Particle-in-cell plasma simulation with OmpSs-2

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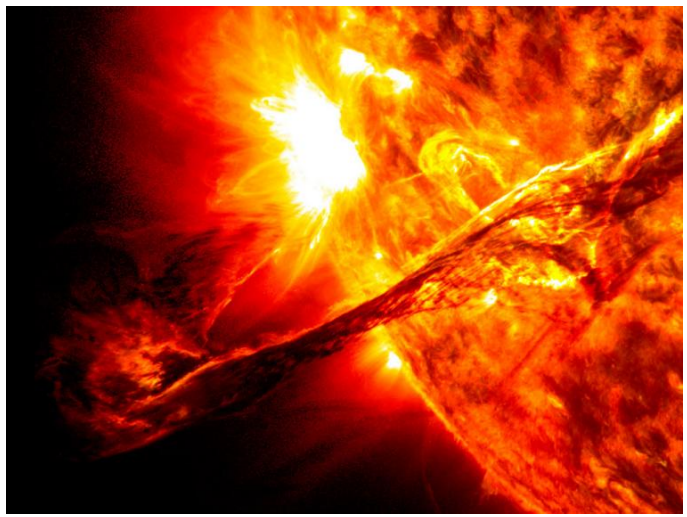
Outline

Introduction

A plasma is an almost neutral gas of charged and neutral particles which exhibits collective behavior.



Simulation can provide insight in the behavior of plasma without expensive laboratory equipment.

Motivation

Simulation of plasma is a real case scenario where we can test the **OmpSs-2** programming model as well as the **TAMPI** library and measure the performance and programmability.

The challenges found during the development can be used to improve the current solutions of the programming model and to propose new alternatives.

Vlaslov equation

The Vlaslov equation describes the evolution of a plasma, with long range iteration between particles.

$$\frac{\partial f_j}{\partial t} + \boldsymbol{v} \cdot \frac{\partial f_j}{\partial \boldsymbol{x}} + \frac{q_j}{m_j} \left(\boldsymbol{E} + \frac{\boldsymbol{v} \times \boldsymbol{B}}{c} \right) \cdot \frac{\partial f_j}{\partial \boldsymbol{v}} = 0 \qquad (1)$$

Where $f_j(\boldsymbol{x}, \boldsymbol{v}, t)$ is the distribution function of the specie j (particles with same mass and charge), and the fields electric $\boldsymbol{E}$ and magnetic $\boldsymbol{B}$ are determined by Maxwell equations.

Maxwell equations

The evolution of the fields is governed by the Maxwell equations

$$\begin{aligned} \nabla \cdot \boldsymbol{E} &= \frac{\rho}{\epsilon_0} & \nabla \times \boldsymbol{E} &= -\frac{\partial \boldsymbol{B}}{\partial t} \\ \nabla \cdot \boldsymbol{B} &= 0 & \nabla \times \boldsymbol{B} &= \mu_0 \left(\boldsymbol{J} + \epsilon_0 \frac{\partial \boldsymbol{E}}{\partial t} \right) \end{aligned} \tag{2}$$

Where ρ is the charge density distribution, $\boldsymbol{J}$ the current field and ϵ_0 and μ_0 are constants.

Electrostatic approximation

In our model, we will only have a **strong fixed magnetic field** $\boldsymbol{B}_0$ and the Maxwell equations can be simplified.

$$\nabla \cdot \boldsymbol{E} = \frac{\rho}{\epsilon_0} \qquad \nabla \times \boldsymbol{E} = 0 \tag{3}$$

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As the electric field is irrotational, we can introduce a scalar field ϕ, the electric potential, and rewrite $\boldsymbol{E}$ as a gradient $\boldsymbol{E} = -\nabla\phi$.
Finally, if we solve for ϕ we obtain the Poisson equation:

$$\nabla^2\phi = -\frac{\rho}{\epsilon_0}, \tag{4}$$

This approximation is called **electrostatic** as opposed to the **electromagnetic** case, when $\boldsymbol{B}$ varies with time.

The particle-in-cell method

Solving the Vlaslov equation directly is very **computationally expensive**. The current solution is to introduce a spatial grid where the Maxwell equations are solved.

The distribution function f_j is then modeled by macro-particles which interact with the grid by an interpolation method.

This method is known as **particle-in-cell** (PIC).

The particle-in-cell method

The PIC method has four main steps

- **Charge accumulation**: The charge density ρ is interpolated in the grid from the particle positions.

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- **Interpolation of electric field**: The electric field is interpolated back to the particle positions.
- **Particle motion**: The force is computed from the electric field at the particle position and the particle is moved accordingly.

Charge accumulation

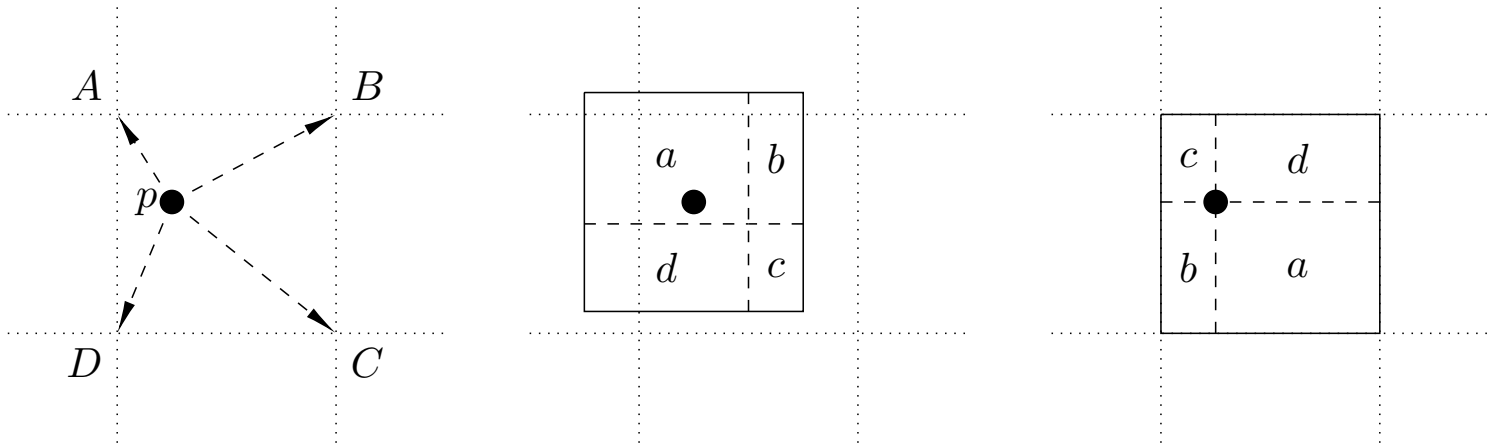

Figure: Interpolation of particle p charge into the four grid points A to D.

