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Utregning av det elektromagnetiske feltet i Monte Carlo transport simulering

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Master i fysikk og matematikk

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Implementation of Maxwell Equation Solver in Full-band Monte Carlo Transport Simulators

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Abstract

This is the master thesis at the end of the Applied Physics and Mahtematics program at the Norwegian University of Science and Technology (NTNU). It has been carried out in cooperation with the Norwebian Defense Research Establishement (FFI) in LillestrÃ¸m. FFI have during the last several years been developing a simulation program for semiconductor devices using the Monte Carlo method. This thesis has been centered around creating a Poisson equation solver using the biconjugate gradient stabilized (BiCGStab) method, an iterative krylov subspace solution method. A working 2D BiCGStab solver for a uniform mesh grid, and a non-uniform mesh has been written and implemented in the Monte Carlo program, in addition to adaptive grid routines to distribute the non-uniform mesh.

Defense Research Establishment (FFI) in LillestrÃ¸m, who

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Chapter 1

Introduction

As electronic and optoelectronic devices get increasingly advanced, it is important to understand their behaviour before starting production or expensive prototyping tests. Whether it is a nuclear reactor or new and smaller transistors, this often means studying the physical behaviour through computer simulation. In this master thesis will will look at Monte Carlo semiconductor transport simulation. More specifically, at the solution of Poisson's equation through the means of the finite difference method and an iterative solver. In doing so, we will also study a practical implementation of in a semiconductor transport simulator, and investigate how one can utilize uniform, or non-uniform meshes.

1.1 The Monte Carlo Method

The Monte Carlo method relies on random or pseudorandom numbers to obtain numerical results[1]. The flow chart 1.1 shows a typical execution of a Monte Carlo device simulation.

1.2 Poisson equation

Calculating the potential and electric field inside the device, means solving Poisson's equation (**??**).

$$\nabla^2\phi = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\phi = -\frac{1}{\epsilon}\rho \tag{1.2.1}$$

The objective of this thesis is to solve equation (1.2.1) with its given boundary conditions, and obtain the potential and the electric field to be used in the Monte Carlo simulation. As mentioned, there are multiple methods one can use to accomplish this. One approach is to use the method of finite differences, which is the approach of choice in this thesis. The following steps were thusly taken in order to find the electric potential and field during simulation:

1. Discretize the domain in which we need to solve Poisson's equation.
2. Approxixmate the derivatives of Poisson's equation using finite differences in the said discretized domain.
3. Collect and solve the resulting set of linear equations for the potential.
4. Calculate the electric field from the newfound potential using, again, finite differences in the discretized domain.

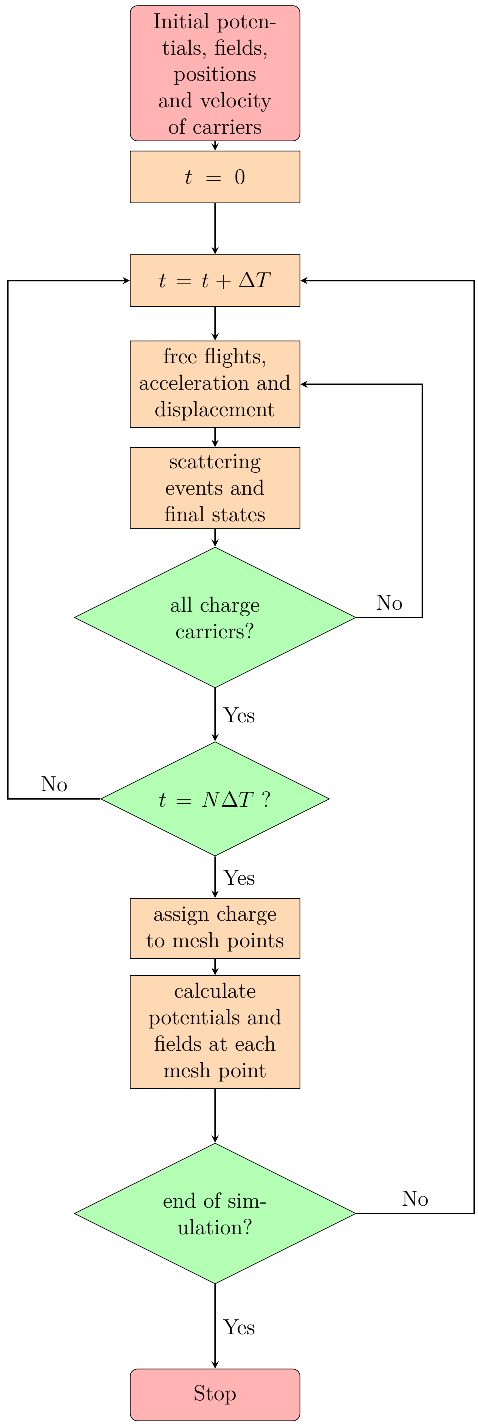

Figure 1.1: Flow chart of typical MC simulation of semiconductor devices[1]

Chapter 2

Solving Poisson's Equation

2.1 Discretizing the Domain

The first step in using the FD-method to solve (1.2.1) is to discretize the domain of the device in question. In the FD-method this consists of distributing $N_{x,y,z}$ grid points along the x, y, z-directions of the device, with spacings $h_{i,j,k}$ between the grid points such that $\sum_{i,j,k=1}^{N_{x,y,z}-1} h_{i,j,k} = L_{x,y,z}$. Here, $L_{x,y,z}$ is the length of the device in the x, y, z-directions, respectively. The resulting discrete mesh can have uniform or non-uniform grid spacings, and it can be constant during simulation, or adapt to the changing charge distributions over the iterations (adaptive grid).

Using a uniform mesh entails having $h_i = h_j = h_k = h$ for all i, j, k. This has the benefit of uniform finite difference coefficients, which makes the resulting linear system easy to handle, with little or no memory requierements for the system matrix. The accuracy of the finite difference derivative approximations will also be known and well-behaved over the entire mesh, depending only on the type of FDM used. However, one does potentially waste grid points in regions where a less dense mesh is required, and when h is to be constant, the number of required gridpoints along x, y, z-direction has to be handled with h-in mind.

When using a mesh with non-uniform grid spacings, one can economize with the number of gridpoints one has to use by packing them more densely in regions that requires it, thus getting a mesh with better resolution with fewer grid points. This does however mean that the finite difference coefficients are no longer uniform, and the resulting linear system is now more complex to handle, and has a system matrix that must, or should, be stored in memory. Said matrix is now no longer necessarily symmetric, which limits the types of iterative solvers that can be used such as the conjugate-gradient method. Also, the accuracy of the FD-approximation now depends on how the gridpoints are distributed.

2.1.1 Uniform Grid Spacing

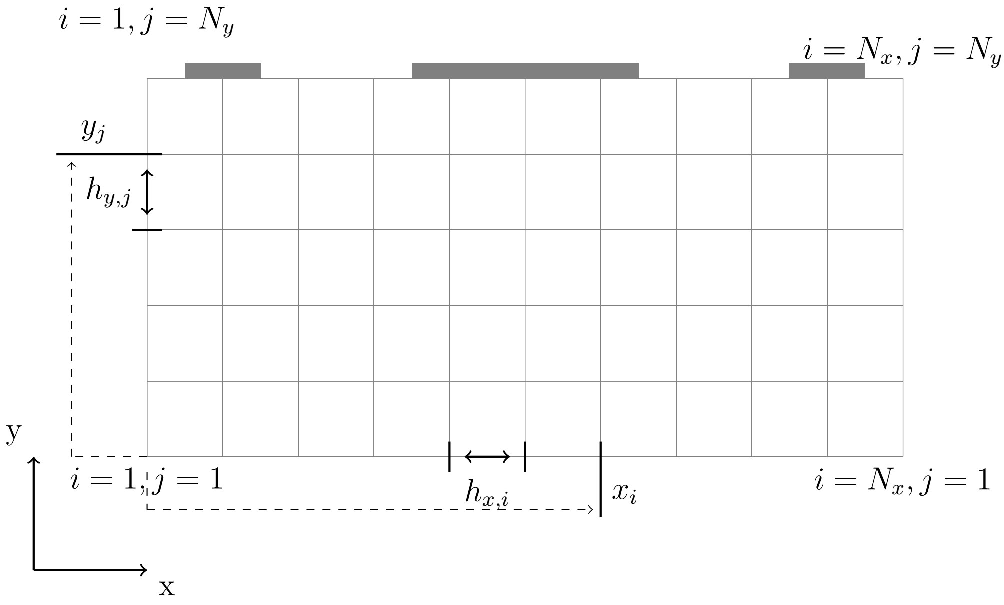

Figure 2.1: Uniform grid representation

Figure 2.1.1 shows a representation of a discrete mesh on a device. $h_{x,i}$ is the distance between grid points i and $i+1$, x_i is the x-position of grid points with index i. The same convention applies to the y-direction. $\phi_{i,j}$ is now the potential at grid point (i,j) and is equal to $\phi(x_i, y_j)$. If the grid is uniform, then $h_{x,i} = h_{y,j} = h$, for all i and all j, giving $x_i = (i-1) \cdot h$.

