# Parallel Computing, 2025S

## Assignment 2: Heat Equation (2D) with MPI

# SOLVING HEAT EQUATION IN 2D

**The heat equation is a Partial Differential Equation**

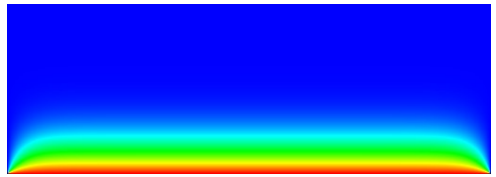
$$\frac{\partial u}{\partial t} = \alpha\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right)$$

**Using Jacobi iterative method (simplified):**

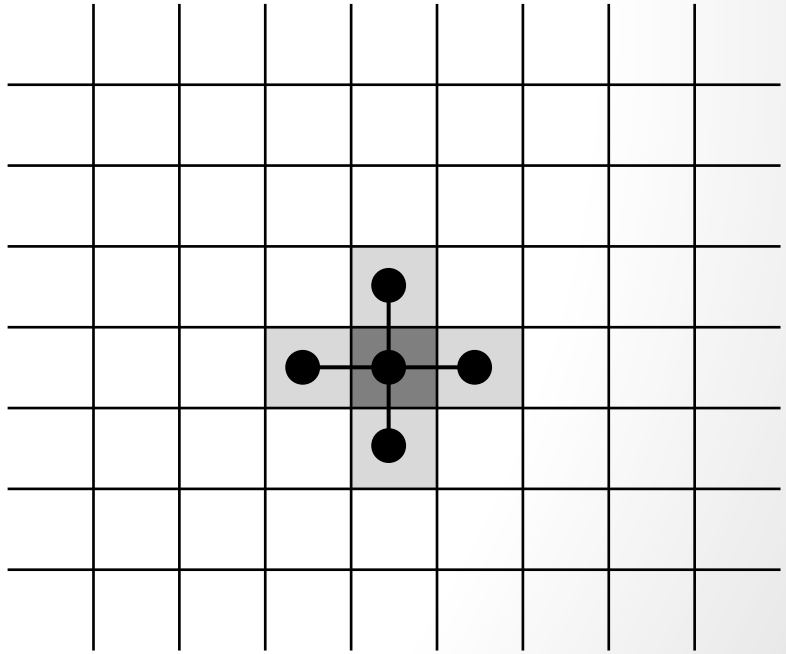
$$v_{m.l}^{n+1} = \frac{1}{4}\left(v_{m+1,l}^{n} + v_{m-1,l}^{n} + v_{m.l+1}^{n} + v_{m.l-1}^{n}\right) - \frac{h^2}{4} f_{ml}$$

Zero

- NxM Matrix (M rows and N columns)
- Basically, a five-point stencil
  - Calculation of averages



