

Poiseuille flow simulation via Lattice Boltzmann method

Parallel Computing in Mathematical Modeling
and Data-Intensive Applications

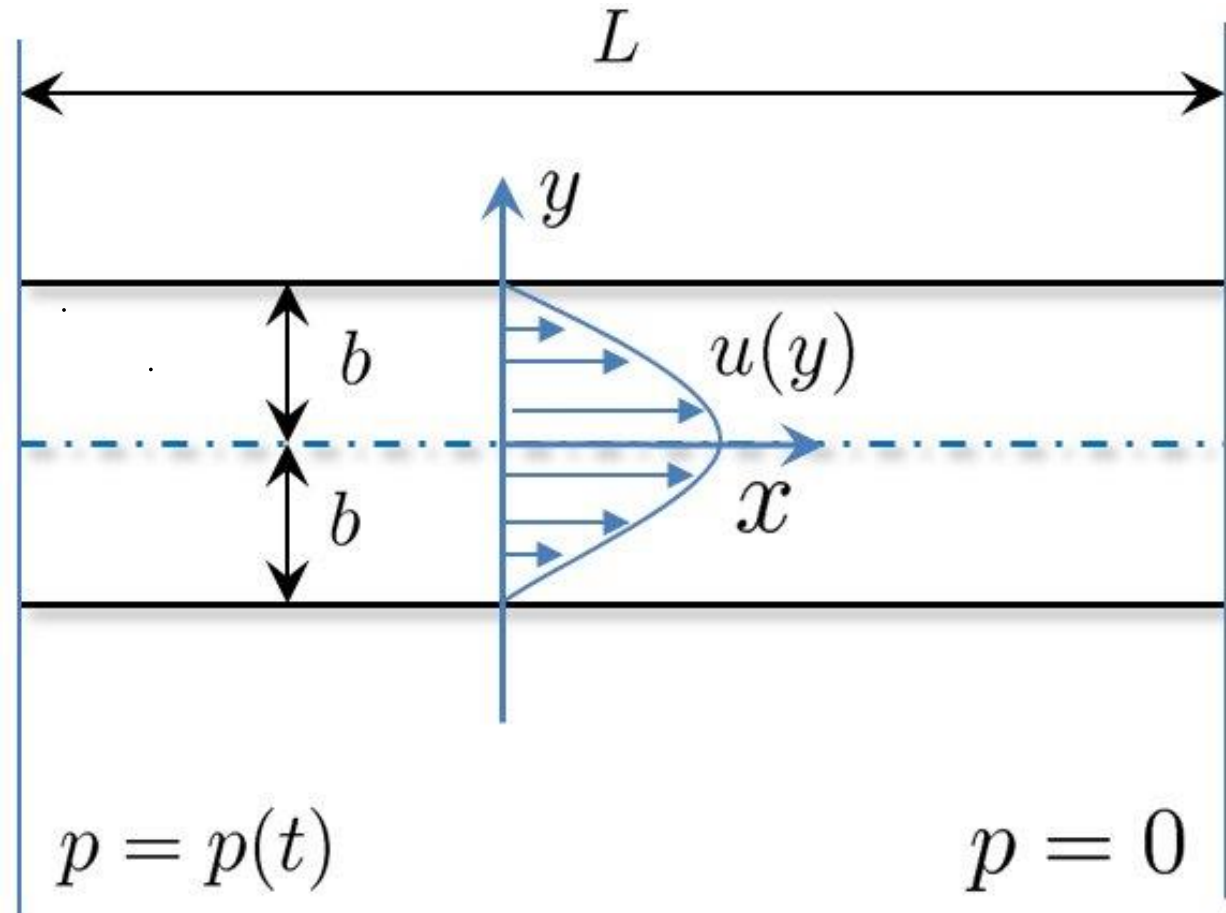
Task description

- Optimize given sequential Lattice Boltzmann method code
- Develop the parallelized code from sequential
- Profile. Measure timing and plot speedup plot depending on number of processes/threads.
- Conclude. Is the speedup You obtained is approximately linear?

