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Chapter 1

Method

1.1 Poisson Solvers

In the Particle in Cell method, instead of calculating the forces directly between the particles, we first calculate the electric field from all the particles and then use that to calculate the individual force on the particles. From the particles we use a weighting scheme to obtain a charge density on a grid. Then we can use Poisson's equation eq. (1.1) to calculate the electric potential from the charge density, before computing the electric field from the potential. So we need an efficient Poisson solver.

$$\nabla^2 \Phi = -\rho \quad \text{in} \quad \Omega \quad (1.1)$$

The problem also need boundary conditions in which we will focus on periodic, Dirichlet and Neumann boundary conditions.

1.1.1 Spectral Methods

The spectral methods is based on Fourier transforms of the problem and solving the problem in it's spectral version, see **Shen1994** for an implementation of an spectral poisson solver. They are efficient solvers that can be less, but can be inaccurate for complex geometries.

When looking for a solution with a spectral method we first rewrite the functions as Fourier series, which for the three-dimensional Poisson equation would be

$$\nabla^2 \sum A_{j,k,l} e^{i(jx+ky+lz)} = \sum B_{j,k,l} e^{i(jx+ky+lz)} \quad (1.2)$$

From there we get a relation between the coefficients

$$A_{j,k,l} = -\frac{B_{j,k,l}}{j^2 + k^2 + l^2} \quad (1.3)$$

Then we compute the Fourier transform of the right hand side obtaining the coefficients $B_{j,k,l}$. We compute all the coefficients $A_{j,k,l}$ from the relation between the coefficients. At last we perform a inverse Fourier transform of the left hand side obtaining the solution.

(1.4)

1.1.2 Finite Element Methods

The finite element is a method to numerically solve a partial differential equations (PDE) first transforming the problem into a variational problem and then constructing a mesh and local trial functions, see **Sandve2011** for a more complete discussion.

To transform the PDE to a variational problem we first multiply the PDE by a test function v , then it is integrated using integration by parts on the second order terms. Then the problem is separated into two parts, the bilinear form $a(u, v)$ containing the unknown solution and the test function and the linear form $L(v)$ containing only the test function.

$$a(u, v) = L(v) \quad v \in \hat{V} \quad (1.5)$$

Next we construct discrete local function spaces of that we assume contain the trialfunctions and testfunctions. The function spaces often consists of locally defined functions that are 0 except in a close neighbourhood of a mesh point, so the resulting matrix to be solved is sparse and can be computed quickly. The matrix system is then solved by a suiting linear algebra algorithm, before the solution is put together.

1.2 Multigrid

The multi grid, MG, method used to solve the Poisson equation and obtain the electric field is a widely used and highly efficient solver for elliptic equations, having a theoretical scaling of $\mathcal{O}(N)$ (**Press1987**), where N is the grid points. Here I will go through the main theory and algorithm behind the method, as explained in more detail in (**Press1987; Trottenberg2000**) as well as go through some of possible algorithms to parallelize the method.

We want to solve a linear elliptic problem,

$$\mathcal{L}u = f \quad (1.6)$$

where \mathcal{L} is a linear operator, u is the solution and f is a source term. In our specific case the operator is given by the laplacian, the source term is given by the charge density and we solve for the electric potential.

We discretize the equation onto a grid of size q .

$$\mathcal{L}_q u_q = f_q \quad (1.7)$$

Let the error, v_q be the difference between the exact solution and an approximate solution to the difference equation (1.7), $v_q = u_q - \tilde{u}_q$. Then we define the residual as what is left after using the approximate solution in the equation.

$$d_q = \mathcal{L}_q \tilde{u}_q - f_q \quad (1.8)$$

Since \mathcal{L} is a linear operator the error satisfies the following relation

$$\mathcal{L}_q v_q = \mathcal{L}(u_q - \tilde{u}_q) + (f_q - f_q) \quad (1.9)$$

$$\mathcal{L}_q v_q = -d_q \quad (1.10)$$

In the multigrid methods instead of solving the equation directly here, we set up a system nested coarser square grids, $\mathfrak{T}_1 \subset \mathfrak{T}_2 \subset \dots \subset \mathfrak{T}_\ell$, where 1 is the coarsest grid and ℓ is the finest. Then the main thought behind the methods is that instead of solving the problem directly on the initial grid, we use restriction, \mathcal{R} , and interpolation, \mathcal{P} , operators to change the problem between the different grid levels and solve them on there. (Fix previous sentence) Due to the fewer grid points the problem is faster to solve on the coarser grid levels than on the fine grid.

If we then apply a restriction operator on the residual we go down a level on the grids and the opposite for the interpolation operator.

$$\mathcal{R}d_q = d_{q-1} \quad \text{and} \quad \mathcal{P}d_q = d_{q+1} \quad (1.11)$$

1.2.1 Algorithm

A sequential algorithm for a two grid V shaped algorithm, where the coarse grid and fine grid has respectively $q = 1, 2$.

- Initial approximation. \tilde{u}
- for $i < \text{nCycles}$:
 - Presmooth: $\hat{u}_2 = S_{pre}(u)_2$

- Calculate defect: $d_2 = f_2 - \mathcal{L}\hat{u}_2$
- Restrict defect: $d_1 = Rd_2$
- Initial guess: $\tilde{u}_1 = 0$
- Solve (G-S RB): $L_1\tilde{u}_1 = d_1$
- Interpolate: $\tilde{u}_2 = I\tilde{u}_1$
- Add correction: $u_2^{new} = \hat{u}_2 + \tilde{u}_2$

1.2.2 Smoothing: Gauss-Seidel

Relaxation methods, such as Gauss-Seidel, work by looking for the setting up the equation as a diffusion equation, and then solve for the equilibrium solution.

So suppose we want to solve the elliptic equation

$$\mathcal{L}u = \rho \quad (1.12)$$

Then we set it up as a diffusion equation

$$\frac{\partial u}{\partial t} = \mathcal{L}u - \rho \quad (1.13)$$

By starting with an initial guess for what u could be the equation will relax into the equilibrium solution $\mathcal{L}u = \rho$. By using a Forward-Time-Centered-Space scheme to discretize, along with the largest stable timestep $\Delta t = \Delta^2/2^d$ (Double check the factor.), we arrive at Jacobi's method, which is an averaging of the neighbors in addition to a contribution from the source term. By using the already updated values for in the calculation of the u^{new} we arrive at the method called Gauss-Seidel which for two dimensions is the following

$$u_{i,j}^{n+1} = \frac{1}{4} (u_{i+1,j}^n + u_{i-1,j}^{n+1} + u_{i,j+1}^n + u_{i,j-1}^{n+1}) - \frac{\Delta^2 \rho_{i,j}}{4} \quad (1.14)$$

To achieve a vectorization of the calculation of $u_{i,j}^{n+1}$ we will use Red and Black ordering, first calculating the odd nodes and then the even nodes, so the method has the available information.

1.3 Parallelization

For the parallelization of an algorithm there is two obvious issues that need to be addressed to ensure that the algorithm retains a high degree of parallelization; communication overhead and load imbalance (**Trottenberg**). Communication overhead means the time the computational nodes spend communicating with each other, if that is longer than the actual time spent computing the speed of

the algorithm will suffer, and load imbalance appears if some nodes need to do more work than others causing some nodes to stand idle.

Here we will focus on multigrid of a 3D cubic (to be expanded to rectangular cubes) grid, where each grid level has half the number of grid points. We will use grid partitioning to divide the domain, GS-RB (Gauss-Seidel Red-Black) as both a smoother and a coarse grid solver.