Consider a device with dimensions are L_x and L_y and we want h, N_x and N_y such that $(N_x - 1) \cdot h = L_x$, and $(N_y - 1) \cdot h = L_y$. If some specific N_x is chosen, we have:

$$\begin{aligned}
(N_x - 1) \cdot h &= L_x \\
h &= \frac{L_x}{N_x - 1} \\
(N_y - 1)\frac{L_x}{Nx - 1} &= L_y \\
N_y &= (Nx - 1)\frac{L_x}{L_y} + 1
\end{aligned} \tag{2.1.1}$$

Equations (2.1.1) show that if N_y is to be an integer, which certainly is a requirement, then $(N_x - 1)L_x$ factorized, has to contain all the factors of L_y factorized. Choosing N_x for a uniform grid means choosing the number of grid points that resolves the device in question accurately enough for FDM, and contains factors such that N_y given by (2.1.1) is a whole number.

2.1.2 Non-uniform Grid Spacing

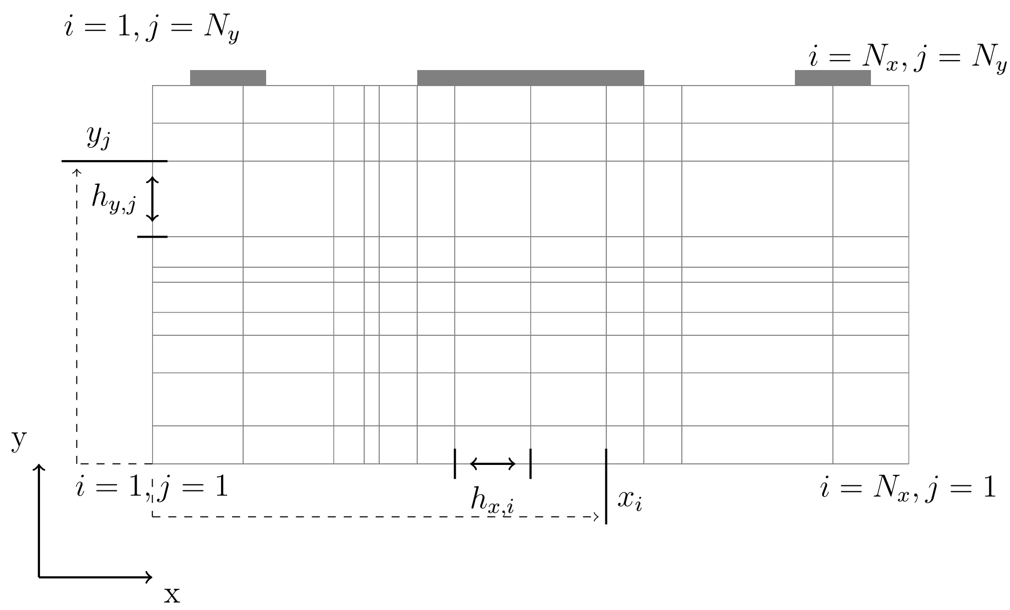

Figure 2.2: Representation of Non-Uniform Mesh

[ht]

A non-uniform grid like the one illustrated in figure 2.1.2 implies that $h_{x,i}$ and/or $h_{y,j}$ is not constant over the domain. Care is not needed to be taken to match the grid spacings like for the uniform grid in section 2.1.1. What matters is to distribute a set of points i and j at positions x_i and y_j that resolves the device accurately, and does not vary so fast as too impede on the accuracy of the FD-approximations. For reasons discussed in the section concerning finite differences, the non-uniform grid should be chosen such that

$$h_i = h_{i-1} \cdot a_i \tag{2.1.2}$$

with a_i being close to 1.

Consider a device with length L_x, where N_x grid points are to be distributed along the x-dimension. To make the distribution of the grid points reflect the distribution of the charges along the x-direction, L_x is divided into n-intervals of length L_k with $k = 1, 2, 3 \ldots n$. Each interval k should contain n_k gridpoints, such that the density of gridpoints is optimal in terms of the needed density distribution of gridpoints during the Monte Carlo simulation. For the n_k intervals we now have:

$$\begin{aligned} \sum_{k=1}^{n} L_k &= L_x \\ \sum_{i=1}^{n_k} h_{k,i} &= L_k \\ \sum_{k=1}^{n}\sum_{i=1}^{n_k} h_{k,i} &= L_x \end{aligned} \tag{2.1.3}$$

The task is now to distribute the grid points according to (2.1.2) and (2.1.3).

$$\begin{aligned} h_{k,i} &= h_{k,i-1}a_{k,i} \\ h_{k,i} &= h_{k,0}\prod_{j=1}^{i} a_{k,j} \\ \sum_{i=1}^{n_k} h_{k,i} &= \sum_{i=1}^{n_k} h_{k,0}\prod_{j=1}^{i} a_{k,j} = L_k \\ \sum_{k=1}^{n}\sum_{i=1}^{n_k} h_{k,i} &= \sum_{k=1}^{n}\sum_{i=1}^{n_k} h_{k,0}\prod_{j=1}^{i} a_{k,j} = L_x \end{aligned} \tag{2.1.4}$$

where

$$h_{k,0} = h_{k-1,n_{k-1}} \tag{2.1.5}$$

for $k = 2, 3, 4 \ldots n$, and

$$h_{1,0} = h_s \tag{2.1.6}$$

As a means to ensure that h fulfills (2.1.2) between the intervals, we will also require that

$$\begin{aligned} a_{k,i} &= a_{k,i-1}a_{k,c} \\ a_{k,i} &= a_{k,0}a_{k,c}^{i-1} \end{aligned} \tag{2.1.7}$$

where

$$a_{k,0} = a_{k-1,n_{k-1}} \tag{2.1.8}$$

for $k = 2, 3, 4 \ldots n$, and

$$\begin{aligned} a_{1,0} &= 1 \\ a_{n,n_k} &= 1 \end{aligned} \tag{2.1.9}$$

Equation (2.1.9) means that the grid should be constant at the gridpoints on the boundary of the device, ensuring the accuracy of the FD-approximations involved with the boundary conditions, while (2.1.8) ensure that $\frac{dh}{dx}$ is continous between intervals.

Distributing the gridpoints along x now consists of solving

$$\begin{aligned} \sum_{i=1}^{n_k} h_{k,i} &= \sum_{i=1}^{n_k} h_{k,0} \prod_{j=1}^{i} a_{k,j} = L_k \\ \sum_{i=1}^{n_k} h_{k,i} &= \sum_{i=1}^{n_k} h_{k,0} \prod_{j=1}^{i} a_{k,0} a_{k,c}^{i-1} = L_k \\ \sum_{i=1}^{n_k} h_{k,i} &= \sum_{i=1}^{n_k} h_{k,0} a_{k,0}^{i} a_{k,c}^{\sum_{j=1}^{i} i-1} = L_k \end{aligned} \tag{2.1.10}$$

and

$$\sum_{k=1}^{n} \sum_{i=1}^{n_k} h_{k,i} = \sum_{k=1}^{n} \sum_{i=1}^{n_k} h_{k,0} a_{k,0}^{i} a_{k,c}^{\sum_{j=1}^{i} i-1} = L_x \tag{2.1.11}$$

With the conditions of (2.1.9), (2.1.8), (2.1.6)(2.1.5) and (2.1.2). This is a problem of exponential spline interpolation.