Field equations

First the electric potential ϕ must be computed from ρ, and then the electric field $\boldsymbol{E}$.

Several methods are available for solving the Poisson equation:

- **Iterative methods**: Jacobi, Gauss-Seidel, Successive Over Relaxation (SOR), Chebyshev...
- **Matrix methods** Thomas Tridiagonal algorithm, Conjugate-Gradient, LU, Incomplete Decomposition...
- **Spectral methods** A family of methods that use the fast Fourier transform (FFT).

We will only focus on two methods: The LU decomposition used as debug, and MFT, a spectral method with complexity $O(N_g \log N_g)$.

Sequential simulator

A sequential version of the simulator was produced to test the model with a visualization module to see the fields in real-time.

Both simulations in 1D and 2D are supported.

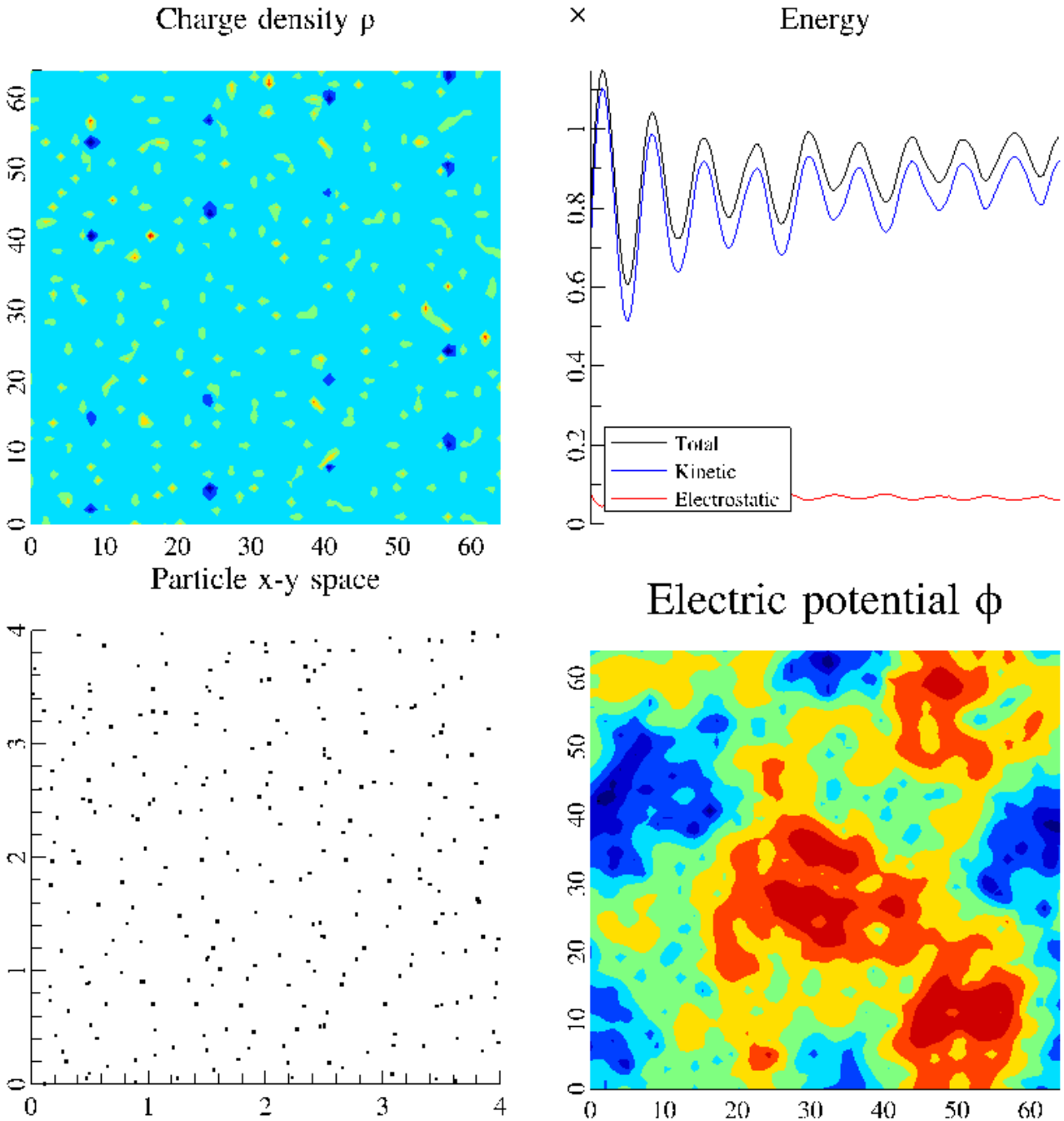

Figure: Example run in 2D of the simulator in debug mode.