We need to investigate how the different steps: interpolation, restriction, smoothing and the coarse grid solver, in a MG method will handle parallelization.

1.3.1 Grid Partition

There are several well explored options for how a multigrid method can be parallelized, for example Domain Decomposition (**Arraras2015**), Algebraic Multigrid (**StUben2001**), see **Chow2006** for a survey of different techniques. Here we will focus on Geometric Multigrid (GMG) with grid partitioning used for the parallelization, as described in the books **Trottenberg2000**; **Trottenberg**

With grid partitioning we divide the grid \mathcal{T} into geometric subgrids, then we can let each processes handle one subgrid each, as we will see it can be useful when using the G-S RB smoothing to let the subgrids overlap 1 layer deep. since it on the edges of the subgrid it will need the adjacent node values.

1.3.2 Distributed and accumulated data

During the parallel execution of the code there can be useful to keep track of the different data structures and what needs to be accumulated over all the computational nodes and what only needs to be distributed on the individual computational nodes.

- u solution (Φ)
- w temporary correction
- d defect
- f source term (ρ)
- \mathcal{L} differential operator
- \mathcal{I} interpolation operator
- \mathcal{R} restriction operator
- **u** Bold means accumulated vector
- $\tilde{\mathbf{u}}$ is the temporary smoothed solution

- Accumulated vectors: $\mathbf{u}_q, \hat{\mathbf{u}}_q, \tilde{\mathbf{u}}_q, \hat{\mathbf{w}}_q, \mathbf{w}_{q-1}, \mathbf{I}, \mathbf{R}$
- Distributed vectors: f_q, d_q, d_{q-1}

Algorithm: P is the number of processes

- If (q == 1): Solve: $\sum_{s=1}^P \mathcal{L}_{s,1} \mathbf{u}_1 = \sum_{s=1}^P f_{s,1}$
- else:
 - Presmooth: $\hat{\mathbf{u}}_q = \mathcal{S}_{pre} \mathbf{u}_q$
 - Compute defect: $d_q = f_q - \mathcal{L}_q \hat{\mathbf{u}}_q$
 - Restrict defect: $d_{q-1} = \mathcal{R} d_q$
 - Initial guess: $\mathbf{w}_{q-1} = 0$
 - Solve defect system: $\mathbf{w}_{q-1} = PMG(\mathbf{w}_{q-1}, d_{q-1})$
 - Interpolate correction: $\mathbf{w}_q = \mathcal{R} \mathbf{w}_{q-1}$
 - Add correction: $\tilde{\mathbf{u}}_q = \hat{\mathbf{u}}_q + \mathbf{w}_q$
 - Post-smooth: $\mathbf{u}_q = \mathcal{S}_{post}$

1.3.3 Smoothing

Will use G-S with R-B ordering, supposedly good parallel properties (**Chow2006**). Follow algorithm I in **Adams2001** (alternatively try to implement the more complicated version)?

We have earlier divided the grid into subgrids, with overlap, as described in subsection 1.3.1 and given each processor responsibility for a subgrid. Then do a GS-RB method we start with an approximation of $u_{i,j}^n$. Then we will obtain the next iteration by the following formula

$$u_{i,j}^{n+1} = \frac{1}{4} (u_{i+1,j}^n + u_{i-1,j}^{n+1} + u_{i,j+1}^n + u_{i,j-1}^{n+1}) - \frac{\Delta^2 \rho_{i,j}}{4} \quad (1.15)$$

We can see that for the inner subgrid we will have no problems since we have all the surrounding grid points. On the edges we will need the adjacent grid points that are kept in the other processors. To avoid the algorithm from asking neighboring subgrids for adjacent grid points each time it reaches a edge we instead update the entire neighboring column at the start. So we will have a 1-row overlap between the subgrids, that need to be updated for each iteration.

1.3.4 Restriction

For the transfer down a grid level, to the coarser grid we will use a half weighting stencil. In two dimensions it will be the following

$$\mathcal{R} = \frac{1}{8} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 4 & 1 \\ 0 & 1 & 0 \end{bmatrix} \quad (1.16)$$

With the overlap of the subgrids we will have the necessary information to perform the restriction without needing communication between the processors (**Trottenberg**).

1.3.5 Interpolation

For the interpolation we will use bilinear interpolation:

$$\mathcal{I} = \frac{1}{4} \begin{bmatrix} 1 & 2 & 1 \\ 2 & 4 & 2 \\ 1 & 2 & 1 \end{bmatrix} \quad (1.17)$$

Since the interpolation is always done after GS-RB iterations the the outer part overlapped part of the grid updated, and we can have all the necessary information.

1.3.6 Scaling

Volume-Boundary effect

While a sequential MG algorithm has a theoretical scaling of $\mathcal{O}(N)$ (**Press1987**), where N is the number of grid points, an implementation will have a lower scaling efficiency due to interprocessor communication. We want a parallel algorithm that attains a high speedup with more added processors P , compared to sequential 1 processor algorithm. Let $T(P)$ be the computational time needed for solving the problem on P processors. Then we define the speedup $S(P)$ and the parallel efficiency $E(P)$ as

$$S(P) = \frac{T(1)}{T(P)} \quad E(P) = \frac{S(P)}{P} \quad (1.18)$$

A perfect parallel algorithm would the computational time would scale inversely with the number of processors, $T(P) \propto 1/P$ leading to $E(P) = 1$. Due to the necessary interprocessor communication that is generally not achievable.

	Cycle	Sequential	Parallel
MG	V	$\mathcal{O}(N)$	$\mathcal{O}(\log N)$
	W	$\mathcal{O}(N)$	$\mathcal{O}(\sqrt{N})$
FMG	V	$\mathcal{O}(N)$	$\mathcal{O}(\log^2 N)$
	W	$\mathcal{O}(N)$	$\mathcal{O}(\sqrt{N} \log N)$

Table 1.1: The parallel complexities of sequential and parallel multigrid cycles

The computational time of the algorithm is also important, if the algorithm is very slow but has good parallel efficiency it is often worse than a fast algorithm with a worse parallel efficiency.

The parallel efficiency of an algorithm is governed by the ratio between the time of communication and computation, T_{comm}/T_{comp} . If there is no need for communication, like on 1 processor, the algorithm is perfectly parallel efficient. In our case the whole grid is divided into several subgrids, which is assigned to different processors. In many cases the time used for computation is roughly scaling with the interior grid points, while the communication time is scaling with the boundaries of the subgrids. If a local solution method is used on a local problem it is only the grid points at the boundary that needs the information from grid points on the other processors. Since the edges has lower dimensionality than the inner grid points. So when the problem is increasing the time for computation grows faster than the time for communication, and a parallel algorithm often has a higher parallel efficiency on a larger problem. This is called the Boundary-Volume effect.

Parallel complexity

The complexities, as in needed computational work, of sequential and parallel MG cycles is calculated in **Trottenberg** and is shown in table 1.1. In the table we can see that in the parallel case there is a substantial increase in the complexity in the case of W cycles compared to V cycles. In the sequential case the change in complexity when going to a W cycle is not dependent on the problem size, but it is in the parallel case.