Solution algorithm of exponential splines of grid

To solve the exponential spline interpolation problem of equations (2.1.10) and (2.1.11), one can use a suitable numerical root-finding method to find the root of

$$f(h_s) = L_x - \sum_{k=1}^{n} \sum_{i=1}^{n_k} h_{k,0} a_{k,0}^{i} a_{k,c}^{\sum_{j=1}^{i} i-1} \tag{2.1.12}$$

and

$$f(a_{k,c}) = L_k - \sum_{i=1}^{n_k} h_{k,0} a_{k,0}^{i} a_{k,c}^{\sum_{j=1}^{i} i-1} \tag{2.1.13}$$

Below follows a flow chart that describes the alghorithm used to to fit the grid points of the non-uniform mesh.

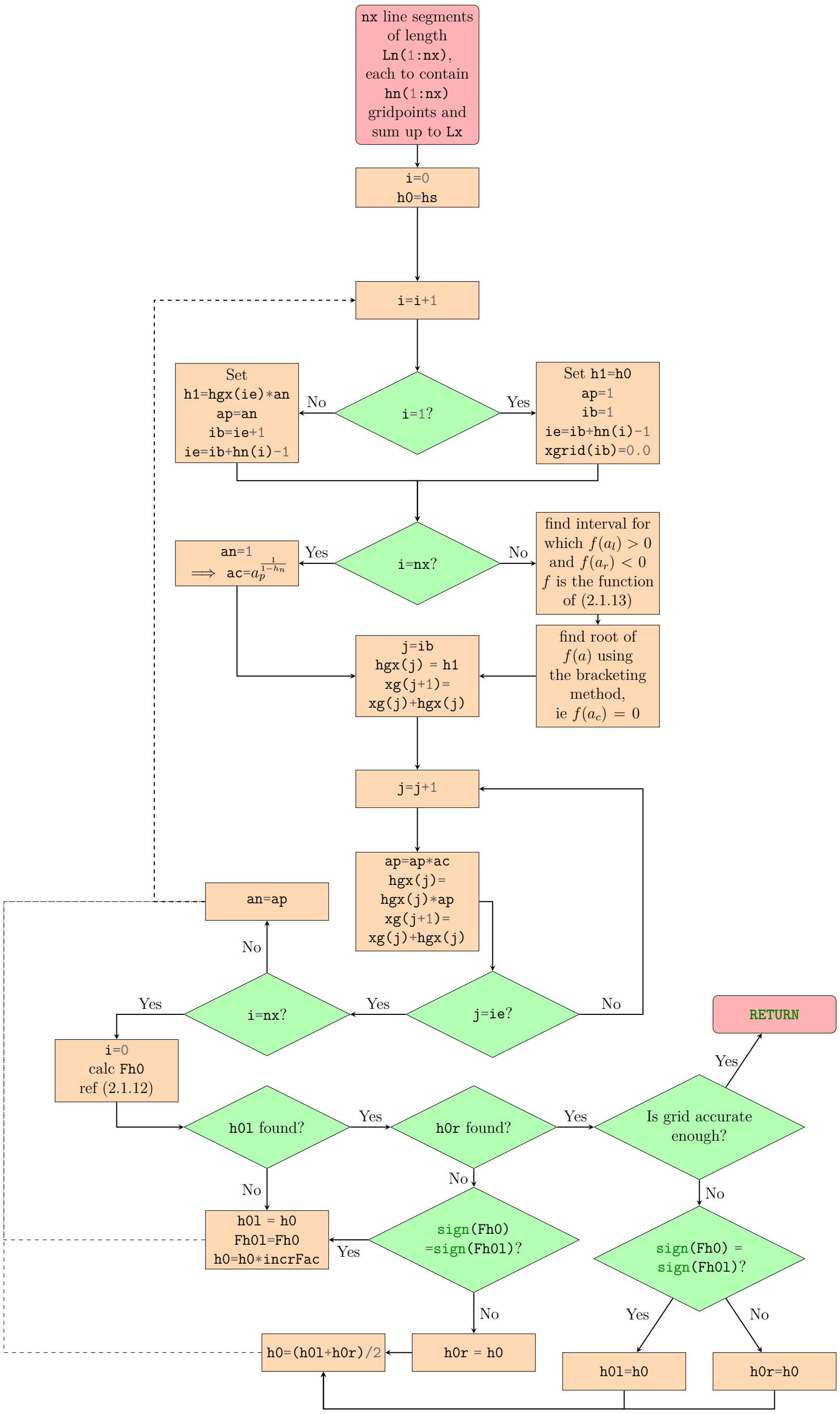

Figure 2.3: Flow chart illustrating the alghorithm used to fit the non-uniform mesh

2.2 Finite Difference Approximation

Once the domain of (1.2.1) has been discretized, one can use the differences of the values of the potential at discrete neighbouring points, to approximate the second the derivatives in Poisson's equation. This is what is known as the finite difference method. To calculate the derivatives, for instance with respect to x, using the finite difference method, one starts with the taylor series expansion of the potential ϕ around some point a:

$$\begin{aligned} \phi(x) = \phi(a) + (x-a)\cdot\phi'(a) - \frac{(x-a)^2}{2!}\phi''(a) \\ + \frac{(x-a)^3}{3!}\phi'''(a)\cdots + (-1)^{n+1}\frac{(x-a)^n}{(n-1)!}\phi^{(n)}(a) \\ + \mathcal{O}((x-a)^{n+1}) \end{aligned} \tag{2.2.1}$$

where $\mathcal{O}$ is the remainder, or error, term.

From the taylor series expansions around the value of the potential at the mesh, one then seek to express Poisson's equation with its boundary equation by a linear set of equation which in turn is solveable by a suitable numerical method. In this section, the finite differences used in the for the uniform and non-uniform case will be presented and explained. For a thorough presentation of how the FD-coefficients and such were calculated, we refer to appendix (A)

2.2.1 Uniform Grid

For a mesh with uniform grid spacing, h is the same between every grid point (2.1.1). Taylor series expansion, like (2.2.1), around (i, j) in the x- and y-directions can be expressed as follows:

$$\phi_{i+n,j} = \phi_{i,j} + nh\frac{\partial\phi_{i,j}}{\partial x} - n^2h^2\frac{\partial^2\phi_{i,j}}{2\partial x^2} + n^3h^3\frac{\partial^3\phi_{i,j}}{6\partial x^3}\cdots + \mathcal{O} \tag{2.2.2}$$

$$\phi_{i,j+n} = \phi_{i,j} + nh\frac{\partial\phi_{i,j}}{\partial y} - n^2h^2\frac{\partial^2\phi_{i,j}}{2\partial y^2} + n^3h^3\frac{\partial^3\phi_{i,j}}{6\partial y^3}\cdots + \mathcal{O} \tag{2.2.3}$$

Through algebraic manipulation of (2.2.2) and (2.2.3) on an adequate number of points on the mesh, one seeks to find suitably accurate approximations of the first and second derivatives of ϕ.

Second Derivative

The second derivative in the uniform case is found using points at (i, j), $(i \pm 1, j)$ and $(i, j \pm 1)$ on the mesh:

$$\begin{aligned} \frac{\partial^2 \phi(x_i, y_j)}{\partial x^2} &\approx \frac{\phi_{i-1,j} - 2\phi_{i,j} + \phi_{i+1,j}}{h^2} \\ \frac{\partial^2 \phi(x_i, y_j)}{\partial y^2} &\approx \frac{\phi_{i,j-1} - 2\phi_{i,j} + \phi_{i,j+1}}{h^2} \end{aligned} \tag{2.2.4}$$

This is called the central difference formulation for the second derivative, and the remainder term is $\mathcal{O}(h^2)$, 2nd order accuracy.

