1d diffusion.