Example output



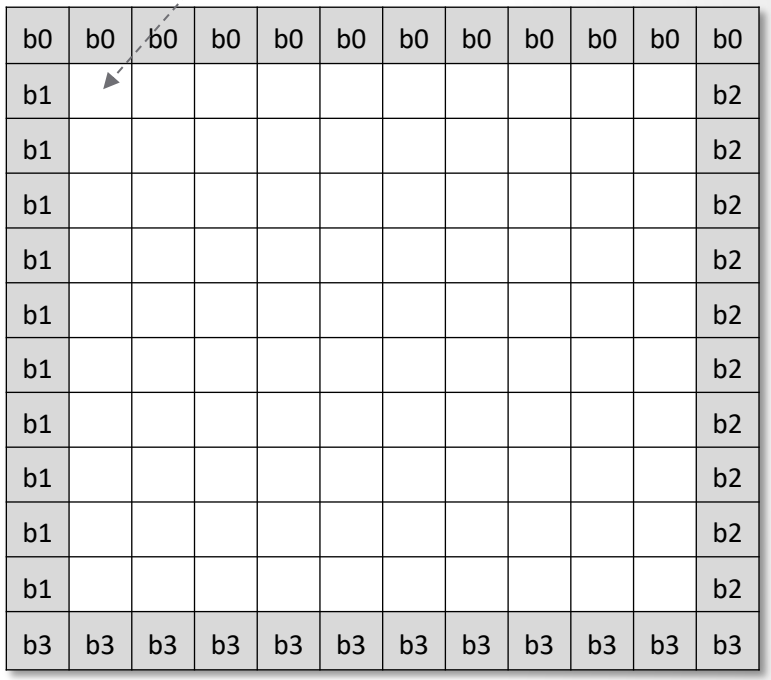
Five-point stencil

# CORE OF THE SEQUENTIAL CODE

```
//...
iteration_count = 0;
do
{
  iteration_count++;
  diffnorm = 0.0;

  /* Compute new values (but not on boundary) */
  for (i = 1; i < M - 1; ++i) {
    for (j = 1; j < N - 1; ++j) {
      W[i][j] = (U[i][j+1] + U[i][j-1] + U[i+1][j] + U[i-1][j]) * 0.25;
      diffnorm += (W[i][j] - U[i][j]) * (W[i][j] - U[i][j]);
    }
  }

  // Only transfer the interior points
  for (i = 1; i < M - 1; ++i)
    for (j = 1; j < N - 1; ++j)
      U[i][j] = W[i][j];

  diffnorm = sqrt(diffnorm);

} while (epsilon <= diffnorm && iteration_count < max_iterations);
//...
```

exit criteria

We start from here




Boundary conditions

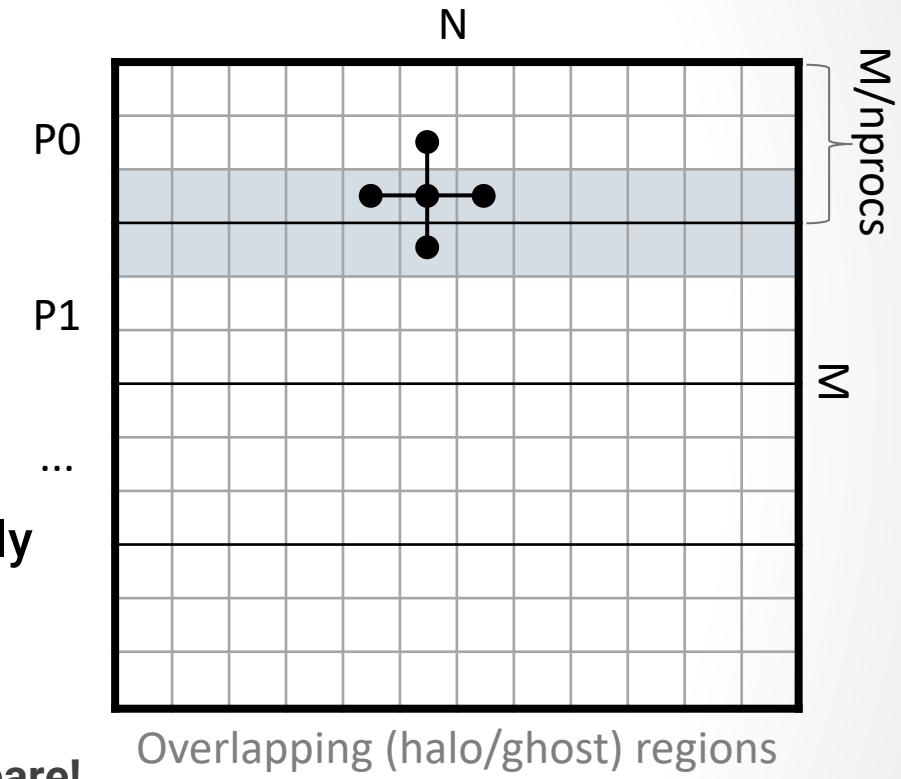
b0 = 0.02, b1 = 0.05, b2 = 0.1, b3 = 0.2

Note: Note that in most cases the code will reach the maximum number of iterations with the current setup