Test: Conservation of energy

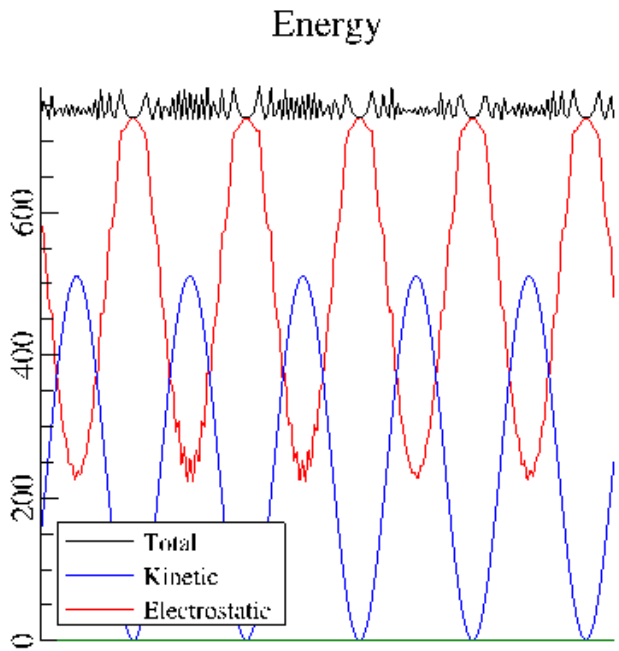

Figure: Energy conservation in two particle test as shown in the simulator.

Parallelization

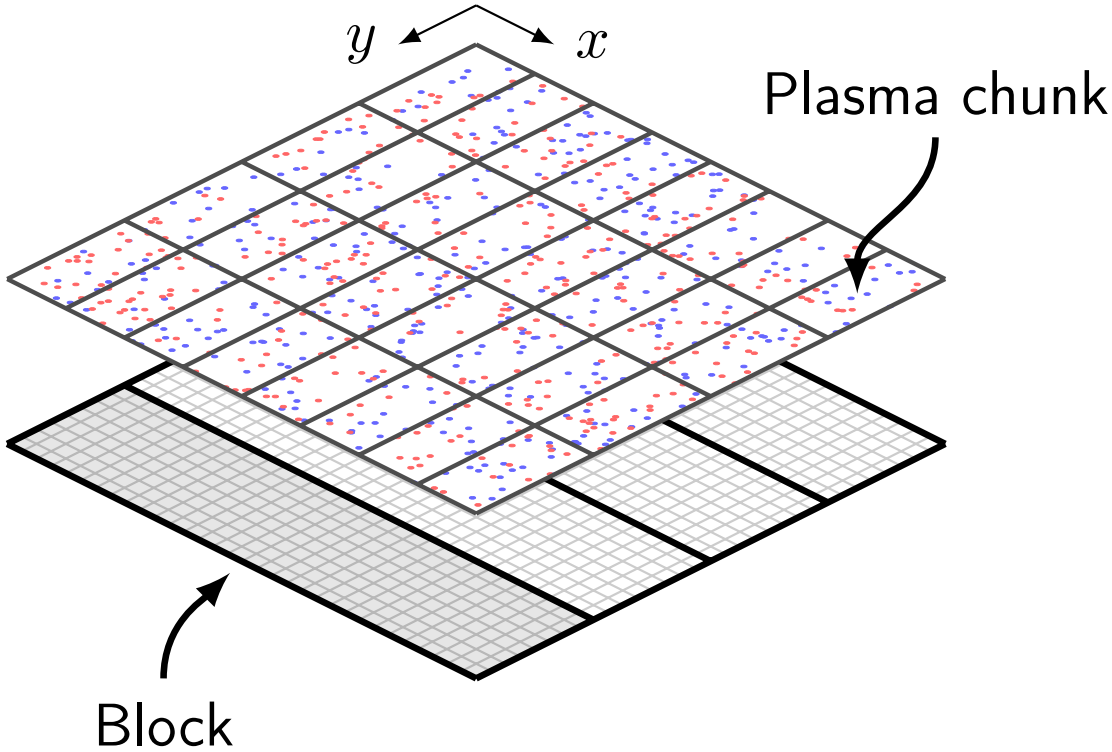

Figure: Domain decomposition: The plasma is divided into chunks in both directions and the fields into blocks in the Y dimension only

Communication

In order to exchange data (particles and fields) we use:

- MPI between processes in Y.
- Shared memory between chunks in X.

The communication of particles is done first in X and then in Y.

Communication: Particles in X

The particles are moved in the X direction for each chunk.

- A dependency over both neighbour chunks is needed
- If we use `inout` we create a **chain of dependencies**.

```
#pragma oss task inout(*chunk, *prev_chunk, \
      *next_chunk) label(exchange_particles_x)
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- We can use inout with coloring (advance the chunks by 3)

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for(color = 0; color < 3; color++) {
      for(i = color; i < nchunks; i+=3) {
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            ...
```
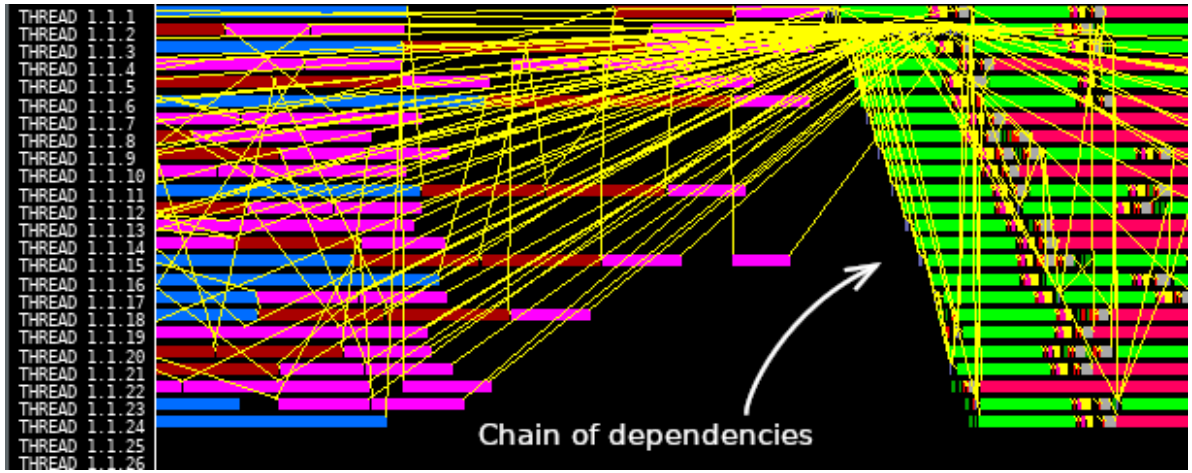
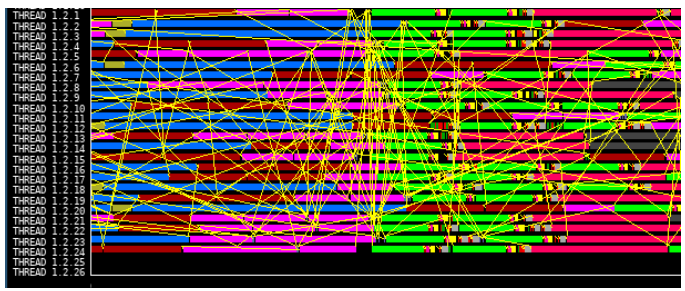