Task description

Dimensionless parameters of simulation:

Sign	Description	Value
N_x	Length of tube, equivalent to L	1000
N_y	Diameter of tube, equivalent to $2*b$	200
ρ_{in}	Inlet pressure in LBM units.	1
ρ_{out}	Outlet pressure in LBM units	0.95
τ	Relaxation time	1
nt	Number of time steps	20000



Task description

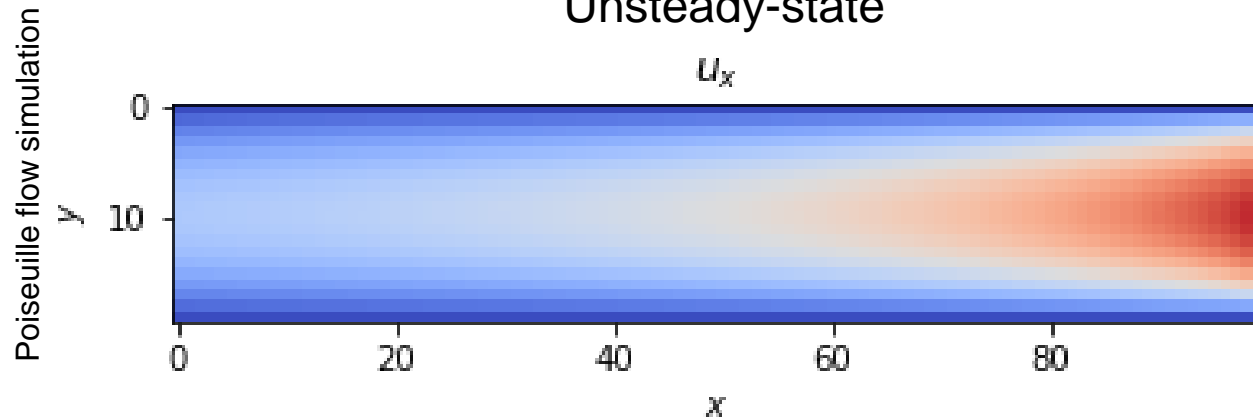
$$\tilde{f}_i(r, t) = f_i(r + \vec{v}_i, t + 1)$$

Streaming step

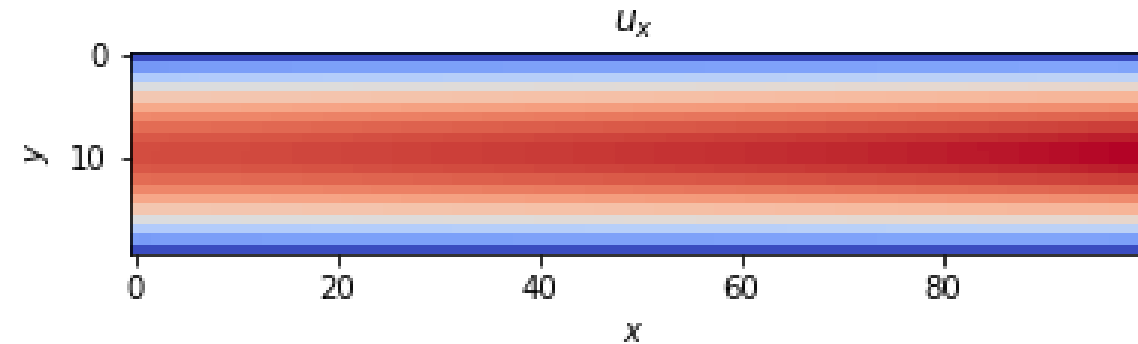
$$f_i(r, t) = \tilde{f}_i(r, t) - \frac{\tilde{f}_i - f_i^{eq}}{\tau}$$

Collision step

Unsteady-state



Steady-state



Poiseuille velocity profile:

$$u(y) = -\frac{\Delta p}{4\rho\nu L}(b^2 - y^2)$$

Lattice units:

$$\tau = \frac{\nu}{c_s^2} + 0.5$$

ν – kinematic
viscosity of fluid

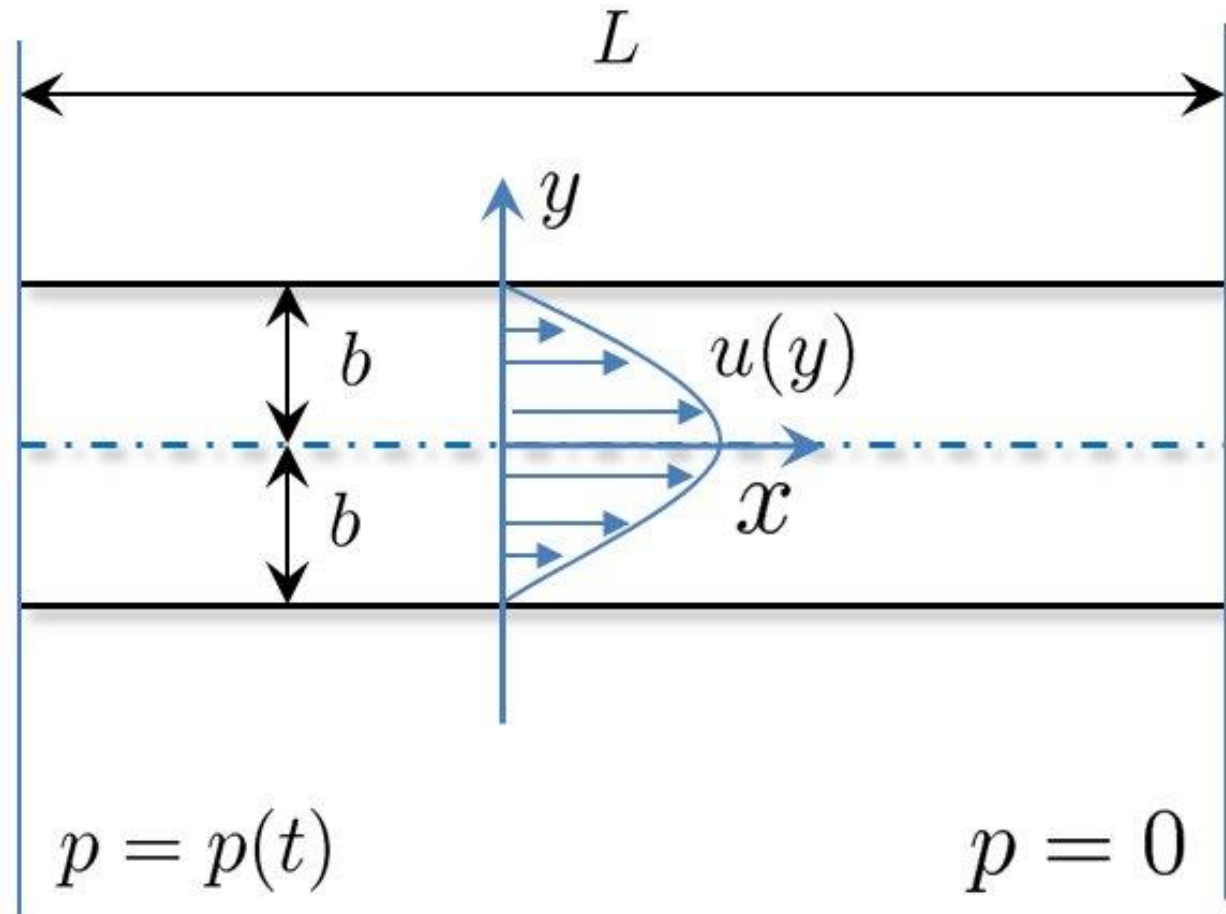
$$\rho_{phys} \neq \rho_{LB}$$

$$p_{LB} = c_s^2 \rho_{LB}$$

Task description

Several **Sequential** codes in shared folder:

/gpfs/gpfs0/ParallelComputingShared/Lattice
_Boltzmann_2021



Task description

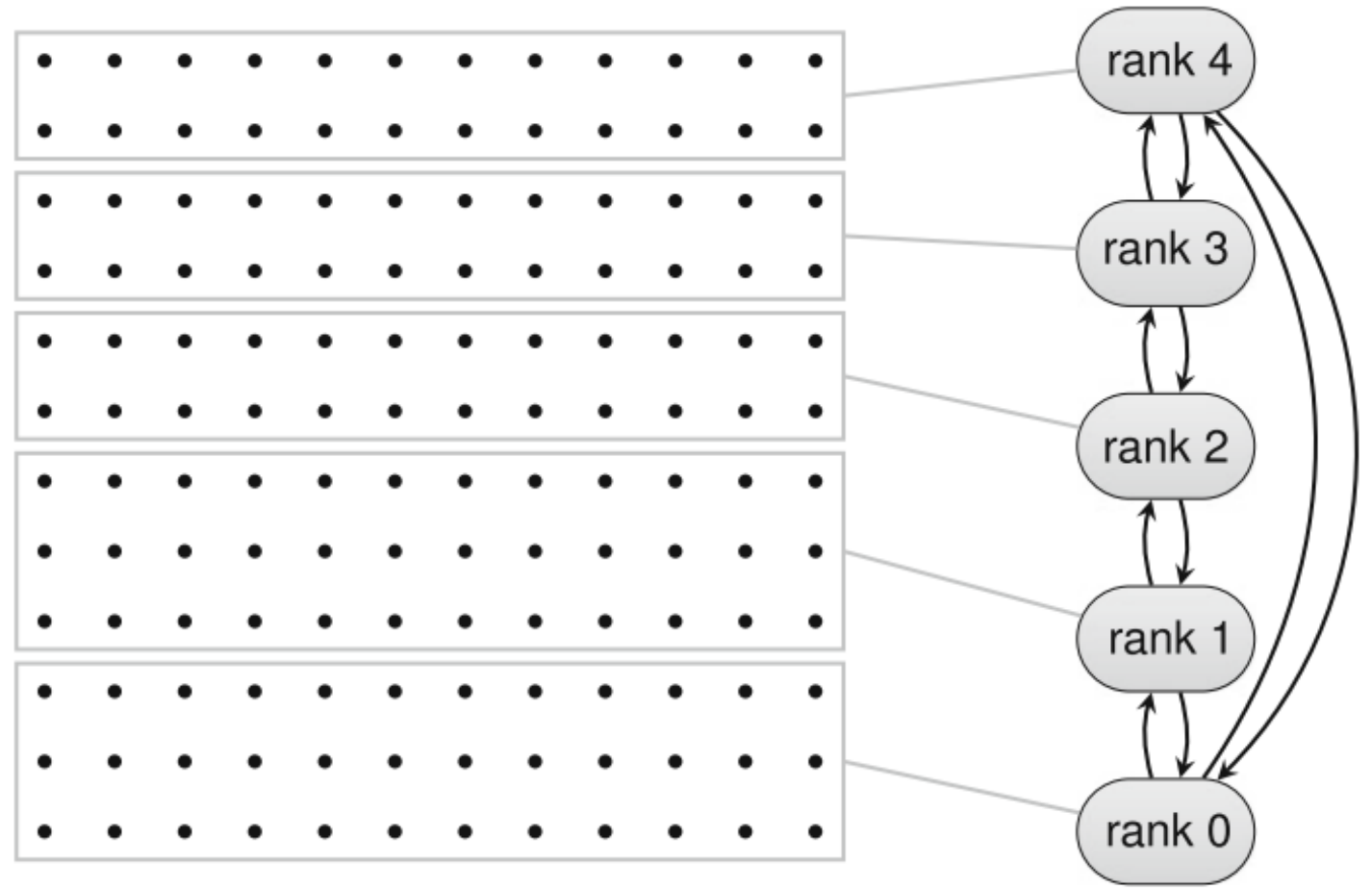
```
If (rank < NX % nprocs): //ranks that are  
less than reminder
```

```
    rank_nx = NX/nprocs+1;  
    rank_xstart = rank*rank*nx;
```

```
else:
```

```
    rank_nx = NX/nprocs;  
    rank_xstart = NX-(nprocs-  
rank)*rank_nx
```

```
print("Rank %d: %d nodes from y = %d  
to y = %d\n", % (rank, rank_nx,  
rank_xstart, rank_xstart+rank_nx-1))
```



Task description

```
# streaming and collision step
def streaming_and_collision(f):
    ... # streaming
    ... for j in range(Ny-1, 0, -1):
    ...     for i in range(0, Nx-1):
    ...         f[i,j,2] = f[i,j-1,2]
    ...         f[i,j,6] = f[i+1,j-1,6]
```

→

```
def streaming_and_collision(f, ranknx, rank_xstart):
    ...
    for j in range(Ny-1, 0, -1):
        for l in range(rank_xstart, ranknx):
```

Blocking realization

```

if(rank % 2 == 0) // even ranks send then receive
{
    // send below, i.e. rank-1
    MPI_Send(send_buffer, count, MPI_DOUBLE,
            rankml, tag, MPI_COMM_WORLD);
    // receive from above, i.e. rank+1
    MPI_Recv(recv_buffer, count, MPI_DOUBLE,
            rankpl, tag, MPI_COMM_WORLD,
            status);
}
else // odd ranks receive then send
{
    // receive from above, i.e. rank+1
    MPI_Recv(recv_buffer, count, MPI_DOUBLE,
            rankpl, tag, MPI_COMM_WORLD,
            status);
    // send below, i.e. rank-1
    MPI_Send(send_buffer, count, MPI_DOUBLE,
            rankml, tag, MPI_COMM_WORLD);
}