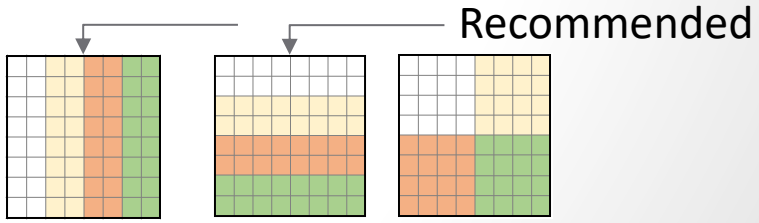
# HEAT2D WITH MPI

**Realize an efficient parallel implementation of the serial code for iteratively solving heat equation using MPI**

1. **Distribute data over all processes**
   - Horizontal blocks (you can also choose vertical or 2D)
   - Initialize in a distributed fashion (!)
   - Each process gets only a part of the matrix
   - Support (M % nprocs != 0)
     - e.g., have larger last block
2. **Use point-to-point communication to communicate the overlapping regions**
3. **Make sure that you get the termination criteria correctly**
   - The results must be the same as if executed with the sequential code
4. **Verify/compare to the sequential version**
   - **Use collectives to transfer data to rank 0, and then compare!**
     - Also measure the time required to collect data on rank 0
   - **Results must be the same!**



Overlapping (halo/ghost) regions



Other configurations

Hints: First support M%nprocs == 0 and then improve

Useful MPI routines: MPI_Isend/Recv, MPI_Allreduce, MPI_Gather, MPI_Gatherv

# DATA DISTRIBUTION (HORIZONTAL)

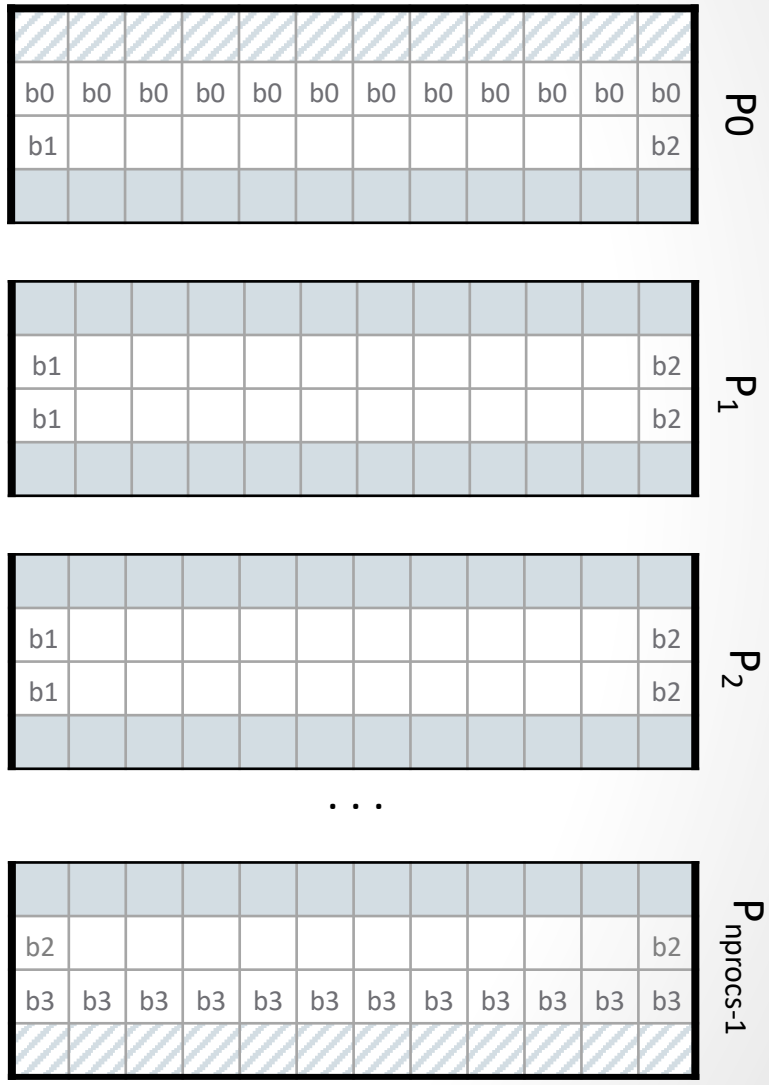
**Each process gets a part of the MxN matrix**

- e.g., each process gets ~M/nprocs (the # of processes) and additional rows for transfering the overlapping rows

**Neighbouring blocks need to exchange data so that the 5-point stancil can be computed**

**Example M=8, nprocs=4**

- Local matrix size → 8/4 = 2 ( + 2 for the halo region)
- Blue rows = extra rows to handle the “overlapping/halo” region
- You can have same local size for all process
  - Pattern fill ignored rows for this case
  - Tends to be easier
- Alternativelly, you can have smaller local sizes for the top and bottom processes (tends to be more complex)