- Or `commutative` to avoid the chain.

```
#pragma oss task commutative(*chunk, *prev_chunk, \
     *next_chunk) label(collect_local_particles)
```

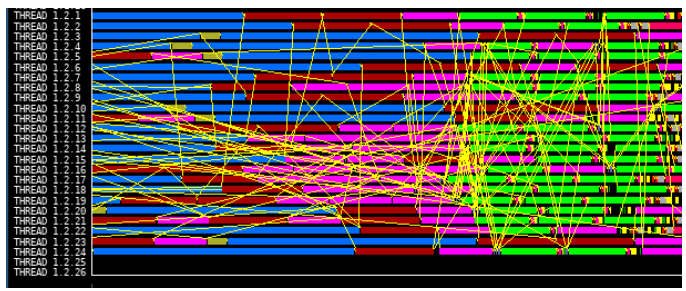
Chain of dependencies



(a) Chain of dependencies observed with inout



(b) Coloring+inout



(c) Commutative

Figure: Comparison of three `paraver` traces using: inout, coloring and commutative. Similar performance was found between both coloring and commutative.

Communication: Fields and particles in Y

Additionally to sending particles that are outside our block, we need to send the ghost frontiers.

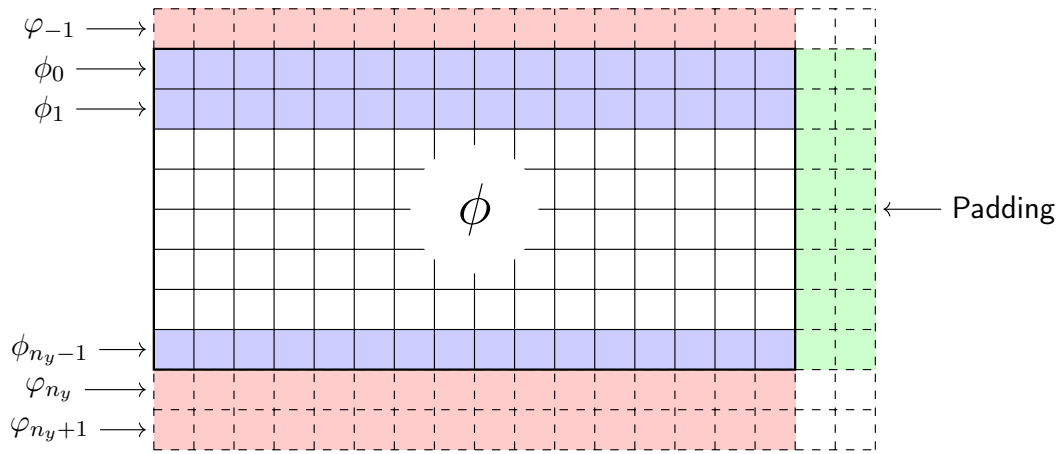


Figure: The electric potential ϕ with the ghost rows (red) and padding (green)

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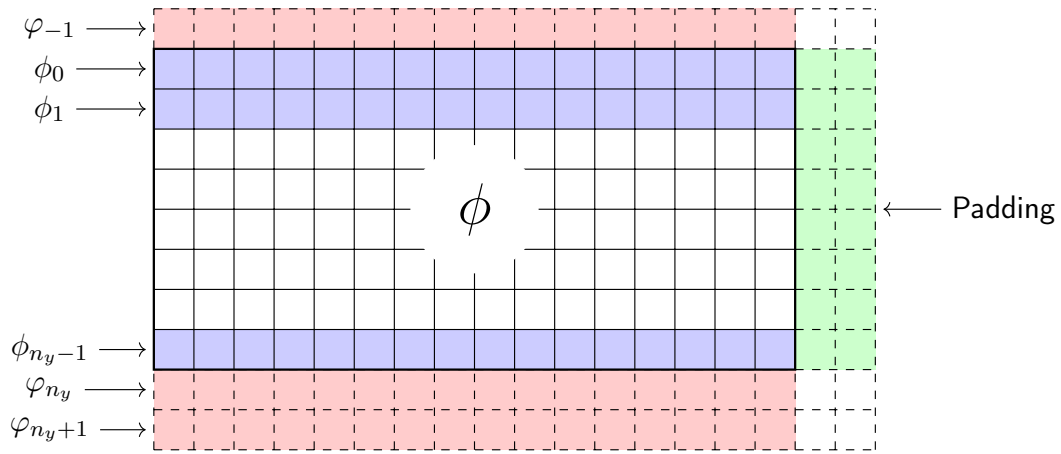


Figure: The electric potential ϕ with the ghost rows (red) and padding (green)

For the vertical communication we tested MPI and TAMPI.

- MPI requires special care to avoid deadlocks: Same tag for each chunk, receive the first message and process it.
- With TAMPI we can use a tag per chunk, but we need buffering for particles as cannot use `MPI_Probe`.