Chapter 2

Implementation of MG parts

2.1 Restriction

The multigrid method (MG) has several grids of different resolution, and we need to convert the problem between the different grids during the overarching the MG-algorithm. The restriction algorithm has the task of translating from a fine grid to a coarser grid. In this implementation we use a half weight stencil to restrict a quantity from a fine grid to a coarse grid. To get the coarse grid value it gives half weighting to the fine grid point corresponding directly to the coarse grid point, and gives the remaining half to the adjacent fine grid values, see (2.1), for 1D, 2D and 3D examples.

$$\begin{aligned}\mathcal{R}_{1D} &= \frac{1}{4} \begin{bmatrix} 1 & 2 & 1 \end{bmatrix} \\ \mathcal{R}_{2D} &= \frac{1}{8} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 4 & 1 \\ 0 & 1 & 0 \end{bmatrix} \\ \mathcal{R}_{3D} &= \frac{1}{12} \left(\begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 1 & 0 \\ 1 & 6 & 1 \\ 0 & 1 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \right)\end{aligned}\tag{2.1}$$

In our implementation we first cycle through all of the true coarse grid points, then the two main tasks is to find the specific fine grid point corresponding to the specific coarse grid point, and finding the indexes of the fine grid points surrounding the grid point.

Since the value in both grids are stored in a first order lexicographical array, we should treat the grid points in the same fashion, so the values are stored close to each other in the array. The first dimension is treated first, then the next is dimension is incremented followed by treating the first dimension again, then increment the next and so on. The fine grid has twice the resolution of the coarse grid, so for each time the coarse grid index is incremented, the fine grid index is

incremented twice.

Along the x-axis each incrementation is the number of values stored in the grid, which for scalars is 1 (This is only used for scalars, so now the 1 is hardcoded, I will need to test if using `size[0]` instead affects speed), and 2 for the fine index. The fine index will in addition need to skip 1 row each time, each time the y-axis is incremented, due to the finer resolution and 1 layer each time the z-axis is incremented.

At the edges of the grid we have ghost layers, which have equal thickness for both the grids, so the coarse grid needs to increment over the ghost values, in the x-direction, each time y is incremented. When z is incremented the index need to skip over a row of ghost values. The fine index follows the same procedure as the coarse index when dealing with the ghost layers.

When correct fine grid index is found, corresponding to a coarse grid index, the stencil needs to be applied around that grid value. This is done by first calculating the index of the first coarse and find indexes and setting the correct indexes for the surrounding grid values, then the surrounding grid indexes can be incremented exactly as the fine grid index and they will keep their shape around the fine grid index. Since our indexes in x, y and z are labeled j,l,k, the next value along the x-axis is labeled 'fj' and the previous is labeled 'fjj'. The coarse and fine grid indexes are label 'c' and 'f' respectively.

```
//Indexes
long int c = cSizeProd[1]*nGhostLayers[1] +
            cSizeProd[2]*nGhostLayers[2] +
            cSizeProd[3]*nGhostLayers[3];

long int f = fSizeProd[1]*nGhostLayers[1] +
            fSizeProd[2]*nGhostLayers[2] +
            fSizeProd[3]*nGhostLayers[3];
long int fj  = f + fSizeProd[1];
long int fjj = f - fSizeProd[1];
long int fk  = f + fSizeProd[2];
long int fkk = f - fSizeProd[2];
long int fl  = f + fSizeProd[3];
long int fll = f - fSizeProd[3];
```

Listing 2.1: Setting the stencil indexes

```

//Cycle Coarse grid
for(int l = 0; l < cTrueSize[3]; l++){
    for(int k = 0; k < cTrueSize[2]; k++){
        for(int j = 0; j < cTrueSize[1]; j++){
            cVal[c] = coeff*(6*fVal[f] + fVal[fj] + fVal[fjj] +
                fVal[fk] + fVal[fkk] + fVal[fl] + fVal[fll]);
            c++;
            f +=2;
            fj +=2;
            fjj +=2;
            fk +=2;
            fkk +=2;
            fl +=2;
            fll +=2;
        }
        c += cKEdgeInc;
        f += fKEdgeInc;
        fj += fKEdgeInc;
        fjj += fKEdgeInc;
        fk += fKEdgeInc;
        fkk += fKEdgeInc;
        fl += fKEdgeInc;
        fll += fKEdgeInc;
    }
    c += cLEdgeInc;
    f += fLEdgeInc;
    fj += fLEdgeInc;
    fjj += fLEdgeInc;
    fk += fLEdgeInc;
    fkk += fLEdgeInc;
    fl += fLEdgeInc;
    fll += fLEdgeInc;
}

```

Listing 2.2: The four loop doing the calculations

As of now there is 2 separate implementations, for 2 and 3 dimensions.

2.2 Prolongation

Along with the restriction operator described in the previous section, we also need prolongation operator to go from a coarse grid to a finer grid. Here we will use bilinear interpolation, for two dimensions and trilinear interpolation for 3 dimensions. In bilinear interpolation separate linear interpolation is done in the x- and y-direction, then those are combined to give a result on the wanted spot. (Note to self: Add source here) The same concept is expanded to give trilinear interpolation. The two and three dimensional stencils is given in (2.2)

$$\begin{aligned}
\mathcal{I}_{2D} &= \frac{1}{4} \begin{bmatrix} 1 & 2 & 1 \\ 2 & 4 & 2 \\ 1 & 2 & 1 \end{bmatrix} \\
\mathcal{I}_{3D} &= \frac{1}{8} \left(\begin{bmatrix} 1 & 2 & 1 \\ 2 & 4 & 2 \\ 1 & 2 & 1 \end{bmatrix}, \begin{bmatrix} 2 & 4 & 2 \\ 4 & 8 & 4 \\ 2 & 4 & 2 \end{bmatrix}, \begin{bmatrix} 2 & 2 & 1 \\ 2 & 4 & 2 \\ 1 & 2 & 1 \end{bmatrix} \right)
\end{aligned} \tag{2.2}$$

The algorithm implemented for the interpolation is based on the method, described in ?? has the following steps, which is also shown for a 2D case in 2.1.

1. Direct insertion: Coarse- \rightarrow Fine
2. Interpolation on highest Dimension: $f(x) = \frac{f(x+h)+f(x-h)}{2h}$
3. Fill needed ghosts.
4. Interpolation on next highest Dimension

The interpolation should always first be done on the highest dimension, because the grid values are stored further apart along the highest axis in the memory, and the each successive interpolation needs to apply to more grid points. (Note to self: should test)