```

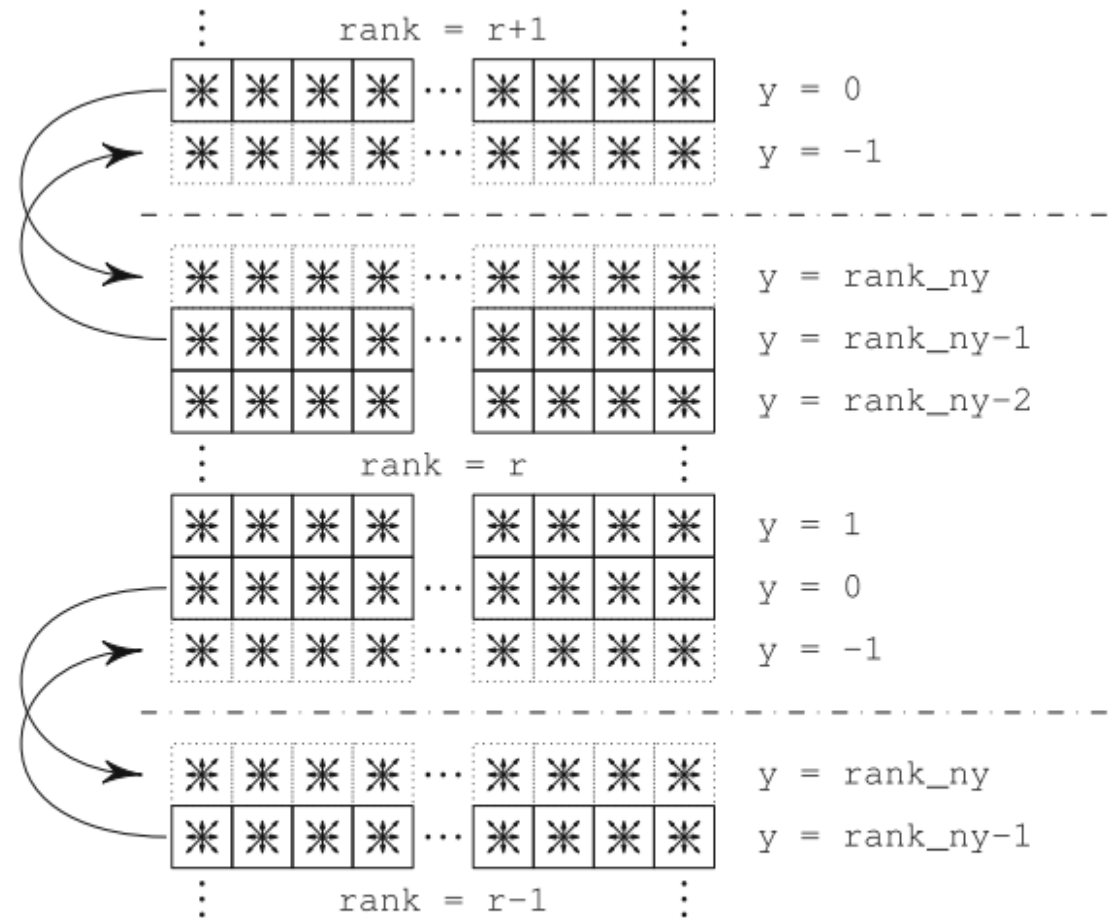


Fig. 13.10 Diagram showing the rows of data that need to be transferred across subdomain boundaries between processes. Boxes with solid outlines denote the nodes of the subdomain updated by each rank, while boxes with dotted outlines denote the extra rows used to store data from adjacent subdomains that are handled by different ranks

Blocking realization

```

MPI_Sendrecv(&f1[fieldn_index(0,rank_ny-1,1)],
             transfer_doubles,MPI_DOUBLE,
             rankp1,rank,
             &f1[fieldn_index(0,-1,1)],
             transfer_doubles,MPI_DOUBLE,
             rankm1,rankm1,
             MPI_COMM_WORLD,MPI_STATUS_IGNORE);

MPI_Sendrecv(&f1[fieldn_index(0, 0,1)],
             transfer_doubles,MPI_DOUBLE,
             rankm1,rank,
             &f1[fieldn_index(0,rank_ny,1)],
             transfer_doubles,MPI_DOUBLE,
             rankp1,rankp1,
             MPI_COMM_WORLD,MPI_STATUS_IGNORE);
    
```

```
size_t transfer_doubles = (ndir-1)*NX;
```