Comparison: MPI and TAMPI

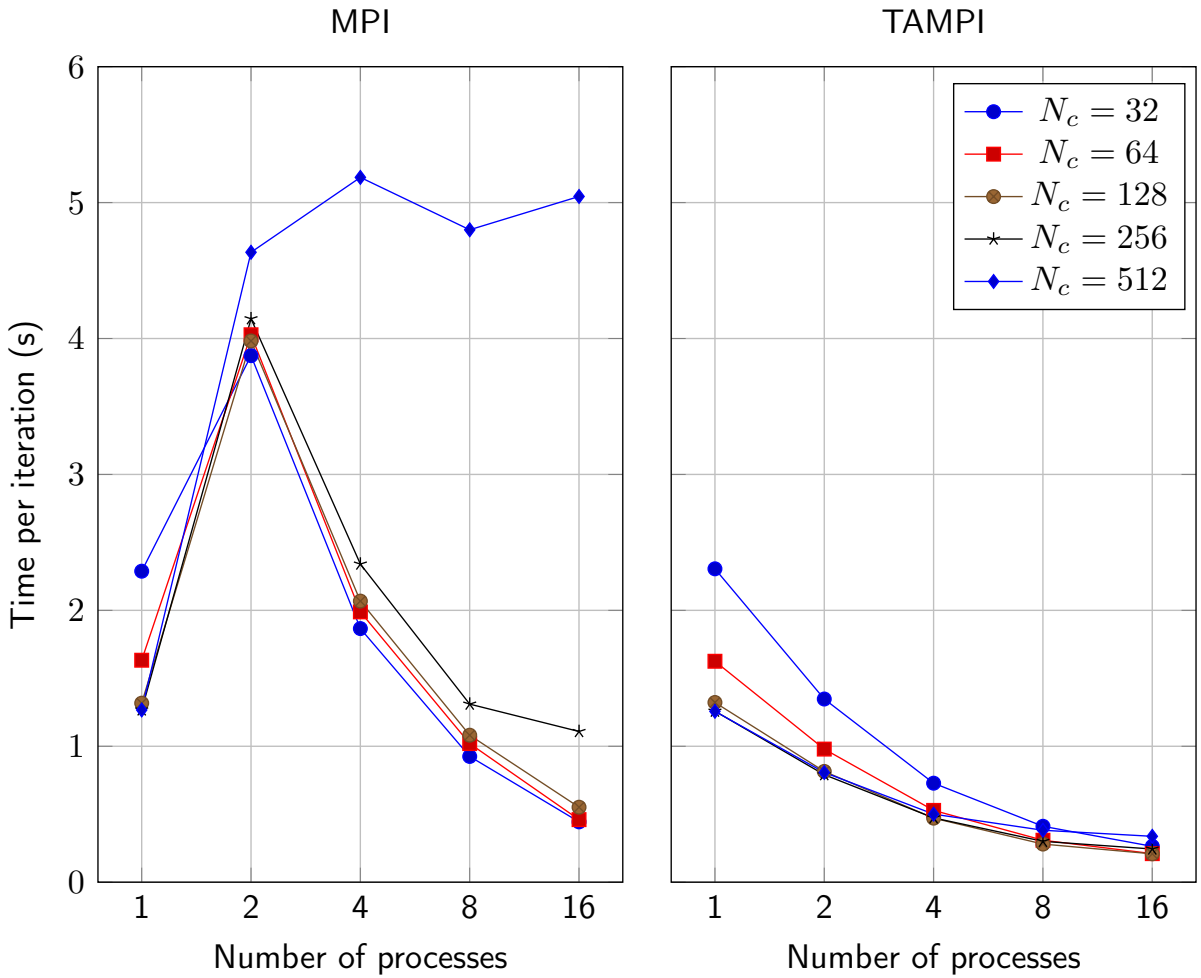


Figure: Comparison of MPI and TAMPI: Using one process per node.

Solving the fields

- In order to compute the electric field, the MFT method is used to solve the Poisson equation in each iteration.

$$\nabla^2 \phi = -\frac{\rho}{\epsilon_0} \tag{5}$$

- The FFT needs to be computed and the FFTW library provides distributed and multithreading support.
- However we found a very bad performance using threads.

Multithread FFTW

The FFTW library has a very bad performance with threads.

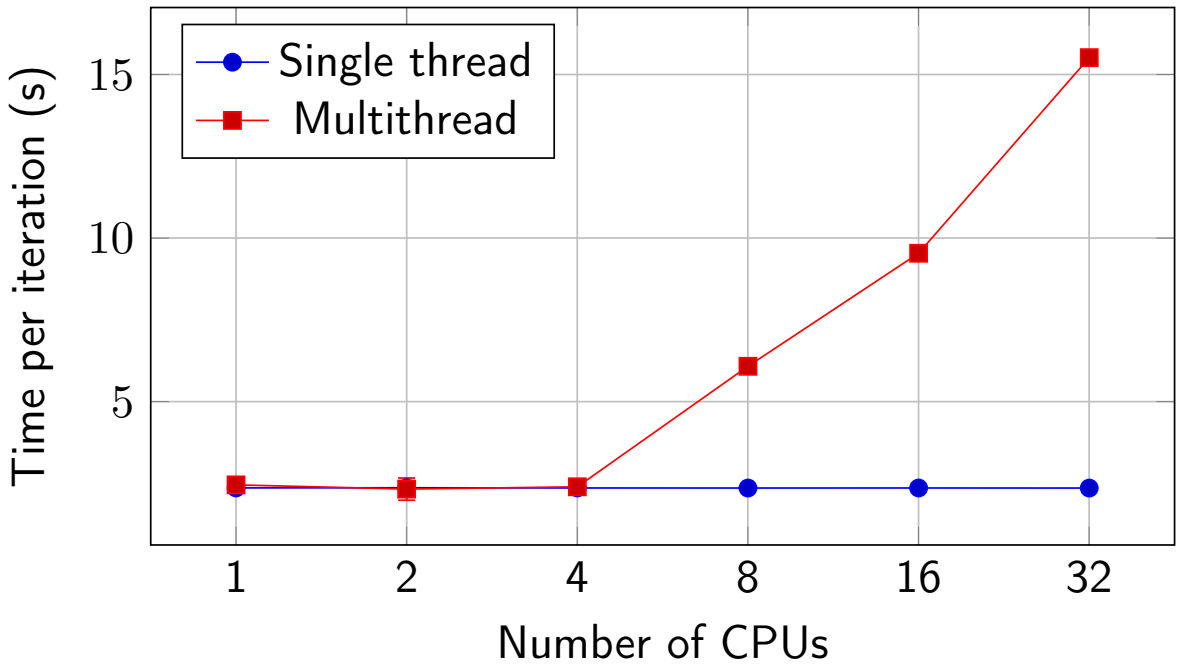


Figure: The number of CPUs is increased with only one process: the solver cannot scale and the time per iteration increases. Configuration used: $N_p = 5 \times 10^5$, $N_g = 8192^2$.