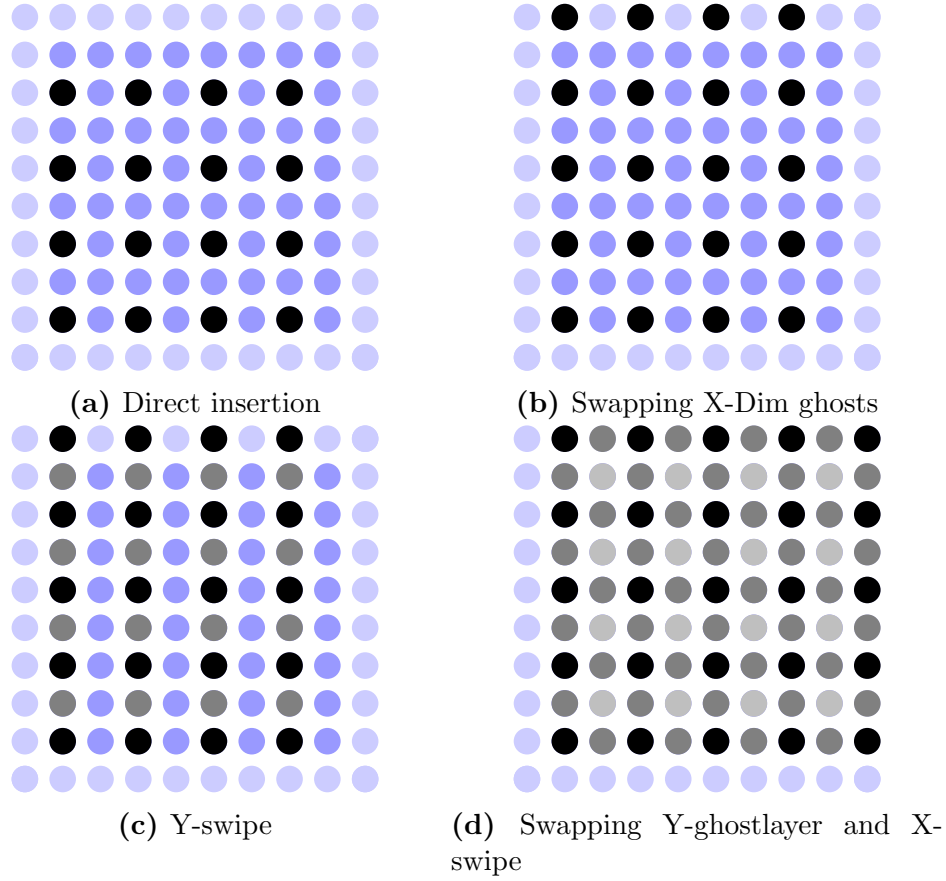


Figure 2.1: This figure shows the steps in computing the prolongation stencil in an $[8 \times 8]$ grid. First a direct insertion from the coarse grid is performed (2.1a), followed by filling the ghostlayer perpendicular to the x-axis from the neighbouring grid (2.1b). Then a swipe is performed in the y-direction filling the grid points between, taking half the value from the node above, and half from the node below (2.1c). Then a ghost swap is performed before doing a swap in the x-direction (2.1d).

The direct insertion is done similar to the previously described in the restriction section, ??.

```
//Interpolation 3rd Dim
f = fSizeProd[1] + fSizeProd[2] + 2*fSizeProd[3];
fNext = f + fSizeProd[3];
fPrev = f - fSizeProd[3];

for(int l = 0; l < fTrueSize[3]; l+=2){
    for(int k = 0; k < fSize[2]; k+=2){
        for(int j = 0; j < fSize[1]; j+=2){
            fVal[f] = 0.5*(fVal[fPrev]+fVal[fNext]);
            f +=2;
            fNext +=2;
            fPrev +=2;
        }
        f +=fSizeProd[2];
        fNext +=fSizeProd[2];
        fPrev +=fSizeProd[2];
    }
    f +=fSizeProd[3];
    fNext +=fSizeProd[3];
    fPrev +=fSizeProd[3];
}

gSwapHalo(fine, mpiInfo, 2);

//Interpolation 2nd Dim
f = fSizeProd[1] + 2*fSizeProd[2] + fSizeProd[3];
fNext = f + fSizeProd[2];
fPrev = f - fSizeProd[2];

for(int l = 0; l < fTrueSize[3]; l++){
    for(int k = 0; k < fSize[2]; k+=2){
        for(int j = 0; j < fSize[1]; j+=2){
            fVal[f] = 0.5*(fVal[fPrev]+fVal[fNext]);
            f +=2;
            fNext +=2;
            fPrev +=2;
        }
        f +=fSizeProd[2];
        fNext +=fSizeProd[2];
        fPrev +=fSizeProd[2];
    }
}

gSwapHalo(fine, mpiInfo, 1);

//Interpolation 2nd Dim
f = 2*fSizeProd[1] + fSizeProd[2] + fSizeProd[3];
fNext = f + fSizeProd[1];
```



```

fPrev = f - fSizeProd[1];

for(int l = 0; l < fTrueSize[3]; l++){
    for(int k = 0; k < fTrueSize[2]; k++){
        for(int j = 0; j < fSize[1]; j+=2){
            fVal[f] = 0.5*(fVal[fPrev]+fVal[fNext]);
            f +=2;
            fNext +=2;
            fPrev +=2;
        }
    }
    f +=2*fSizeProd[2];
    fNext +=2*fSizeProd[2];
    fPrev +=2*fSizeProd[2];
}

```

Listing 2.3: Codesnippet for the Z Y and X sweeps

Notes

- Restriction algorithm
 - I tried to make a simpler algorithm, that just cycled through all the values and didn't care about the ghost layers. The problem was that the fine grid needed to increment twice as fast as the coarse grid, except at the edge where it needed to increment the same as the coarse grid, due to having the same number of ghost cells.
- Prolongation
 - All the dimensional swipes repeats itself so much that it should easily be able to modified to an nDim algorithm instead of a 2D and 3D case.
 - When filling ghost layer in a particular direction, we already know that only one side has values. So transferring both sides of the ghost layer is unnecessary.
- Should time everything, test performance/improvements

2.3 Jacobian and Gauss-Seidel RB

The main iterative ODE solver, in this version of the multigrid program, is a Gauss-Seidel Red-Black, in addition a Jacobian solver was developed as a stepping stone and testing purposes. It is a modification of the Jacobian method, where the updated values are used where available, which lead to a doubled converging rate **NumReci**

Our problem is given by $\nabla^2\phi = -\rho$, one way to think of the jacobian method is as a diffusion problem, and with the equilibrium solution as our wanted solution. If we then discretize the diffusion problem by a Forward-Time-Centralized-Space scheme, we arrive at the Jacobian method, which is shown explicitly below for 1 dimension.

$$\frac{\partial\phi}{\partial t} = \nabla^2\phi + \rho \quad (2.3)$$

The subscript j indicates the spatial coordinate, and the superscript n is the 'temporal' component.

$$\frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} = \frac{\phi_{j+1}^n - 2\phi_j^n + \phi_{j-1}^n}{\Delta x^2} + \rho_j \quad (2.4)$$

This is numerically stable if $\Delta t/\Delta x^2 \leq 1/2$, so using the timestep $\Delta t = \Delta x^2/2$ we get

$$\phi_j^{n+1} = \phi_j^n + \frac{1}{2} (\phi_{j+1}^n - 2\phi_j^n + \phi_{j-1}^n) + \frac{\Delta x^2}{2} \rho_j \quad (2.5)$$

Then we arrive at the Jacobian method

$$\phi_j^{n+1} = \frac{1}{2} (\phi_{j+1}^n + \phi_{j-1}^n + \Delta x^2 \rho_j) \quad (2.6)$$

The Gauss-Seidel method uses updated values, where available, and is given by

$$\phi_j^{n+1} = \frac{1}{2} (\phi_{j+1}^n + \phi_{j-1}^{n+1} + \Delta x^2 \rho_j) \quad (2.7)$$

Following the same procedure we get the Gauss-Seidel method for 2 and 3 dimensions.

$$\phi_{j,k}^{n+1} = \frac{1}{4} (\phi_{j+1,k}^n + \phi_{j-1,k}^{n+1} + \phi_{j,k+1}^n + \phi_{j,k-1}^{n+1} + \Delta x^2 \rho_{j,k}) \quad (2.8)$$

$$\phi_{j,k,l}^{n+1} = \frac{1}{8} (\phi_{j+1,k,l}^n + \phi_{j-1,k,l}^{n+1} + \phi_{j,k+1,l}^n + \phi_{j,k-1,l}^{n+1} + \phi_{j,k,l+1}^n + \phi_{j,k,l-1}^{n+1} + \Delta x^2 \rho_{j,k,l}) \quad (2.9)$$

Here we have implemented a different version of the Gauss-Seidel algorithm called Red and Black ordering, which has conceptual similarities to the leapfrog algorithm, where usually position and velocity is computed at t and $t + (\delta t)/2$. Every other grid point is labeled a red point, and the remaining is black. When updating a red node only black nodes are used, and when updating black nodes only red nodes are used. Then a whole cycle consists of two halfsteps which calculates the red and black nodes separately.