On the edges of the device, the central difference formulation can not be used outright. With neumann boundary conditions on the first derivative, one can use so called ghost nodes outside the device, which are solved for through the boundary condition. One can also use forward, or backwards differences. In that case, an approximation for the second derivative is obtained using points at (i, j), $(i + 1, j)$, $(i, j + 1)$, $(i + 2, j)$ and $(i, j + 2)$

$$\begin{aligned} \frac{\partial^2 \phi(x_i, y_j)}{\partial x^2} &\approx \frac{-\frac{7}{2}\phi_{i,j} + 4\phi_{i+1,j} - \frac{1}{2}\phi_{i+2,j}}{h^2} - \frac{3}{h}\frac{\partial \phi(x_i, y_j)}{\partial x} \\ \frac{\partial^2 \phi(x_i, y_j)}{\partial y^2} &\approx \frac{-\frac{7}{2}\phi_{i,j} + 4\phi_{i,j+1} - \frac{1}{2}\phi_{i,j+2}}{h^2} - \frac{3}{h}\frac{\partial \phi(x_i, y_j)}{\partial y} \end{aligned} \tag{2.2.5}$$

The first derivative is given, due to Von Neumann boundary conditions along the sides of the device.

First Derivative

A finite difference expression for the first derivative of ϕ is also needed, to find the electric field:

$$E = -\nabla \phi \tag{2.2.6}$$

For this we have chosen to use a 4th order accurate finite difference approximation:

$$\begin{aligned} E_{x,(i,j)} &\approx \frac{-\phi_{i+2,j} + 8\phi_{i+1,j} - 8\phi_{i-1,j} + \phi_{i-2,j}}{12h} \\ E_{y,(i,j)} &\approx \frac{-\phi_{i,j+2} + 8\phi_{i,j+1} - 8\phi_{i,j-1} + \phi_{i,j-2}}{12h} \end{aligned} \tag{2.2.7}$$

Which is a center difference, and as for the second derivative we neeed forward- and backwards difference for the edges as well:

$$\begin{aligned} E_{x,(i,j)} &\approx \frac{-25\phi_{i,j} + 48\phi_{i+1,j} - 36\phi_{i+2,j} + 16\phi_{i+3,j} - 3\phi_{i+4,j}}{12h} \\ E_{y,(i,j)} &\approx \frac{-25\phi_{i,j} + 48\phi_{i,j+1} - 36\phi_{i,j+2} + 16\phi_{i,j+3} - 3\phi_{i,j+4}}{12h} \end{aligned} \tag{2.2.8}$$

These are both forward differences, and to get the backward difference, simply multiply (2.2.8) with -1, and flip the sign of the indices

2.2.2 Non-Unifrom Grid

In the non-uniform case, the grid spacing is **not** equal over the device. Taylor series expension of ϕ around (x_i, y_j) is now:

$$\begin{aligned}\phi(x_{i+n}, y_j) = \phi_{i,j} &+ \left(\sum_{k=1}^{n} h_{x,k}\right) \frac{\partial \phi_{i,j}}{\partial x} - \left(\sum_{k=1}^{n} h_{x,k}\right)^2 \frac{\partial^2 \phi_{i,j}}{2\partial x^2} + \left(\sum_{k=1}^{n} h_{x,k}\right)^3 \frac{\partial^3 \phi_{i,j}}{6\partial x^3} - \dots \\ &+ (-1)^{N-2} \left(\sum_{k=1}^{n} h_{x,k}\right)^{N-1} \frac{\partial^{(N-1)} \phi_{i,j}}{(N-1)!\partial x^{(N-1)}} + \mathcal{O}\left(\left(\sum_{k=1}^{n} h_{x,k}\right)^N\right)\end{aligned} \tag{2.2.9}$$

and

$$\begin{aligned}\phi(x_i, y_{j+n} = \phi_{i,j} &+ \left(\sum_{k=1}^{n} h_{y,k}\right) \frac{\partial \phi_{i,j}}{\partial y} - \left(\sum_{k=1}^{n} h_{y,k}\right)^2 \frac{\partial^2 \phi_{i,j}}{2\partial y^2} + \left(\sum_{k=1}^{n} h_{y,k}\right)^3 \frac{\partial^3 \phi_{i,j}}{6\partial y^3} - \dots \\ &+ (-1)^{N-2} \left(\sum_{k=1}^{n} h_{y,k}\right)^{N-1} \frac{\partial^{(N-1)} \phi_{i,j}}{(N-1)!\partial y^{(N-1)}} + \mathcal{O}\left(\left(\sum_{k=1}^{n} h_{y,k}\right)^N\right)\end{aligned} \tag{2.2.10}$$

$\mathcal{O}$ is still the remainder, or error, term.

To find the finite difference approximations of the derivatives on the non-uniform mesh, follow the same procedure as for the uniform mesh. The difference is that the algebra is more difficult when h is not constant.

Second Derivative

The second derivative is found around (i, j), $(i \pm 1, j)$ and $(i, j \pm 1)$, same as for the uniform case. The result is the is the following central difference expression:

$$\begin{aligned}\frac{1}{2}\frac{\partial^2 \phi(x_i, y_j)}{\partial x^2} = &\frac{\phi_{i-1,j}}{h_{x,i}(h_{x,i} + h_{x,i-1})} + \frac{\phi_{i+1,j}}{h_{x,i}(h_{x,i} + h_{x,i-1})} \\ &- \phi_{i,j}\left(\frac{1}{h_{x,i}(h_{x,i} + h_{x,i-1})} + \frac{1}{h_{x,i-1}(h_{x,i} + h_{x,i-1})}\right)\end{aligned} \tag{2.2.11}$$

and forward/backwards difference on edges, with first derivative for boundary condition:

$$
\begin{aligned}
\frac{1}{2}\frac{\partial^2\phi(x_i,y_j)}{\partial x^2} &= \phi_{i,j}\left(\frac{h_{x,i}^3-(h_{x,i}+h_{x,i+1})^3}{h_{x,i}^2h_{x,i+1}(h_{x,i}+h_{x,i+1})^2}\right)+\phi_{i+1,j}\left(\frac{h_{x,i}+h_{x,i+1}}{h_{x,i}^2+h_{x,i}}\right)\\
&-\phi_{i+2,j}\left(\frac{h_{x,i}}{(h_{x,i}+h_{x,i+1})^2h_{x,i+1}}\right)\\
&-\frac{\partial\phi(x_i,y_j)}{\partial x}\left(\frac{(h_{x,i}+h_{x,i+1})(h_{x,i}^3(h_{x,i}+h_{x,i+1}^2))}{(h_{x,i}+h_{x,i+1})^2h_{x,i+1}}\right)
\end{aligned}
\tag{2.2.12}
$$

First Derivative

$$\frac{\partial\phi(x_i,y_j)}{\partial x}=a_0\phi_{i,j}+a_1\phi_{i+1}+a_2\phi_{i+2,j}+a_3\phi_{i+3,j}+a_4\phi_{i+4,j}$$

where

$$a_0=-(a_1+a_2+a_3+a_4)$$

and

$$
\begin{aligned}
a_1 &= \frac{h_{x,2}^*h_{x,3}^*h_{x,4}^*}{h_{x,1}^*(h_{x,4}^*-h_{x,1}^*)(h_{x,3}^*-h_{x,1}^*)(h_{x,2}^*-h_{x,1}^*)}\\
a_2 &= -\frac{h_{x,1}^*h_{x,3}^*h_{x,4}^*}{h_{x,2}^*(h_{x,4}^*-h_{x,2}^*)(h_{x,3}^*-h_{x,2}^*)(h_{x,2}^*-h_{x,1}^*)}\\
a_3 &= \frac{h_{x,1}^*h_{x,2}^*h_{x,4}^*}{h_{x,3}^*(h_{x,4}^*-h_{x,3}^*)(h_{x,3}^*-h_{x,2}^*)(h_{x,1}^*-h_{x,1}^*)}\\
a_4 &= -\frac{h_{x,1}^*h_{x,2}^*h_{x,3}^*}{h_{x,4}^*(h_{x,4}^*-h_{x,3}^*)(h_{x,4}^*-h_{x,2}^*)(h_{x,4}^*-h_{x,1}^*)}
\end{aligned}
\tag{2.2.13}
$$