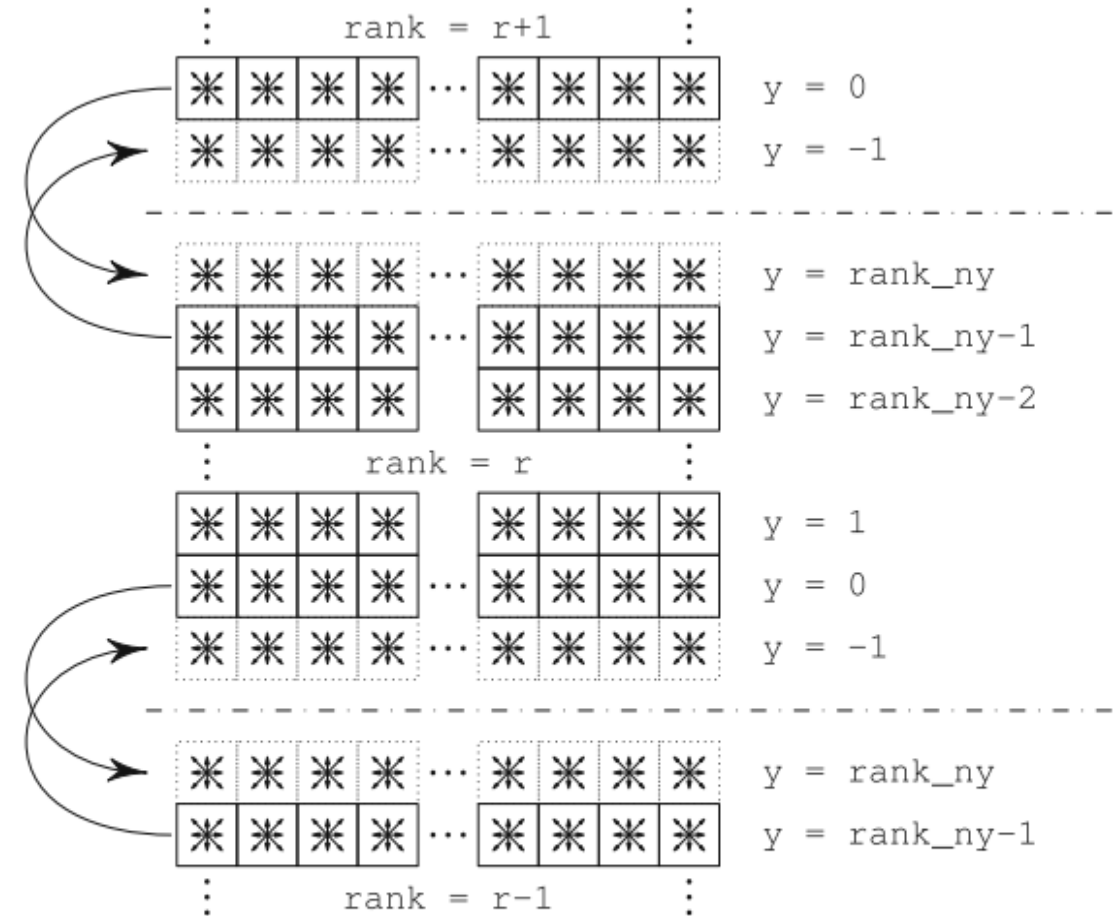


Fig. 13.10 Diagram showing the rows of data that need to be transferred across subdomain boundaries between processes. *Boxes with solid outlines* denote the nodes of the subdomain updated by each rank, while *boxes with dotted outlines* denote the extra rows used to store data from adjacent subdomains that are handled by different ranks

Non-Blocking realization

```
// Start a nonblocking send
int MPI_Isend(const void *buf,
             int count, MPI_Datatype datatype,
             int dest, int tag,
             MPI_Comm comm, MPI_Request *request

// Start a nonblocking receive
int MPI_Irecv(void *buf,
             int count, MPI_Datatype datatype,
             int source, int tag,
             MPI_Comm comm, MPI_Request *request
```

```
MPI_Request reqs[4];
MPI_Status  stats[4];
```