- For all red points:

$$\phi_{j,k,l}^{n+1/2} = \frac{1}{8} (\phi_{j+1,k,l}^n + \phi_{j-1,k,l}^n + \phi_{j,k+1,l}^n + \phi_{j,k-1,l}^n + \phi_{j,k,l+1}^n + \phi_{j,k,l-1}^n + \Delta x^2 \rho_{j,k,l})$$

- For all black points:

$$\phi_{j,k,l}^{n+1} = \frac{1}{8} (\phi_{j+1,k,l}^{n+1/2} + \phi_{j-1,k,l}^{n+1/2} + \phi_{j,k+1,l}^{n+1/2} + \phi_{j,k-1,l}^{n+1/2} + \phi_{j,k,l+1}^{n+1/2} + \phi_{j,k,l-1}^{n+1/2} + \Delta x^2 \rho_{j,k,l})$$

2.3.1 Implementation

Jacobi's method

The implementation of the jacobian algorithm is straightforward, but it has the downside of slow convergence and bad smoothing properties, in addition to needing an additional created. When ϕ_i^{n+1} is computed we need access to the previous value ϕ_{i-1}^n , and more values in higher dimensions, so either the previous values need to be stored separately, or ϕ_i^{n+1} can be computed on a new grid and then copied over after completing the cycle. In this implementation we computed on a temporary grid and then copied over, since it was mostly for debugging purposes and efficiency was not a concern.

The computation is done by starting at index $g = 0$, computing the surrounding grid indexes, gj, gjj, \dots , where gj is the next grid point along the x-axis, and gjj is the previous value. Then the entire grid is looped through over, incrementing both g and the surrounding grid indexes gj, gjj, \dots . The computation on the ghost layers will be incorrect but those will be overwritten when swapping halos. See 2.3.2 for an example code in 2D.

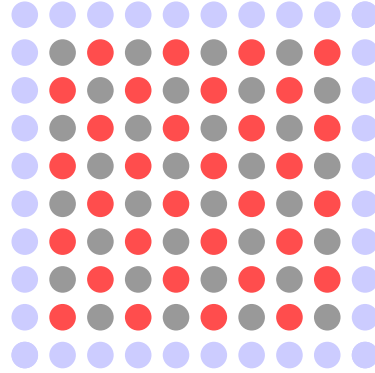
Gauss-Seidel Red and Black

In the implementation of Gauss-Seidel algorithm we use a clever ordering of the computations, called Red and Black ordering, both to increase the smoothing properties of the algorithm as well as avoiding creating a temporary grid to store ϕ^{n+1} in. Every grid point where the indexes sum up to an even number is labeled a red point and the odd index groupings are labeled black points, see fig. 2.2a. Then each red point is directly surrounded by only black points and vice versa.

A cycle is then divided into 2 halfcycles, where each halfcycle computes ϕ^{n+1} for the red and black points respectively.

1. for(int c = 0; c<nCycles; c++)

- Cycle through red points and compute ϕ^{n+1}
- Swap Halo
- Cycle through black points and compute ϕ^{n+1}



(a) Red and Black ordering

- Swap Halo

For the 2 dimensional case the cycling is done first for the odd rows and even rows separately, due to the similarity between all the red points in the odd rows, and between the red points in the even rows. Then the cycling could be generalized into a static inline function used for all the cycling. See 2.3.3 for the 2D implementation.

For the 3 dimensional case there is now did two different takes on the problem, one where the iteration through the grid is streamlined, but needing several loops through the grid taking care of a subgroup of the grid points each loop. The other algorithm uses one loop through the grid, with different conditions on the edges to make it go through the correct grid points in each line.

When the loops are streamlined the edges the loop go through the entire grid, but when it reaches an edge in it either needs to add or subtract 1 to the iterator index. In we want to do a red pass, computing all the red values, the grid is cycled through increasing by 2 each time. Then it will access up the indexes, 36, 38, 40, 42, \dots . In the second row we want it to use the index 43, instead of 42, so we need to increase it by 1 when it reaches the edge. When it reaches the end of the second line, we want it to increase from 47 to 48, so then we need to subtract 1. In the next layer we need to shift the behaviour on the edges to the opposite. See

.
48	49	49	50	51	52
42	43	44	45	46	47
36	37	38	39	40	41

In the other implementation I tried something similar to the 2D implementation, where it does several loops through the grid, computing an easier subgroup of the red nodes each time, so the iterator index can increase by just to each time. So for the red points it computes the odd and even layers and rows separately.

- Compute Odd layers, odd rows
- Compute Odd layers, even rows
- Compute Even Layers, odd rows
- Compute Even layers, even rows

2.3.2 Jacobian code

```
for(int c = 0; c < nCycles; c++){
    // Index of neighboring nodes
    int gj = sizeProd[1];
    int gjj = -sizeProd[1];
    int gk = sizeProd[2];
    int gkk = -sizeProd[2];

    for(long int g = 0; g < sizeProd[rank]; g++){
        tempVal[g] = 0.25*( phiVal[gj] + phiVal[gjj] +
                           phiVal[gk] + phiVal[gkk] + rhoVal[g]);

        gj++;
        gjj++;
        gk++;
        gkk++;
    }

    for(int q = 0; q < sizeProd[rank]; q++) phiVal[q] =
        tempVal[q];
    for(int d = 1; d < rank; d++) gSwapHalo(phi, mpiInfo,
        d);
}
```

Listing 2.4: Code snippet 2D jacobian

2.3.3 GS-RB 2D

```

for(int c = 0; c < nCycles;c++){

    //Increments
    int kEdgeInc = nGhostLayers[2] + nGhostLayers[rank +
        2] + sizeProd[2];

    /******
     *   Red Pass
     *****/
    //Odd numbered rows
    g = nGhostLayers[1] + sizeProd[2];
    loopRedBlack2D(rhoVal, phiVal, sizeProd, trueSize,
        kEdgeInc, g, gj, gjj, gk, gkk);

    //Even numbered columns
    g = nGhostLayers[1] + 1 + 2*sizeProd[2];
    loopRedBlack2D(rhoVal, phiVal, sizeProd, trueSize,
        kEdgeInc, g, gj, gjj, gk, gkk);

    for(int d = 1; d < rank; d++) gSwapHalo(phi, mpiInfo,
        d);

    /******
     *   Black pass
     *****/
    //Odd numbered rows
    g = nGhostLayers[1] + 1 + sizeProd[2];
    loopRedBlack2D(rhoVal, phiVal, sizeProd, trueSize,
        kEdgeInc, g, gj, gjj, gk, gkk);

    //Even numbered columns
    g = nGhostLayers[1] + 2*sizeProd[2];
    loopRedBlack2D(rhoVal, phiVal, sizeProd, trueSize,
        kEdgeInc, g, gj, gjj, gk, gkk);

    for(int d = 1; d < rank; d++) gSwapHalo(phi, mpiInfo,
        d);
}

return;
}

```

Listing 2.5: Main loop

```

gj = g + sizeProd[1];
gjj = g - sizeProd[1];