$$h_{x,l}^*=\sum_{n=0}^{l-1}h_{x,i+n} \tag{2.2.14}$$

$$\frac{\partial\phi(x_i,y_j)}{\partial x}=a_{-2}\phi_{i-2,j}+a_1\phi_{i-1}+a_{-1}\phi_{i-1,j}+a_0\phi_{i,j}+a_1\phi_{i+1,j}+a_2\phi_{i+2,j}$$

where

$$a_0=-(a_{-1}+a_{-2}+a_1+a_2)$$

and

$$
\begin{aligned}
a_{-2} &= \frac{h^*_{x,1}h^*_{x,-1}h^*_{x,2}}{h^*_{x,-2}(h^*_{x,1}+h^*_{x,-2})(h^*_{x,-2}-h^*_{x,-1})(h^*_{x,1}+h^*_{x,-2})} \\
a_{-1} &= -\frac{h^*_{x,2}h^*_{x,1}h^*_{x,-2}}{h^*_{x,-1}(h^*_{x,-1}+h^*_{x,1})(h^*_{x,-2}-h^*_{x,-1})(h^*_{x,2}+h^*_{x,-1})} \\
a_{1} &= \frac{h^*_{x,2}h^*_{x,-1}h^*_{x,-2}}{h^*_{x,1}(h^*_{x,-1}+h^*_{x,1})(h^*_{x,2}-h^*_{x,-1})(h^*_{x,1}+h^*_{x,-2})} \\
a_{2} &= -\frac{h^*_{x,1}h^*_{x,-1}h^*_{x,-2}}{h^*_{x,2}(h^*_{x,2}+h^*_{x,-2})(h^*_{x,2}-h^*_{x,1})(h^*_{x,2}+h^*_{x,-1})}
\end{aligned}
\tag{2.2.15}
$$

$$
\begin{aligned}
h^*_{x,1} &= h_{x,i} \\
h^*_{x,2} &= h_{x,i} + h_{x,i+1} \\
h^*_{x,-1} &= h_{x,i-1} \\
h^*_{x,-2} &= h_{x,i-2} + h_{x,i-1}
\end{aligned}
\tag{2.2.16}
$$

2.3 Iterative Solvers

2.3.1 Discrete Poisson Equation

Poisson's equation (1.2.1) can now be discretized.

$$
\begin{aligned}
\nabla^2\phi(x_i, y_j) &= -\frac{\rho_(x_i, y_j)}{\epsilon_o\epsilon_r} \\
\frac{\partial^2\phi(x_i, y_j)}{\partial x^2} + \frac{\partial^2\phi(x_i, y_j)}{\partial y^2} &= -\frac{\rho_(x_i, y_j)}{\epsilon_o\epsilon_r}
\end{aligned}
\tag{2.3.1}
$$

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Interior points

$$
\begin{aligned}
\frac{\partial^2\phi(x_i, y_j)}{\partial x^2} + \frac{\partial^2\phi(x_i, y_j)}{\partial y^2} &= -\frac{\rho_(x_i, y_j)}{\epsilon_o\epsilon_r} \\
\phi_{j-1,i} + \phi_{i-1,j} - 4\phi_{i,j} + \phi_{i+1,j} + \phi_{i,j+1} &= -h^2\frac{\rho_(x_i, y_j)}{\epsilon_o\epsilon_r}
\end{aligned}
\tag{2.3.2}
$$

The boundary conditions used in the the specific case of the APD device, is that the potential is known at the contacts (V_p, V_n), and that the normal derivative of the potential at the surfaces around the device is equal to 0, von Neumann boundary condition. The discrete poisson equation as, say at the left side of the device, $i = 1$, $j = 1, 2, 3, \dots N_y$, is now:

$$\begin{gathered}\frac{\partial^2 \phi(x_i, y_j)}{\partial x^2} + \frac{\partial^2 \phi(x_i, y_j)}{\partial y^2} = -\frac{\rho_(x_i, y_j)}{\epsilon_o \epsilon_r} \\ \phi_{i,j-1} - \frac{11}{2}\phi_{i,j} + 4\phi_{i+1,j} - \frac{1}{2}\phi_{i+2,j} + \phi_{i,j+1} = -h^2 \frac{\rho_(x_i, y_j)}{\epsilon_o \epsilon_r}\end{gathered} \tag{2.3.3}$$

NUM

Interior points

$$\begin{aligned}\frac{1}{2}\nabla^2 \phi(x_i, y_j) = {} & \frac{\phi_{i-1,j}}{h_{x,i}(h_{x,i} + h_{x,i-1})} + \frac{\phi_{i+1,j}}{h_{x,i}(h_{x,i} + h_{x,i-1})} + \frac{\phi_{i,j-1}}{h_{y,j}(h_{y,j} + h_{y,j-1})} \\ & + \frac{\phi_{i,j+1}}{h_{y,j}(h_{y,j} + h_{y,j-1})} - \phi_{i,j}\left(\frac{1}{h_{x,i}(h_{x,i} + h_{x,i-1})}\right. \\ & \left. + \frac{1}{h_{x,i-1}(h_{x,i} + h_{x,i-1})} + \frac{1}{h_{y,j}(h_{y,j} + h_{y,j-1})} + \frac{1}{h_{y,j}(h_{y,j} + h_{y,j-1})}\right) \\ & = -\frac{\rho(x_i, y_j)}{2\epsilon_0 \epsilon_r}\end{aligned} \tag{2.3.4}$$

At the edges, the boundary condition is the same as the uniform case, and for $i = 1$, $j = 1, 2, 3, \dots, N_y$ we have

$$\begin{aligned}\frac{1}{2}\nabla^2 \phi(x_i, y_j) = {} & \phi_{i,j}\left(\frac{h_{x,i}^3 - (h_{x,i} + h_{x,i+1})^3}{h_{x,i}^2 h_{x,i+1}(h_{x,i} + h_{x,i+1})^2} + \frac{1}{h_{y,j}(h_{y,j} + h_{y,j-1})}\right. \\ & \left. + \frac{1}{h_{y,j}(h_{y,j} + h_{y,j-1})}\right) + \phi_{i+1,j}\left(\frac{h_{x,i} + h_{x,i+1}}{h_{x,i}^2 h_{x,i+1}}\right) \\ & - \phi_{i+2,j}\left(\frac{h_{x,i}}{(h_{x,i} + h_{x,i+1})^2 h_{x,i+1}}\right) + \frac{\phi_{i,j-1}}{h_{y,j}(h_{y,j} + h_{y,j-1})} \\ & + \frac{\phi_{i,j+1}}{h_{y,j}(h_{y,j} + h_{y,j-1})} \\ & = -\frac{\rho(x_i, y_j)}{2\epsilon_0 \epsilon_r}\end{aligned} \tag{2.3.5}$$

2.3.2 Linear System Representation

The collected discrete poisson equations, now consist of one expression for each grid point, totalling $N_x \cdot N_y = N$ linear equations. Figure 2.3.2 shows

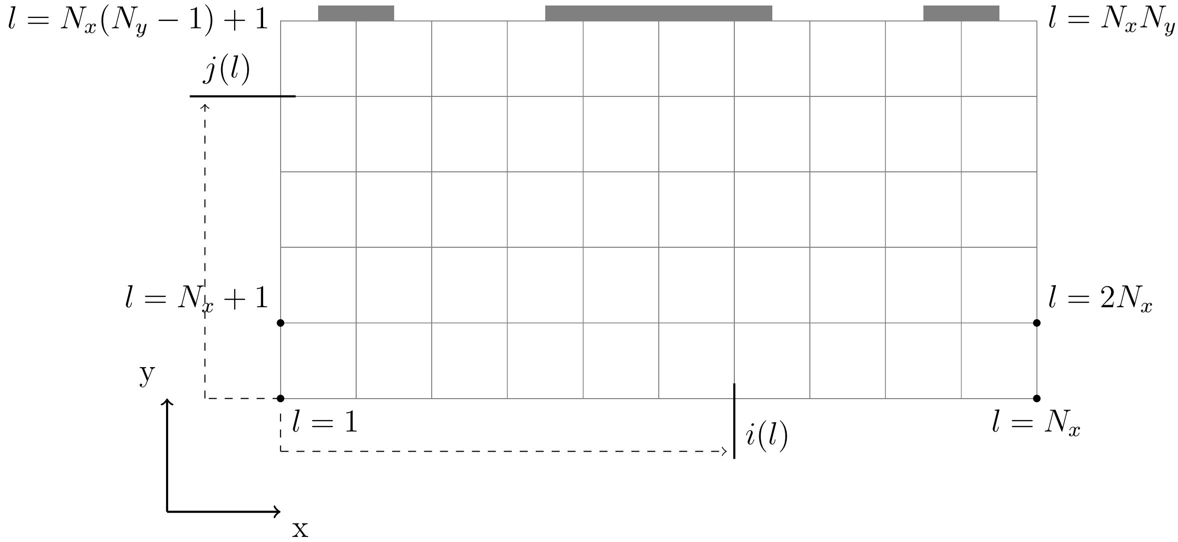

Figure 2.4: Linearization of (i,j)