# COMMUNICATION

**Red arrows**

- Sends from process below to process above
- e.g,: MPI_Send/ISend from the process below, sending its second row (the first after the padding) to process above → e.g., MPI_Send(&U[1][0], N, … )

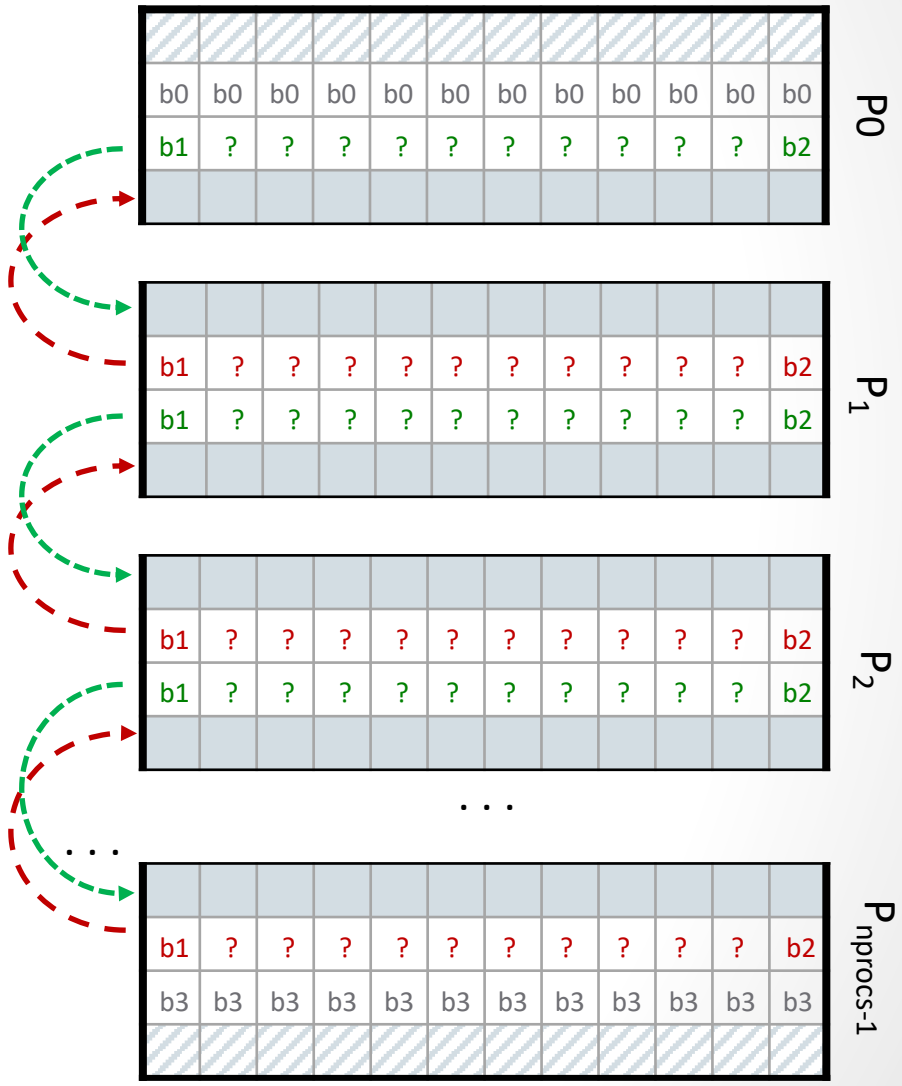
**Green arrows**

- A message from process above to process below
- E.g., using MPI_Send to send its last row (befor the padding) to the process below