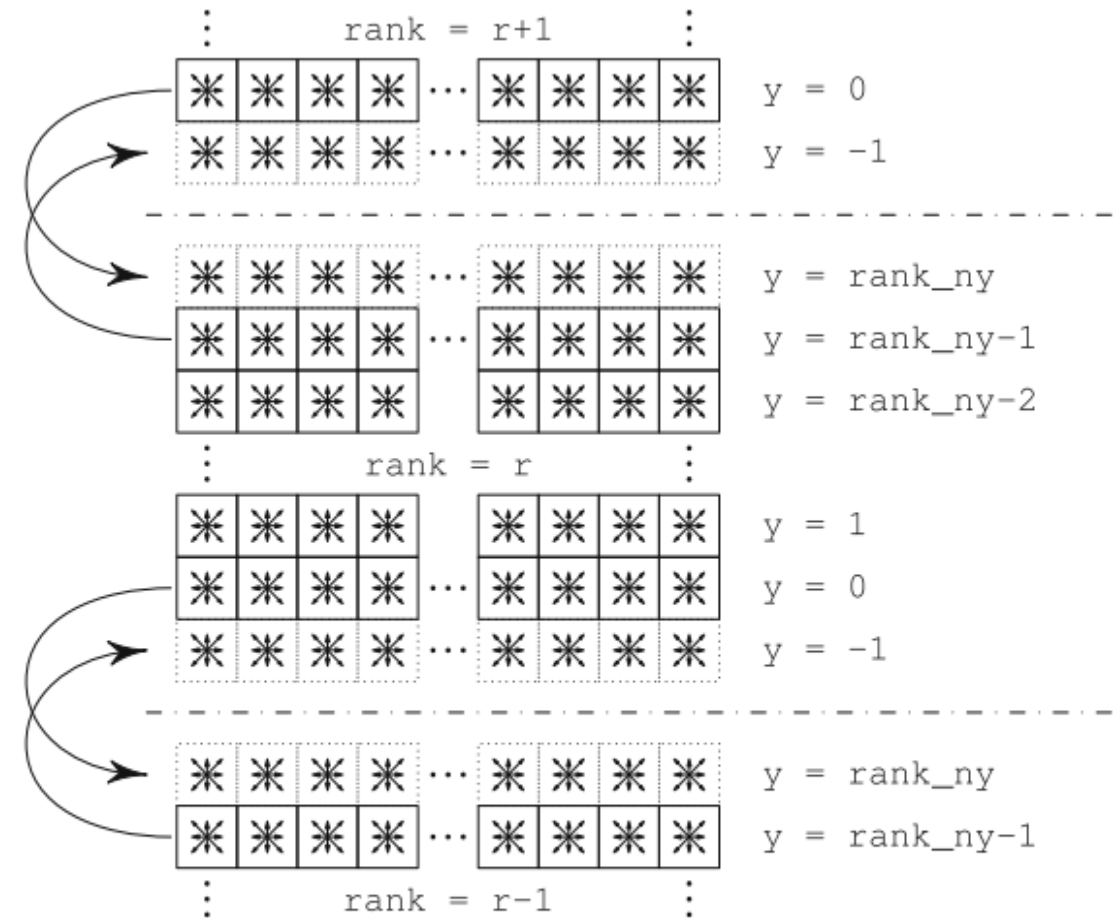


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Non-Blocking realization

```
MPI_Request reqs[4];
MPI_Status stats[4];
```

```
MPI_Isend(&f1[fieldn_index(0,rank_ny-1,1)],
         transfer_doubles,MPI_DOUBLE,
         rankp1,rank, MPI_COMM_WORLD,&reqs[0]);
MPI_Irecv(&f1[fieldn_index(0,-1,1)],
         transfer_doubles,MPI_DOUBLE,
         rankm1,rankm1,
         MPI_COMM_WORLD,&reqs[1]);
```

```
MPI_Isend(&f1[fieldn_index(0,0,1)],
         transfer_doubles,MPI_DOUBLE,
         rankm1,rank,
         MPI_COMM_WORLD,&reqs[2]);
MPI_Irecv(&f1[fieldn_index(0,rank_ny,1)],
         transfer_doubles,MPI_DOUBLE,
         rankp1,rankp1,
         MPI_COMM_WORLD,&reqs[3]);
```

```
int MPI_Waitall(int count,
               MPI_Request *array_of_requests,
               MPI_Status *array_of_statuses)
```

```
int MPI_Testall(int count,
               MPI_Request *array_of_requests,
               int *flag,
               MPI_Status *array_of_statuses)
```