shows how one can number these equations by the index l where $l = 1, 2, 3, \cdots, N$. l is now given by

$$l(i, j) = N_x(j - 1) + i \tag{2.3.6}$$

While i, and j are given by

$$\begin{aligned} j(l) &= \left\lfloor \frac{l}{N_x} \right\rfloor \\ i(l) &= l \bmod N_x \end{aligned} \tag{2.3.7}$$

$$A\phi_v = \rho_v \tag{2.3.8}$$

A is an N by N matrix, N being $N_x \cdot N_y$, and ϕ_v and ρ_v are column vectors of length N

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$$T_0 = \begin{bmatrix} -\frac{11}{2} & 4 & -\frac{1}{2} & \dots & 0 & 0 & 0 & 0 & 0 \\ 1 & -4 & 1 & 0 & \dots & 0 & 0 & 0 & 0 \\ 0 & 1 & -4 & 1 & 0 & \dots & 0 & 0 & 0 \\ 0 & 0 & 1 & -4 & 1 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & & & \ddots & & & \vdots & \vdots \\ \vdots & \vdots & \vdots & & & \ddots & & \vdots & \vdots \\ 0 & \dots & \dots & \dots & 0 & 1 & -4 & 1 & 0 \\ 0 & \dots & \dots & \dots & 0 & 0 & 1 & -4 & 1 \\ 0 & \dots & \dots & \dots & 0 & 0 & -\frac{1}{2} & 4 & -\frac{11}{2} \end{bmatrix} \tag{2.3.9}$$

$$T_c = \begin{bmatrix} -11 & 4 & -\frac{1}{2} & \dots & 0 & 0 & 0 & 0 & 0 \\ 1 & -4 & 1 & 0 & \dots & 0 & 0 & 0 & 0 \\ 0 & 1 & -4 & 1 & 0 & \dots & 0 & 0 & 0 \\ 0 & 0 & 1 & -4 & 1 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & & & \ddots & & & \vdots & \vdots \\ \vdots & \vdots & \vdots & & & \ddots & & \vdots & \vdots \\ 0 & \dots & \dots & \dots & 0 & 1 & -4 & 1 & 0 \\ 0 & \dots & \dots & \dots & 0 & 0 & 1 & -4 & 1 \\ 0 & \dots & \dots & \dots & 0 & 0 & -\frac{1}{2} & 4 & -11 \end{bmatrix} \tag{2.3.10}$$

$$A = \begin{bmatrix} T_c & 4I & -I\frac{1}{2} & 0 & \dots & \dots & 0 & 0 & 0 \\ I & T_0 & I & 0 & 0 & \dots & \dots & 0 & 0 \\ 0 & I & T_0 & I & 0 & 0 & \dots & \dots & 0 \\ 0 & 0 & I & T_0 & I & 0 & 0 & \dots & 0 \\ \vdots & \vdots & & & \ddots & & \vdots & \vdots & \\ 0 & \dots & \dots & \dots & I & T_0 & I & 0 & 0 \\ 0 & 0 & \dots & \dots & 0 & I & T_0 & I & 0 \\ 0 & 0 & 0 & \dots & 0 & 0 & I & T_0 & I \\ 0 & 0 & 0 & \dots & 0 & 0 & -I\frac{1}{2} & 4I & T_c \end{bmatrix} \tag{2.3.11}$$

$$A\phi = A \begin{bmatrix} \phi_{1,1} \\ \phi_{2,1} \\ \phi_{3,1} \\ \vdots \\ \phi_{Nx-1,1} \\ \phi_{Nx,1} \\ \phi_{1,2} \\ \phi_{2,2} \\ \phi_{3,2} \\ \vdots \\ \phi_{1,Ny-1} \\ \phi_{2,Ny-1} \\ \vdots \\ \phi_{Nx-1,Ny} \\ \phi_{Nx,Ny} \end{bmatrix} = -\frac{h^2}{\epsilon_0 \epsilon_r} \begin{bmatrix} \rho_{1,1} \\ \rho_{2,1} \\ \rho_{3,1} \\ \vdots \\ \rho_{Nx-1,1} \\ \rho_{Nx,1} \\ \rho_{1,2} \\ \rho_{2,2} \\ \rho_{3,2} \\ \vdots \\ \rho_{1,Ny-1} \\ \rho_{2,Ny-1} \\ \vdots \\ \rho_{Nx-1,Ny} \\ \rho_{Nx,Ny} \end{bmatrix} \tag{2.3.12}$$

NUM

$$T = \begin{bmatrix}
X_m(i,j) & a_{x_1}(i) & a_{x_2}(i) & 0 & 0 & \dots & \dots & \dots & 0 \\
a_{x_{-1}}(i) & X_m(i,j) & a_{x_1}(i) & 0 & 0 & \dots & \dots & \dots & 0 \\
0 & a_{x_{-1}}(i) & X_m(i,j) & a_{x_1}(i) & 0 & 0 & \dots & \dots & 0 \\
0 & 0 & a_{x_{-1}}(i) & X_m(i,j) & a_{x_1}(i) & 0 & 0 & \dots & 0 \\
\vdots & \vdots & \vdots & & \ddots & & \vdots & \vdots & \vdots \\
0 & \dots & \dots & 0 & a_{x_{i-1}}(i) & X_m(i,j) & a_{x_1}(i) & 0 & 0 \\
0 & 0 & \dots & \dots & 0 & a_{x_{-1}}(i) & X_m(i,j) & a_{x_1}(i) & 0 \\
0 & 0 & 0 & \dots & \dots & 0 & a_{x_{-1}}(i) & X_m(i,j) & a_{x_1}(i) \\
0 & 0 & 0 & \dots & \dots & 0 & a_{x_{-2}}(i) & a_{x_{-1}}(i) & X_m(i,j)
\end{bmatrix} \tag{2.3.13}$$

$$A = \begin{bmatrix}
T^* & a_{y_1}(j)I & a_{y_2}(j)I & 0 & 0 & \dots & \dots & \dots & 0 \\
a_{y_{-1}}(j)I & T^* & a_{y_1}(j)I & 0 & 0 & \dots & \dots & \dots & 0 \\
0 & a_{y_{-1}}(j)I & T^* & a_{y_1}(j)I & 0 & 0 & \dots & \dots & 0 \\
0 & 0 & a_{y_{-1}}(j)I & T^* & a_{y_1}(j)I & 0 & 0 & \dots & 0 \\
\vdots & \vdots & \vdots & & \ddots & & \vdots & \vdots & \vdots \\
0 & \dots & 0 & 0 & a_{y_{-1}}(j)I & T^* & a_{y_1}(j)I & 0 & 0 \\
0 & \dots & \dots & 0 & 0 & a_{y_{-1}}(j)I & T^* & a_{y_1}(j)I & 0 \\
0 & \dots & \dots & \dots & 0 & 0 & a_{y_{-1}}(j)I & T^* & a_{y_1}(j)I \\
0 & \dots & \dots & \dots & 0 & 0 & a_{y_{-2}}(j)I & a_{y_{-1}}(j)I & T^*
\end{bmatrix} \tag{2.3.14}$$