```

```
gk = g + sizeProd[2];
gkk= g - sizeProd[2];

for(int k = 1; k < trueSize[2]; k +=2){
    for(int j = 1; j < trueSize[1]; j += 2){
        phiVal[g] = 0.25*( phiVal[gj] + phiVal[gjj] +
                           phiVal[gk] + phiVal[gkk] + rhoVal[g]);
        g +=2;
        gj +=2;
        gjj +=2;
        gk +=2;
        gkk +=2;
    }
    g +=kEdgeInc;
    gj +=kEdgeInc;
    gjj +=kEdgeInc;
    gk +=kEdgeInc;
    gkk +=kEdgeInc;
}
```

Listing 2.6: Loop through grid

2.4 GS-RB 3D if tests

```

/*****
 * Red Pass
 *****/
g = sizeProd[3]*nGhostLayers[3];
for(int l = 0; l < trueSize[3]; l++){
    for(int k = 0; k < size[2]; k++){
        for(int j = 0; j < size[1]; j+=2){
            phiVal[g] = 0.125*( phiVal[g+gj] + phiVal[g-gj] +
                                phiVal[g+gk] + phiVal[g-gk] +
                                phiVal[g+gl] + phiVal[g-gl] + rhoVal[g]);
            g +=2;
        }
        if(l%2){
            if(k%2) g+=1; else g-=1;
        } else {
            if(k%2) g-=1; else g+=1;
        }
    }
    if(l%2) g-=1; else g+=1;
}

for(int d = 1; d < rank; d++) gSwapHalo(phi, mpiInfo, d);

```

Listing 2.7: GS-RB with if-tests

2.5 GS-RB 3D without if tests

```

/*****
 * Red Pass
 *****/
//Odd layers - Odd Rows
g = nGhostLayers[1]*sizeProd[1] +
    nGhostLayers[2]*sizeProd[2] +
    nGhostLayers[3]*sizeProd[3];
loopRedBlack3D(rhoVal, phiVal, sizeProd, trueSize,
    kEdgeInc, lEdgeInc,
    g, gj, gjj, gk, gkk, gl, gl);

//Odd layers - Even Rows
g = (nGhostLayers[1]+1)*sizeProd[1] +
    (nGhostLayers[2]+1)*sizeProd[2] +
    nGhostLayers[3]*sizeProd[3];
loopRedBlack3D(rhoVal, phiVal, sizeProd, trueSize,
    kEdgeInc, lEdgeInc,
    g, gj, gjj, gk, gkk, gl, gl);

//Even layers - Odd Rows
g = (nGhostLayers[1])*sizeProd[1] +
    (nGhostLayers[2])*sizeProd[2] +
    (nGhostLayers[3]+1)*sizeProd[3];
loopRedBlack3D(rhoVal, phiVal, sizeProd, trueSize,
    kEdgeInc, lEdgeInc,
    g, gj, gjj, gk, gkk, gl, gl);

//Even layers - Even Rows
g = (nGhostLayers[1] + 1)*sizeProd[1] +
    (nGhostLayers[2]+1)*sizeProd[2] +
    (nGhostLayers[3]+1)*sizeProd[3];
loopRedBlack3D(rhoVal, phiVal, sizeProd, trueSize,
    kEdgeInc, lEdgeInc,
    g, gj, gjj, gk, gkk, gl, gl);

for(int d = 1; d < rank; d++) gSwapHalo(phi, mpiInfo, d);

```

Listing 2.8: main routine

```

inline static void loopRedBlack3D(double *rhoVal, double
    *phiVal, long int *sizeProd, int *trueSize, int
    kEdgeInc, int lEdgeInc,
    long int g, long int gj, long int gjj, long int gk,
    long int gkk, long int gl, long int gl){

    gj = g + sizeProd[1];
    gjj = g - sizeProd[1];

```

```

gk = g + sizeProd[2];
gkk= g - sizeProd[2];
gl = g + sizeProd[3];
gll= g - sizeProd[3];

for(int l = 0; l<trueSize[3]; l+=2){
  for(int k = 0; k < trueSize[2]; k+=2){
    for(int j = 0; j < trueSize[1]; j+=2){
      // msg(STATUS, "g=%d", g);
      phiVal[g] = 0.125*(phiVal[gj] + phiVal[gjj] +
                        phiVal[gk] + phiVal[gkk] +
                        phiVal[gl] + phiVal[gll] + rhoVal[g]);

      g +=2;
      gj +=2;
      gjj +=2;
      gk +=2;
      gkk +=2;
      gl +=2;
      gll +=2;
    }
    g +=kEdgeInc;
    gj +=kEdgeInc;
    gjj +=kEdgeInc;
    gk +=kEdgeInc;
    gkk +=kEdgeInc;
    gl +=kEdgeInc;
    gll +=kEdgeInc;
  }
  g +=lEdgeInc;
  gj +=lEdgeInc;
  gjj +=lEdgeInc;
  gk +=lEdgeInc;
  gkk +=lEdgeInc;
  gl +=lEdgeInc;
  gll +=lEdgeInc;
}

return;
}

```

Listing 2.9: loop routine

In the following description of the steps in the MG method, we will use ϕ , ρ , d and ω to signify the solution, source, defect and correction respectively. A subscript means the grid level, while the superscript 0 implies an initial guess is used. For storage purposes we will use three MG data structures, one containing the solution, ϕ , one containing each levels source term ρ and one that is used for the defect when coarsifying the problem and for the correction when going back to the finer grids.

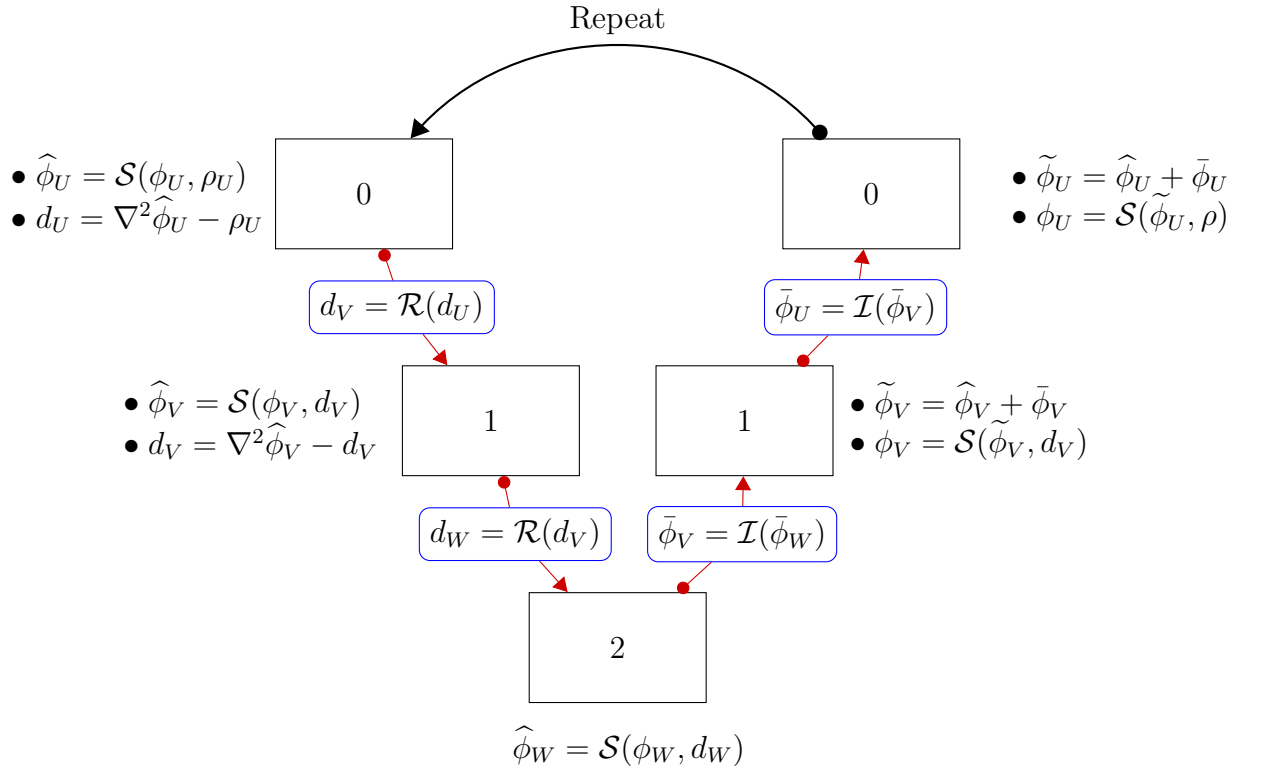


Figure 2.3: Schematic overview of the PIC method. In a three level MG implementation, there is 5 main steps in a cycle that needs to be consider.