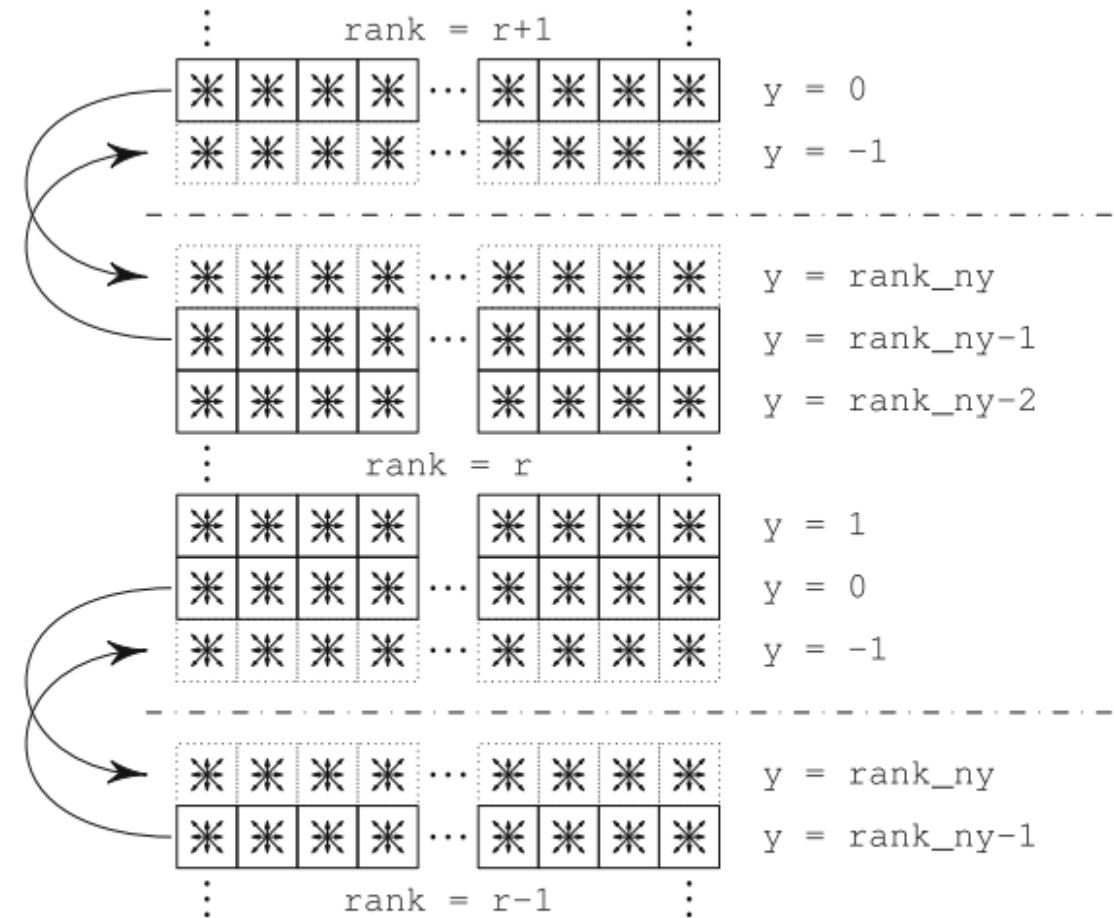


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Non-Blocking realization

Profiling tools for Python

CPU time profiling tools:

1. timeit
2. cProfile
3. line_profiler

Memory profiling tools:

1. memory_profiler
2. heapy

Contacts for questions:

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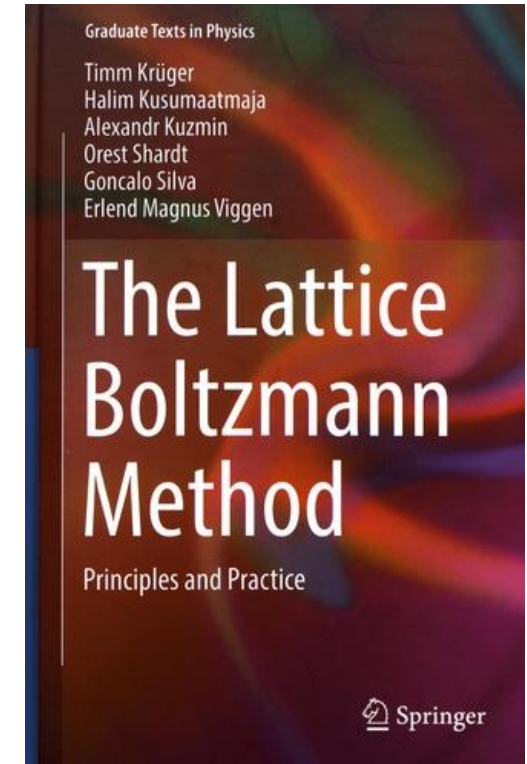
Email: Andrey.Olhin@skoltech.ru

MPI commands for Python:

`/gpfs/gpfs0/ParallelComputingShared/Lattice_Boltzmann_2021 MPI_commands/`

Lattice Boltzmann book

Principles of parallelization of LBM – Chapter 13.4



thx.

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