here

$$a_{x1(i)} = \begin{cases} \frac{1}{h_{x,i}(h_{x,i}+h_{x,i-1})} & : i \in \{2, 3, \ldots, N_x - 2, N_x - 1\} \\ \frac{h_{x,i}+h_{x,i+1}}{h_{x,i}^2 h_{x,i+1}} & : i \in \{1\} \end{cases} \tag{2.3.15}$$

$$a_{x-1(i)} = \begin{cases} \frac{1}{h_{x,i-1}(h_{x,i}+h_{x,i-1})} & : i \in \{2, 3, \ldots, N_x - 2, N_x - 1\} \\ \frac{h_{x,i-1}+h_{x,i-2}}{h_{x,i-1}^2 h_{x,i-2}} & : i \in \{N_x\} \end{cases} \tag{2.3.16}$$

$$a_{x_2} = \begin{cases} -\frac{h_{x,i}}{(h_{x,i}+h_{x,i+1})^2 h_{x,i+1}} & : i \in \{1\} \\ 0 & : i \in \{2, 3, \ldots, N_x - 1, N_x\} \end{cases} \tag{2.3.17}$$

$$a_{x_{-2}} = \begin{cases} -\frac{h_{x,i-1}}{(h_{x,i-1}+h_{x,i-2})^2 h_{x,i-2}} & : i \in \{N_x\} \\ 0 & : i \in \{1, 2, 3, \ldots, N_x - 2, N_x - 1\} \end{cases} \tag{2.3.18}$$

$$X_m(i,j) = -(a_{x_1}(i)+a_{x_2}(i)+a_{x_{-1}}(i)+a_{x_{-2}}(i)+a_{y_1}(j)+a_{y_2}(j)+a_{y_{-1}}(j)+a_{y_{-2}}(j)) \tag{2.3.19}$$

Chapter 3

Simulation Results

The main focus of this thesis has been to create a suitable solution method for poisson's equation using the finite difference method and the BiCGStab solver. In this chapter we will present this work in the context of a Monte Carlo simultion of a CMT photo diode.

3.1 CdHgTe APD

3.1.1 Initial Potential and Particle Positions

Before one can simulate a photon detection event, the device has to be initialized with a suitable number and distribution of electrons and holes. After the particles are released at $t = 0$, the device is then simulated under the specified conditions until it hopefully can model the expected state of a real world device. One can investigate properties such as the depletion length of the pn-junction, potential and distribution of particles in order to decide when this is the case.

The diode in question, has been simulated over 75 ps under a 10 V reverse bias, at 77 K.Figure 3.1 shows the contourplot of the diode after a longer period of simulation. Initial and final states has been saved to file and reloaded for further simulation, and as such, the simulation length is not known excactly. Figure 3.2 shows the same contourplot with arrows indicating the direction of the electric field. Figure 3.3 shows a previous contourplot of the diode after 100 ps simulation under 5 V reverse bias and 77 K. This figure illustrates a problem of the old solver. Holes seem to pile up around the p-contacts, resulting in a deeply negative potential in front of the n-region. For a self-consistent solver, one would expect that these holes would evacuate the region of higher potential, either due to the electric field, or by diffusion, this was however not the case. The underlying problem seemed to be with the way the program handled the contacts of the device, counting the number of super particles in the contact region, and adding it the background impurity charges. For some reason, this resulted in an artificial deficit of charge, and when more holes were injected at the contacts, the resulting potential became artificially high as well. Increasing the bias to 10 V and calculating the surplus charge in the contact region through the charge density matrix, which takes into consideration the particle-mesh coupling that "smears" the charges slightly, seemed to have alleviated the problem. Figures 3.1 and 3.2 seem to be an accurate representation of the diode.

Lastly, we refer to figure 3.4 which shows the particle positions after an extended period of simulation. No unphysical concentration of holes or electrons can be seen, which was the case around the p-contacts previously.

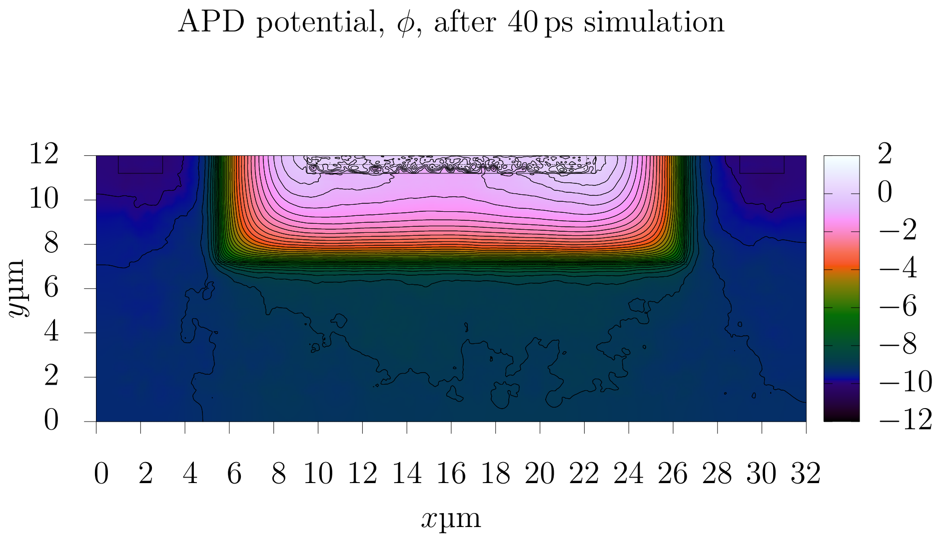

Figure 3.1: Contourplot of potential after > 75ps of simulation

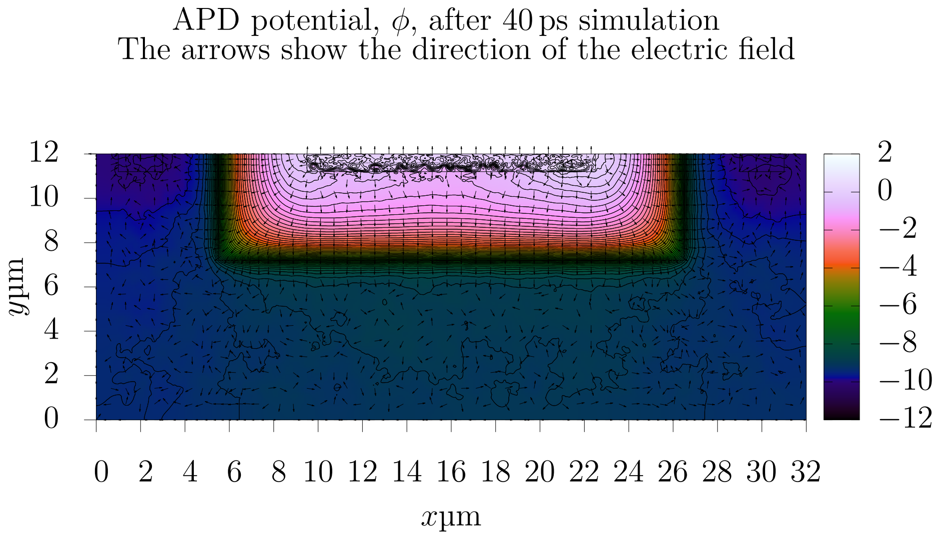

Figure 3.2: Contourplot of potential, ϕ, with arrows indicating the direction of the electric field. > 75 ps simulation.