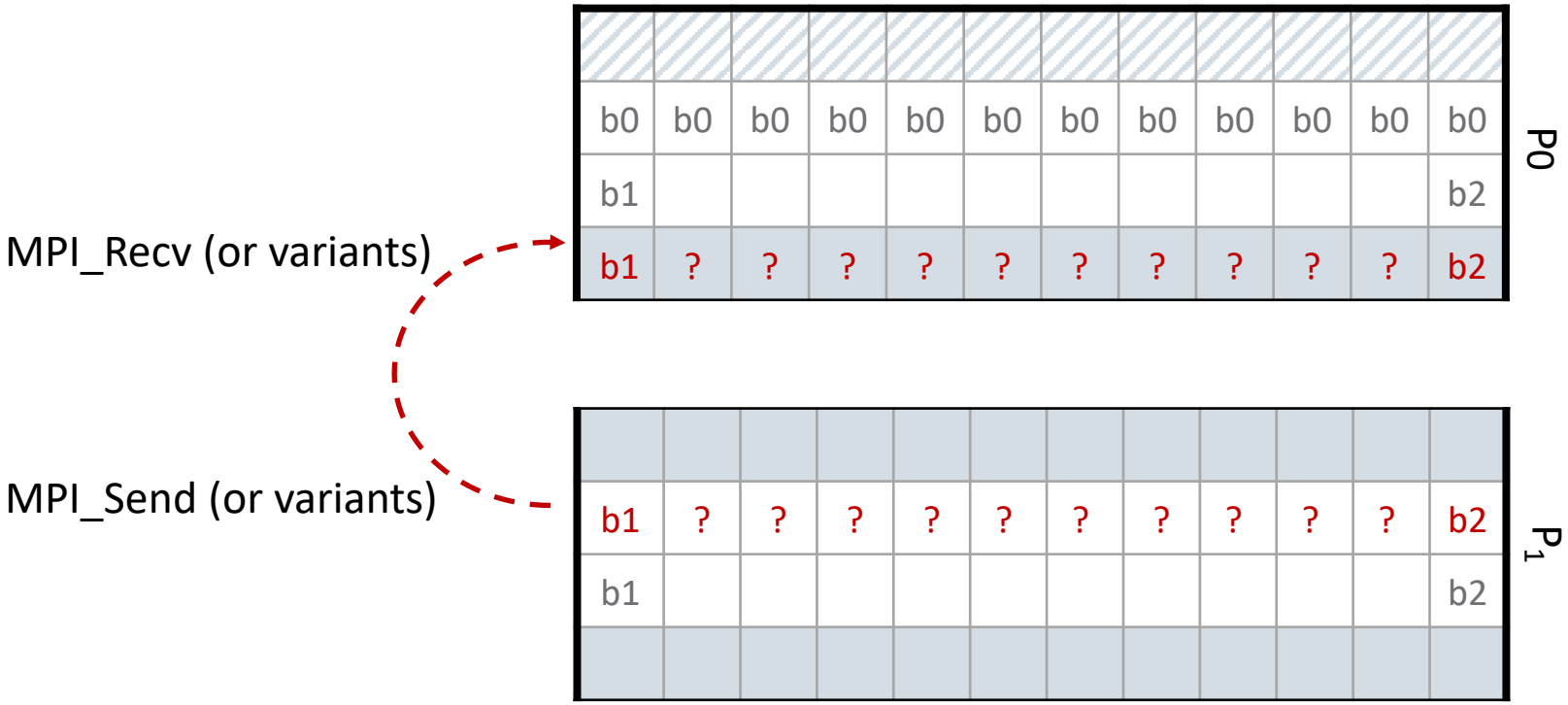
**You need MPI_Send and MPI_Recv on each end**

- Four calls for each neighbour exchange
- Basically 3 different cases
  - Top communicating only with the process below
  - Each middle process with both above and below
  - Bottom communicating with the process above

Note: can also be simplified, and implemented with MPI_Send/Recv, MPI_Isend/Irecv variants and MPI_Sendrecv, …



# COMMUNICATION :: SINGLE MESSAGE




**Example:**

- **P1** sends its first row to **P0**, **P0** receives the row and puts it int its last row (the additional row)
- Point-to-point communication
- E.g., with MPI_Send, MPI_Isend, MPI_Recv, MPI_Irecv, MPI_Sendrecv (avoid deadlocks!)
- *the values in cells are not the actual values

# EXPERIMENTS (MPI)

1. **Your code should work with different sizes of matrix**
   - M rows, N columns (you can assume that matrix is larger than some minimum)

2. **On Alma, run the program with the following configuration using Slurm:**
   a. `mpirun ./heat2d --m 2688 --n 4096 --epsilon 0.01 --max-iterations 1000`

3. **Run** (at least) **using the following cluster configurations:**
   a. 1 node using 2, 4, 8, 16 and 32 MPI processes
   b. 2 nodes, 32 processes
   c. 4 nodes, 64 processes