1. Compute defect on grid 0, the finest grid:

- $\widehat{\phi}_0 = \mathcal{S}(\phi_0, \rho_0)$
- $d_0 = \nabla^2 \widehat{\phi}_0 - \rho_0$
- Restrict defect: $\rho_1 = \mathcal{R}d_0$

2. Compute defect on grid 1:

- $\widehat{\phi}_1 = \mathcal{S}(\phi_1^0, \rho_1)$
- $d_1 = \nabla^2 \widehat{\phi}_1 - \rho_1$
- Restrict defect: $\rho_2 = \mathcal{R}d_1$

3. Solve Coarse Grid for correction ω

- $\phi_2 = \mathcal{S}(\phi_2^0, \rho_2)$
- Interpolate as correction: $\omega_1 = \mathcal{I}\omega_2$

4. Compute correction on level 1:

- $\widetilde{\phi}_1 = \widehat{\phi}_1 + \omega_1$
- $\phi_1 = \mathcal{S}(\widetilde{\phi}_1, \rho_1)$
- Interpolate correction: $\omega_0 = \mathcal{I}\phi_1$

5. Compute solution.

- $\widetilde{\phi}_0 = \widehat{\phi}_0 + \omega_0$
- $\phi_0 = \mathcal{S}(\widetilde{\phi}_0, \rho_0)$

Chapter 3

Unit Tests

TBD

Chapter 4

Optional methods

4.1 MG-Methods

4.1.1 FMG

- 'Easy' to implement.
- Theoretically scales $\mathcal{O}(N)$ (**Press1987**), in reality
- FMG and W cycles are usually avoided in massive parallel computers (**Chow2006**), as they visit the coarsest grid often, due to:
 - At the coarsest level the computation is fast, communication usually the bottleneck
 - Coarsest grid may couple all the domain, needs global communication
- Options to solve the coarse matrix (**Chow2006**)
 - Direct solver: Sequential, if small problem may be done on each processor to avoid communication
 - Iterative method, Gauss-Seidel. Can be parallelized
- Will use G-S with R-B ordering, has good parallel properties

4.2 Other methods worth considering

- MUMPS (MUltifrontal Massive Parallel Solver), tried and compared in **Kacem2012** slower than MG.
 - Solves $Au = \rho$ for a sparse matrix.

Chapter 5

Grid Structs and Partitioning

5.1 Data structures

The fields and quantities in our PiC model is discretized on a three-dimensional grid and comes to use several places in the method. In the multigrid calculation we also have a use for several grids of varying spatial coarseness. So it will be useful for us to organize the data so we have the grid stored as an independent structure available for the program, while the multigrid part uses an extended version where it also has access to the different coarser subgrids. There will also be several types of grid, all with the same specifications, but storing different quantities, so we will use a grid template that all the grids of the same size shares, while we will have a separate struct containing the quantities in the grid and the specifications.

5.2 Domain partitioning

As earlier discussed, in 1.3.1 the physical domain covered by our model will be divided onto several processors that each take care of a subdomain. The subdomains are dependent on each other and we need some communication between them, which we solve by letting each subdomain also store the edge of the neighboring subdomain. Depending on the boundary conditions it could also be useful to store an extra set of values on the outer domain boundary as well, which will be called ghost points, N_G . The extra grid points due to the overlap between the subdomains we will call overlap points, N_O . Let us for simplicity sake consider a regular domain, with equal extent in all dimensions, with N grid points per dimension, d and consider how many grid values we need to store as a singular domain and the grid values needed when it is divided amongst several processors, a 2 dimensional case is depicted in fig. 5.1.

5.2.1 Singular domain

In the case where the whole domain is worked on by one process we need N^d to store the values on the grid representing the physical problem, in addition we see that we also need to store values for the ghost points along the domain boundary. Given that we have one layer of ghost points on all the boundaries, and there is 2 boundaries per dimension, the total number of ghost points is given by $N_G = 2dN$. Since there is only 1 domain we don't need to account for any overlap between subdomains and the total grid points we need to store is:

$$N_{Tot} = N^d + N_G + N_O = N^d + 2dN^{d-1} \quad (5.1)$$

For the 2 dimensional case, in fig. 5.1, that adds up to $N_{Tot} = 8^2 + 2 \times 4 \times 8 = 128$.

5.2.2 Several subdomains

In the case where we introduce several subdomain, in addition to storing the grid values and the ghost points we also need to store an overlap between the subdomains. If we take our whole domain Ω and divide it up into several small domains Ω_S , the smaller domains only take a subsection of the grid points. For simplicity case, and equal load on processors, we let the subdomains as well be regular, with the whole domain being a multiple of the subdomains. Our whole domain has N grid points in each direction, if we then divide that domain into $\#\Omega$ domains, then each of those subdomains will have $N_S = N^d / \#\Omega$ grid points. Each of those subdomains will also need values representing the ghost points and overlap from the neighboring nodes. A boundary of a subdomain will either have overlap points, or ghost points, not both at the same time so for each boundary we need to 1 layer, N_S^{d-1} . Each subdomain will have 2 boundaries per dimension since we have regular subdomains. The total number of grid points needed per subdomain is then

$$N_{Tot,S} = N_S^d + (N_G + N_O) = N_S^d + 2dN_S^{d-1} \quad (5.2)$$

while the total number of grid points is

$$N_{Tot} = \#\Omega N_{Tot,S} \quad (5.3)$$

For the 2 dimensional case discussed earlier we need $N_{Tot,S} = 4^2 + 2 \times 2 \times 4^1 = 32$.

Since the effect of the subdomain boundaries increase the coarser the grid is we should not let the coarsest multigrid level be too small. We also don't need the spatial extent of the grid to be equal on all sides, but it was done here to keep the computations simple.