FFTW scalability problem

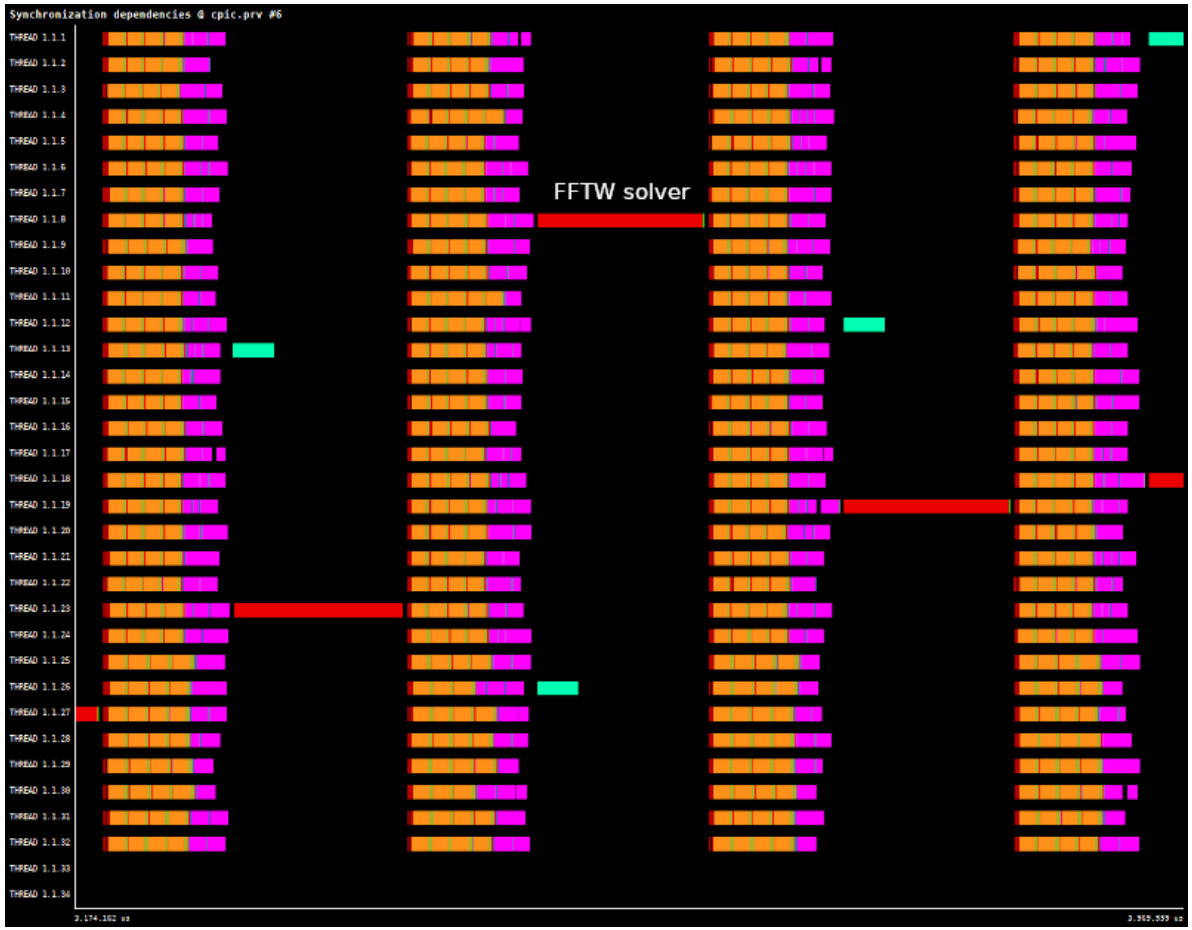


Figure: Trace with the solver shown in red, with 32 CPUs: The FFTW doesn't scale with the number of CPUs