**Achieve a speedup* of ~11 using 4 nodes on the Alma system (using 2.a. and 3.c) and measure the speedup* when using other configurations**

- Note: to test for M % nprocs != 0, then test with different (non-default) value of M

*with respect to the sequential version that uses the same configuration

# DELIVERABLES, REMARKS

**Submit your source code to the online platform (moped.par.univie.ac.at)**

- Only one source file: heat2d.cpp

**Measure speedup on Alma, and enter speedup results on the online platform**

- Create a job script for Slurm on Alma and use it to run your program for performance measurements

**Remarks**

- Remember not to measure on the frontend node
- Some errors may appear only after you test your program on multiple nodes
- To prepare for the test, try to explain the differences (if any) in the performance as M, N, and max-iterations change

# Additional Notes

# COMPILATION, NAMING CONVENTION

## Your starting point is the sequential version of the code (in Moodle):

- **`heat2d.cpp`** (also a template for your solution with comments)
- **`helpers.hpp`**

## Sequential version:

- Compile*: **`g++ -O2 -lm -o heat2d heat2d.cpp`**
- Run: **`./heat2d`** <arguments>
- *you may need to also provide -std=c++17 or -std=c++20 switch on your machine

## MPI version:

- Compile: **`mpic++ -O2 -lm -o heat2d heat2d.cpp`**
- Run: **mpirun -np** <num_processes> **./heat2d** <arguments> (at home)
- Use **Slurm** jobscript to run on Alma (see examples in this slide set)

# SLURM ON ALMA :: JOB SCRIPT EXAMPLE

```
#!/bin/bash
#SBATCH -N 4
#SBATCH --ntasks 16
#SBATCH -t 3
mpirun ./heat2d --m 2688 --n 4096 --epsilon 0.001 --max-iterations 1000
```

4 nodes

MPI tasks

16 processes over 4 nodes

Timeout (in the case of a deadlock)

Submit for execution

```
> sbatch jobscript.sh
Submitted batch job 4242

> squeue
JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
 4242       all jobscrip johndoe  R       0:11      4 alma[01-04]
```

Check if it is running

**The result will be saved in slurm-4242.out when complete**

# MATRIX DATA STRUCTURE AND HELPER FUNCTIONS

**Contains a custom data structure "Mat"**

- Contiguous 2D data structure
- Note the "(" and ")" can also be used: `mat(i,j)`

```
Mat mat(height, width);
for (int i=0; i<mat.height; i++) {
   for (int j = 0; j < mat.width; j++) {
      mat[i][j] = f(x);
   }
}
// with MPI: MPI_Send(&mat[0][0], ... );
```

**And number of member functions that you do not need to modify, but they may be helpful:**

- `void save_to_disk(std::string filename);`
  Purpose: Save data to disk so it can be converted to an image
  Example: `mat.save_to_disk("heat2d.txt");`

- `void print();`
  Purpose: Printing data to standard output
  Example: `mat.print();`

- `bool compare(Mat& m, double eps=std::pow(10, -8));`
  Purpose: Compare data element by elements, used for the verification of the results
  Example: `mat.compare(mat2);`

# OTHER HELPER FUNCTIONS, AND USAGE

**Other functions:**

- ```
  void process_input(int argc, char **argv, int& N, int& M, int& max_iterations,
                     double& epsilon, bool& verify=true, bool& print_config=false);
  ```
  Purpose: Processing of input arguments
  Notes: By default results are verified, and configuration is not printed. Both `verify` and `print_config` are optional.

- ```
  void heat2d_sequential(Mat& mat, int max_iterations,
                         double epsilon, int& iteration_count);
  ```
- Purpose: Compute the data sequentially and use it for verification
  Note1: Matrix `mat` and `iteration_count` are `inout` arguments, they return the resulting sequentially computed data and the number of iterations for verification purposes.

## Usage

```
./heat2d --m <int> --n <int> --max-iterations <int> --epsilon <double> [ --no-verify --print_config ]
```

| | |
|---|---|
| `--m` | The number of rows (required) |
| `--n` | The number of columns (required) |
| `--max-iterations` | Integer value (default == 1000) |
| `--epsilon` | Double value (default == 1.0e-3) |
| `--no-verify` | Disable verification. Could be useful while measuring performance (default == false) |
| `--print_config` | Print the configuration in use (default == false) |