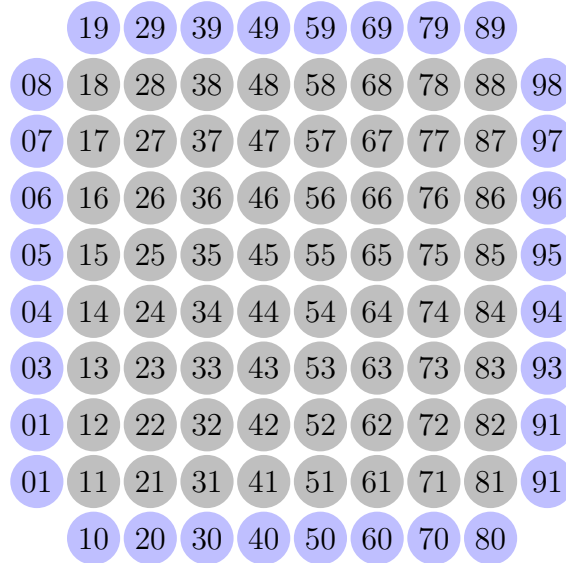
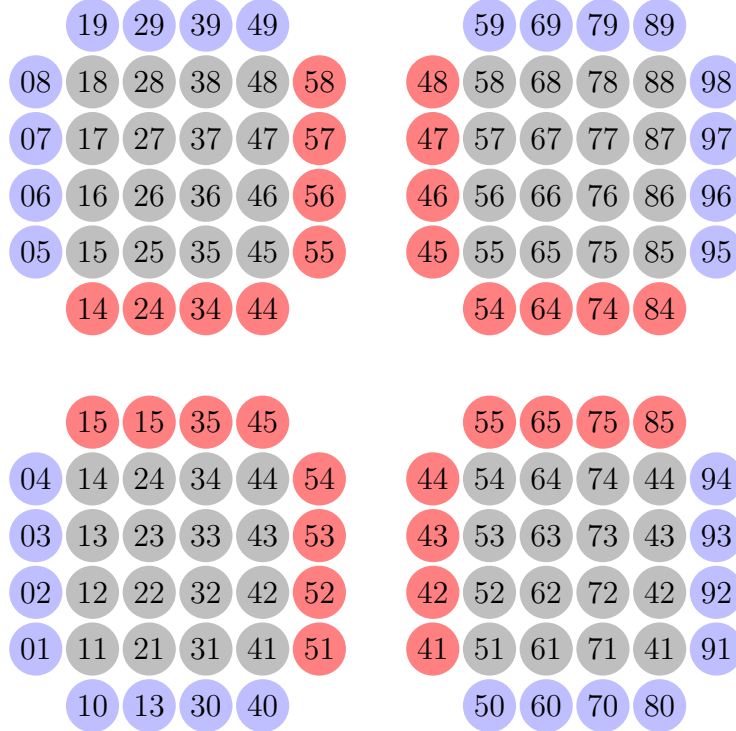
(a) The grid points needed for an 8×8 domain.(b) The 8×8 grid divided into 4 subdomains

Figure 5.1: Each circle in the figures represents 1 grid point, and the first number is the column while the second is the row. The grey colour represents physical space the computational node works on, the blue color is the outer grid points for boundary conditions and the red colour is the overlapping grid points.

Chapter 6

Verification and Testing

The multigrid method has several different steps in the algorithm, as a developmental help and to ensure that the program works correctly during as many different conditions as possible we want to test the whole code, as well as the constituent parts where possible. The method is quite modular and several parts of it can be tested alone. The GS-RB, used for smoothing, can be independently tested, since on it's own it converges to a solution, just at a higher computational cost than the multigrid method. To test it we will use an initial density field with a length between the grid steps that results in an exact answer. The restriction and prolongation operators can also tested to a degree by checking that they preserve a constant grid through several grid level changes.

6.0.3 Prolongation and Restriction

The prolongation and restriction operators with the earlier proposed stencils will average out the grid points when applied. So the idea here is to set up a system with a constant charge density, $\rho(\mathbf{r}) = C$, and then apply a restriction. After performing the restriction we can check that the grid points values are preserved. Then we can do the same with the prolongation. While this does not completely verify that the operators work as wanted, it gives an indication that we have not lost any grid points and the total mass of the charge density should be conserved.

6.0.4 Smoother

The iterative method GS-RB used for the pre- and postsmoothing of the grid in our implementation of the multigrid method is also a direct solver. So we can test it, or most other smoothers, by testing them on a small system where the problem has an analytical solution. Then we can let them run for a while and ensure that they are converging towards the solution. If we let the source term be sinusoidal in one direction, and constant in the other directions it has an easy solution given below

$$\nabla^2 \phi(x, y, z) = \sin(x) \tag{6.1}$$

This has a solution when $\phi(x, y, z) = -\sin(x)$ and we can test that the solver converges to the solution. If we let the source term be constant in the x direction and instead vary in the other directions we can get verify that the solver works in all three directions independently.

6.0.5 Multigrid method

We use both of the aforementioned tests to check that the whole multigrid method works as intended. Since a constant source term will give a trivial solution of the potential, $\phi(x, y, z) = \mathbf{0}$, we use that as a test. In addition we also test that it converges on a sinusoidal source term as we did the smoother.

Chapter 7

Multigrid Libraries

Efficient computation of the poisson equation, or other elliptic equations, is a common problem with many applications, and there exists several predeveloped and optimized libraries to help solve it. These include Parallel Particle Mesh (PPM) ([Sbalzarini2006](#)), Hypre ([Falgout02hypre:a](#)), Muelu ([??](#)), METIS ([METIS](#)) and PETCs ([Gropp2001](#)) amongst others. There is also PiC libraries that can be used PICARD and VORPAL to mention two.

If we want to have an efficient integration of a multigrid library into our PiC model we need to consider how easy it is to use with our scalar and field structures. To have an efficient program we need to avoid having the program convert data between our structures and the library structures. Since our PiC implementation uses the same datastructures for the scalar fields in several other parts, than the solution to the poisson equation, we could have an efficiency problem in the interface between our program and the library.

We could also consider that only part of the multigrid algorithm uses building blocks from libraries. The algorithm is now using the conceptually, and programmatically easy, GS-RB as smoothers, but if we implement compatibility with a library we could easily use several other types of smoothers which could improve the convergence of the algorithm

7.1 Libraries

7.2 PPM - Parallel Particle Mesh

Parallel Particle Mesh is a library designed for particle based approaches to physical problems, written in Fortran. As a part of the library it includes a structured geometric multigrid solver which follows a similar algorithm to the algorithm we have implemented in our project implemented in both 2 and 3 dimensions. For the 3 dimensional case the laplacian is discretized with a 7-point stencil, then it uses a RB-SOR (Red and Black Succesive Over-Relaxation), which equals GS-

RB with the relaxation parameter ω set as 1, as a smoother. The full-weighting scheme is used for restriction and trilinear interpolation for the prolongation, both are described in (**Trottenberg**). It has implementations for both V and W multigrid cycles. To divide up the domains between the computational nodes it uses the METIS library. The efficiency of the parallel multigrid implementation was tested

7.3 Hypre

Hypre is a library developed for solving sparse linear systems on massive parallel computers. It has support for c and Fortran. Amongst the algorithms included is both structured multigrid as well as element-based algebraic multigrid. The multigrid algorithms scales well on up to 100000 cores, for a detailed overview see Baker et al 2012. (bibtex files started to argue, will fix).

7.4 MueLo - Algebraic Multigrid Solver

MueLo is an algebraic multigrid solver, and is a part of the TRILINOS project and has the advantage that it works in conjunction with the other libraries there. It is written as an object oriented solver in cpp. For a investigation into the scaling properties see Lin et. al. 2014.

7.5 METIS - Graph Partitioning Library

METIS is a library that is used for graph partitioning, and could have been used in our program to partition the grids. The partitionings it produces has been shown to be 10% to 50% faster than the partitionings produces by spectral partitioning algorithms (**Karypis**). It is mostly used for irregular graphs, and we are not sure if it could be easily made to work with the datastructures used throughout the program.

7.6 PETSc - Scientific Toolkit

The PETSc is an extensive toolkit for scientific calculation that is used by a multitude of different numerical applications, including FEniCS. It has a native multigrid option, DMDA, where the grid can be constructed as a cartesian grid. In addition there is large amount of inbuilt smoothers that can be used.