Strong scaling with $N_g = 2048^2$

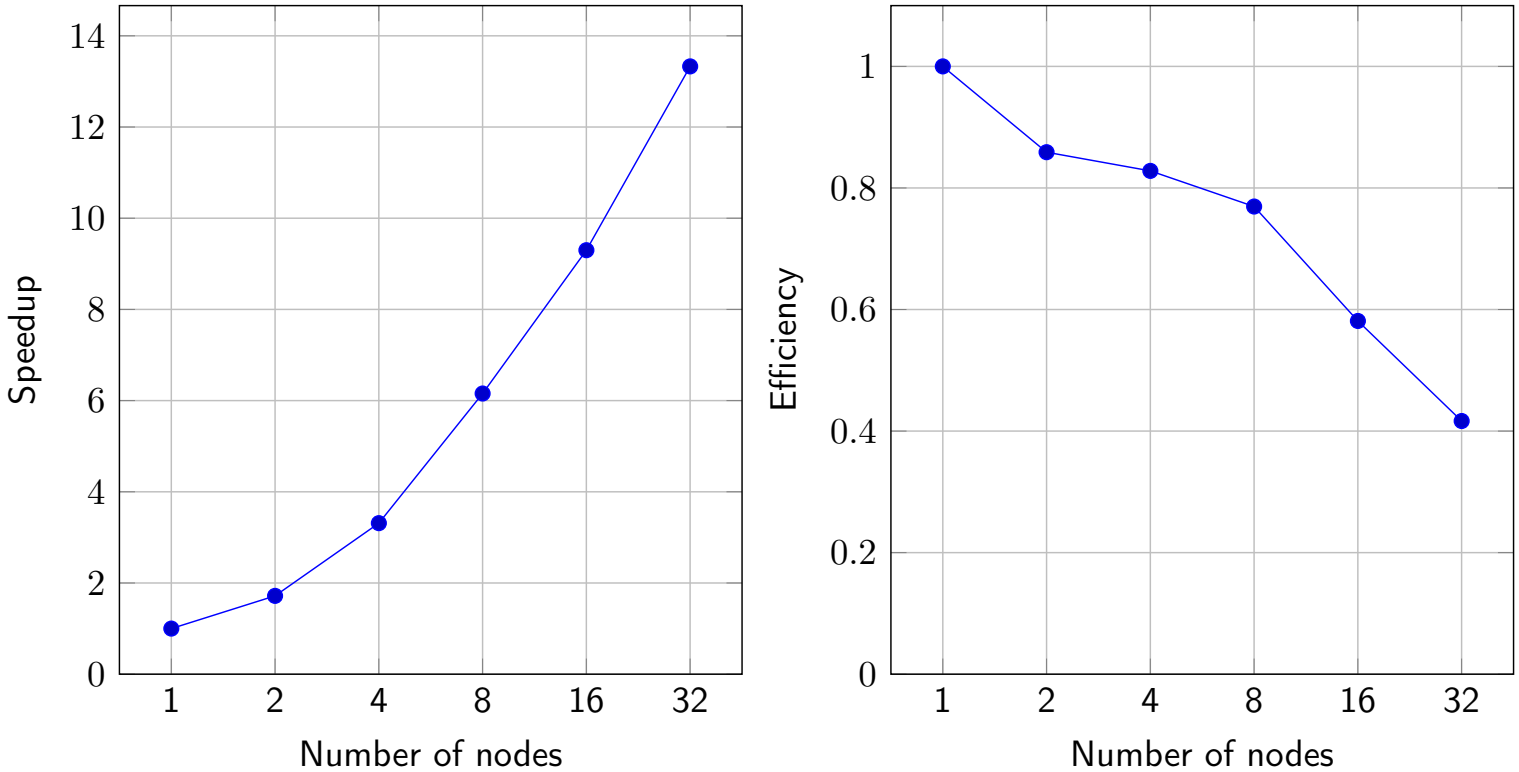


Figure: Strong scaling with configuration: $N_p = 1 \times 10^8$, $N_g = 2048^2$, $N_c = 128$, one process per node, using each 48 cores.

Weak scaling with $N_g = 2048^2$

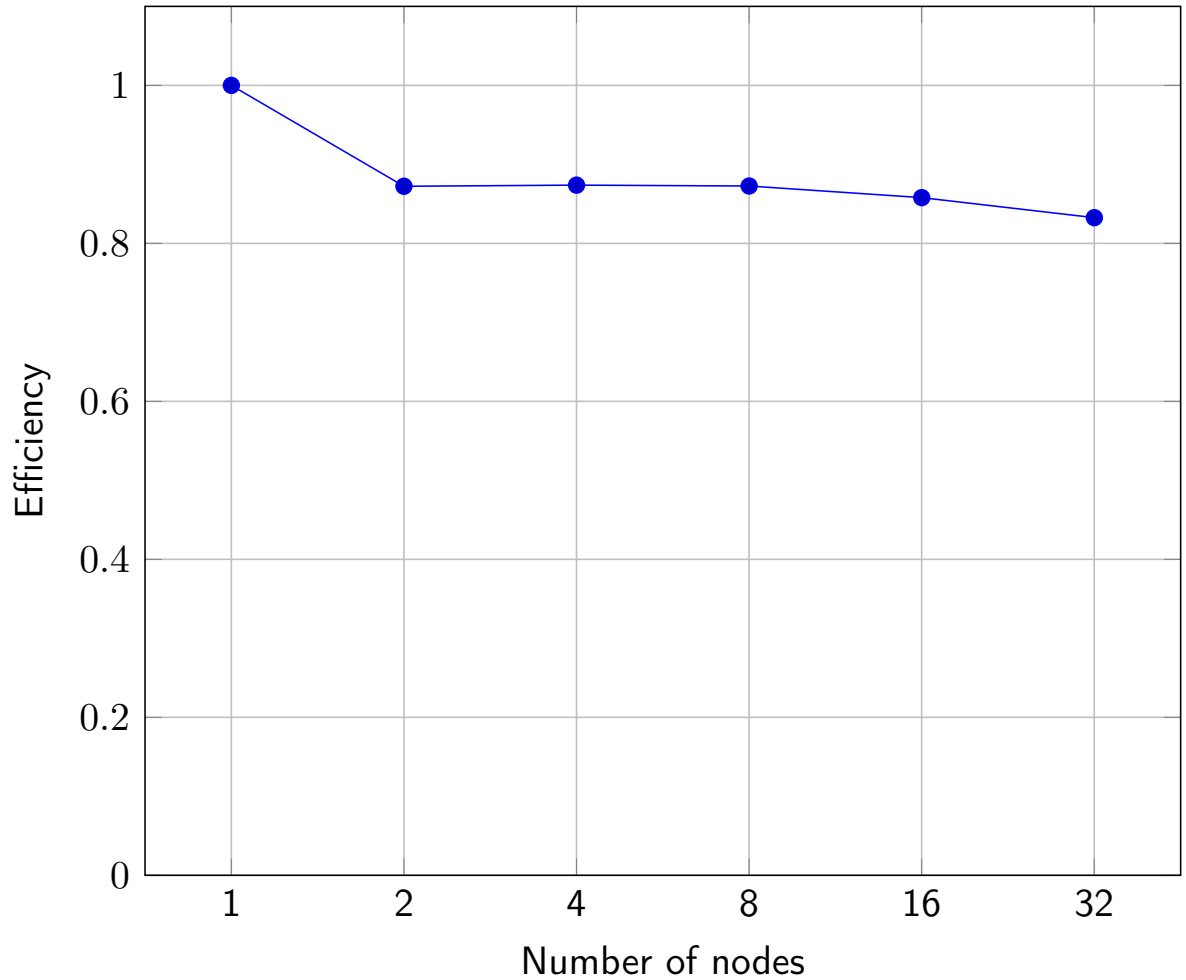
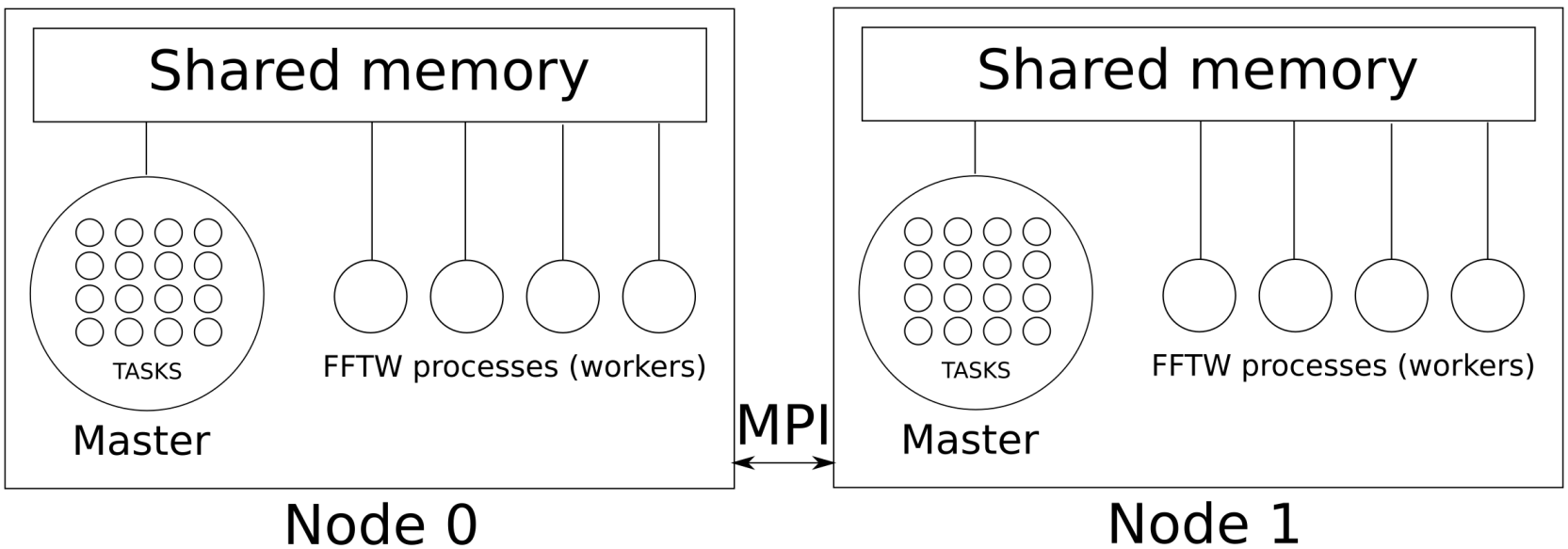


Figure: Weak scaling with 1×10^7 particles per CPU.

FFTW scaling solution

A solution to this problem consists in the use of additional worker processes with shared memory to access the fields.



Preliminary results seem to indicate an improvement in scaling, but a more exhaustive evaluation is required.

Conclusions

By using a real case scenario as plasma simulation we found several challenges to the programming model and FFTW.

- Several solutions to solve a chain of dependences between tasks were provided.
- The performance of MPI and TAMPI was compared.
- The scaling problem of the FFTW library was found and a solution is being developed.

Future work

The first priority is to fix the scalability issue of the FFTW. Other future ideas:

- Fully electromagnetic simulation.
- Better energy conserving codes / interpolation methods.
- Introduce more than 2 dimensions.
- Visualization of big simulations with `paraview`.
- Introduction of probe+receive operations in TAMPI.

End

Thanks for your attention.

The particle-in-cell method

The space of length $\boldsymbol{L}$ is discretized into grid points with a separation $\Delta \boldsymbol{x}$.

The scalar fields ρ and ϕ are now matrices of size $\boldsymbol{G} = (G_x, G_y)$

The vector field $\boldsymbol{E}$ is decomposed into E_x and E_y, which are now matrices of the same size.

Charge accumulation

At each grid point g at $\boldsymbol{x}$, the charge of each particle p at $\boldsymbol{x}_p$ is accumulated using an interpolation function W.

$$\rho(\boldsymbol{x}) = \sum_p q\, W(\boldsymbol{x} - \boldsymbol{x}_p) + \rho_0 \tag{6}$$

Using linear interpolation, we can define W for two dimensions as

$$W(\boldsymbol{x}) = \begin{cases} \left(1 - \dfrac{|x|}{\Delta x}\right)\left(1 - \dfrac{|y|}{\Delta y}\right) & \text{if } -\Delta\boldsymbol{x} < \boldsymbol{x} < \Delta\boldsymbol{x} \\ 0 & \text{otherwise} \end{cases} \tag{7}$$

LU solver

The Poisson equation is transformed in a linear system of N_g equations (one for each grid point).

$$\nabla^2\phi = -\frac{\rho}{\epsilon_0} \quad \rightarrow \quad A\frac{\phi}{\Delta x^2 \Delta y^2} = -\frac{\rho}{\epsilon_0} \quad \rightarrow \quad Ax = b \tag{8}$$

The coefficient matrix A has non-zero coefficients only at $a_{ii} = 4$ and $a_{ij} = -1$ with $j \in \{i+1, i-1, i+N_x, i-N_x\} \mod N_x$, for all $0 \leq i \leq Ng$.

The decomposition $A = LU$ is used to form two systems of equations $Ux = u$ and $Ly = b$, with a computational cost of $O(N_g^3)$ (but only at the beginning), which are solved in each iteration with cost $O(N_g^2)$.

MFT solver