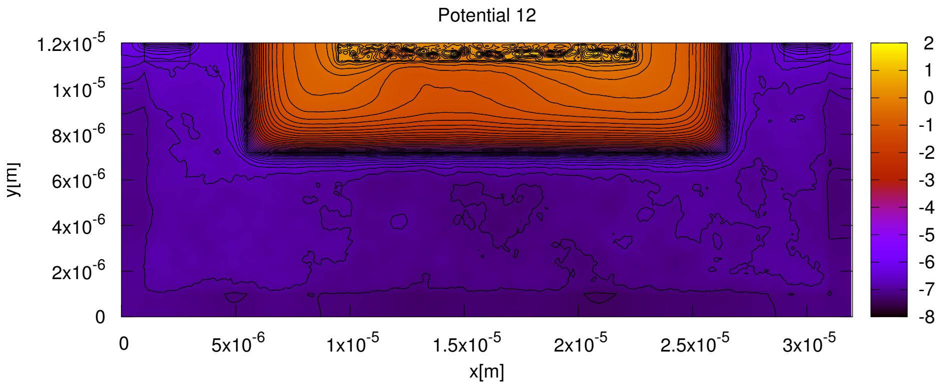

Figure 3.3: Previous simulation result; controuplot of potential after 100 ps simulation, 5 V reverse bias at 77 K

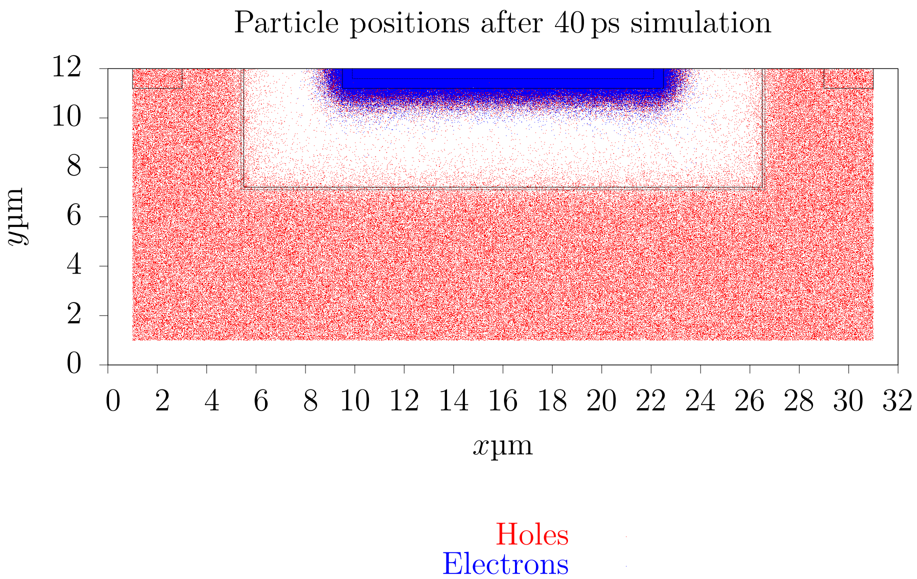

Figure 3.4: Particle positions. Faintly dashed line represents the depletion length

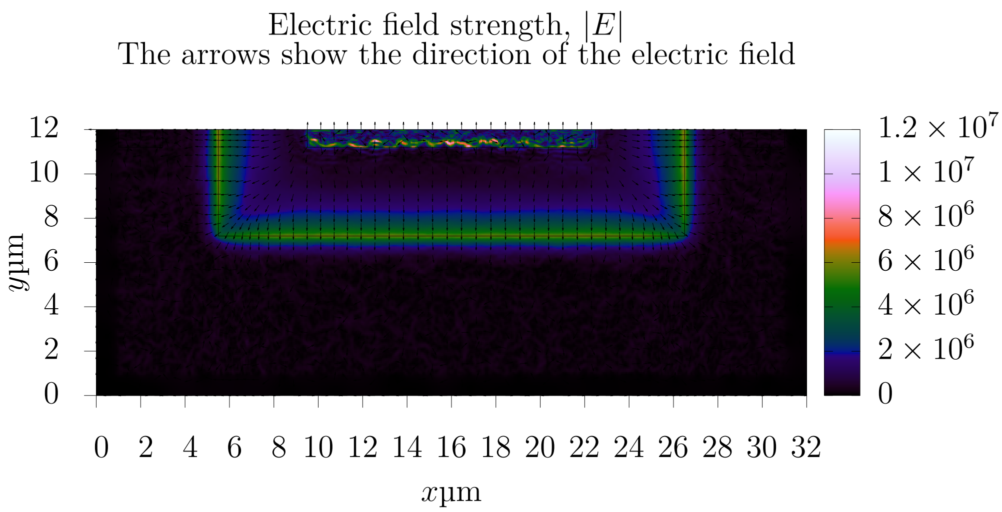

Figure 3.5: Absolute value of electric field, and arrow indicators of direction

3.1.2 APD event simulation

Figures 3.7, 3.8 and 3.6 show some of the results from a simulation of a generated electron-hole from photon excitation. The enclosed file ”APDdetection.avi” should show the particle position under the impactionisation and recombination.

3.2 Non-uniform Mesh in Simulation

During initial Monte Carlo simulation in order for the device to stabilize, we fitted the grid spacing relative to the absolute value of the electric field, every 3rd call to the poisson solver. For the x-direction, we fitted n_k grid points to N_k subdivisions of the total length L_x. Using $k > 19$ subdivisions became perhaps too taxing for the chosen solution method, causing long solution times and crashes due too floating point errors. 15 subdivisions in the x-direction, and 7 for the y-grid seemed to be a good compromise in speed, accuracy and stability. Figures 3.9 and 3.10 shows the gridpoint distribution after an extended period of simulation.

Figures 3.12, 3.13 and 3.11 further illustrates the distribution of grid points after simulation

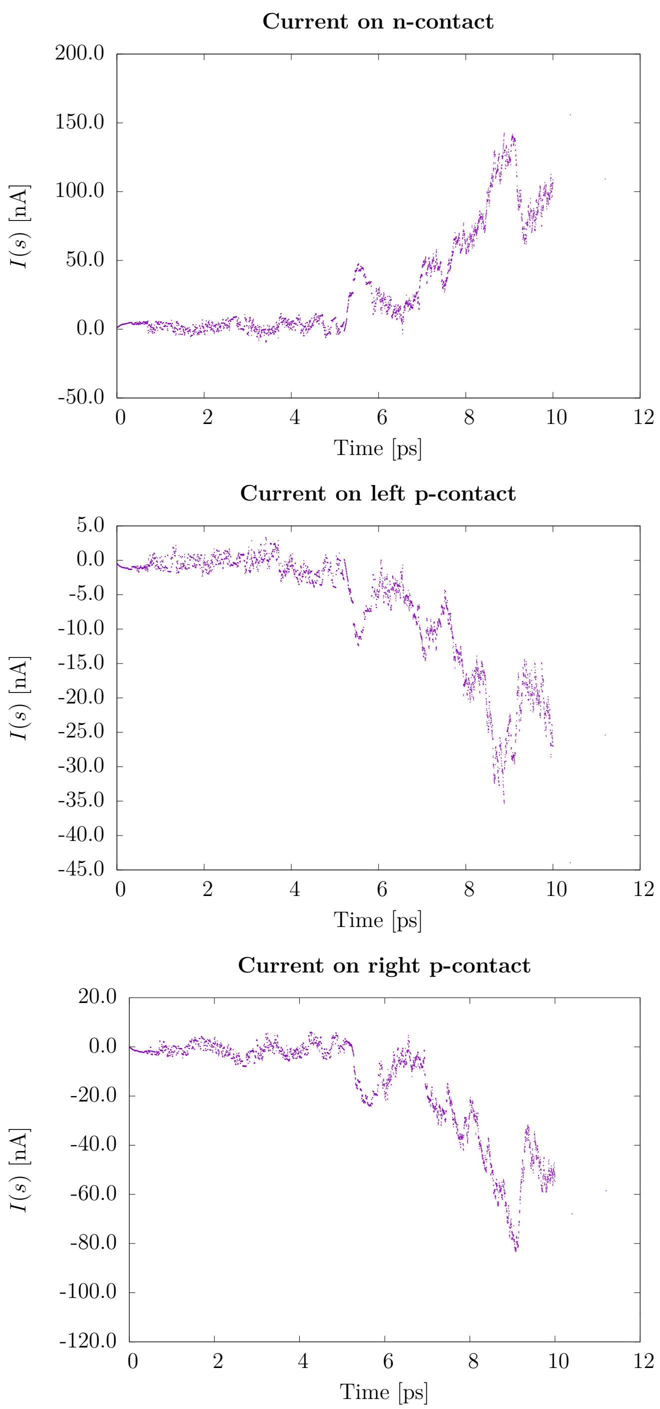

Figure 3.6: Current on contacts as due to Shockley-Ramo

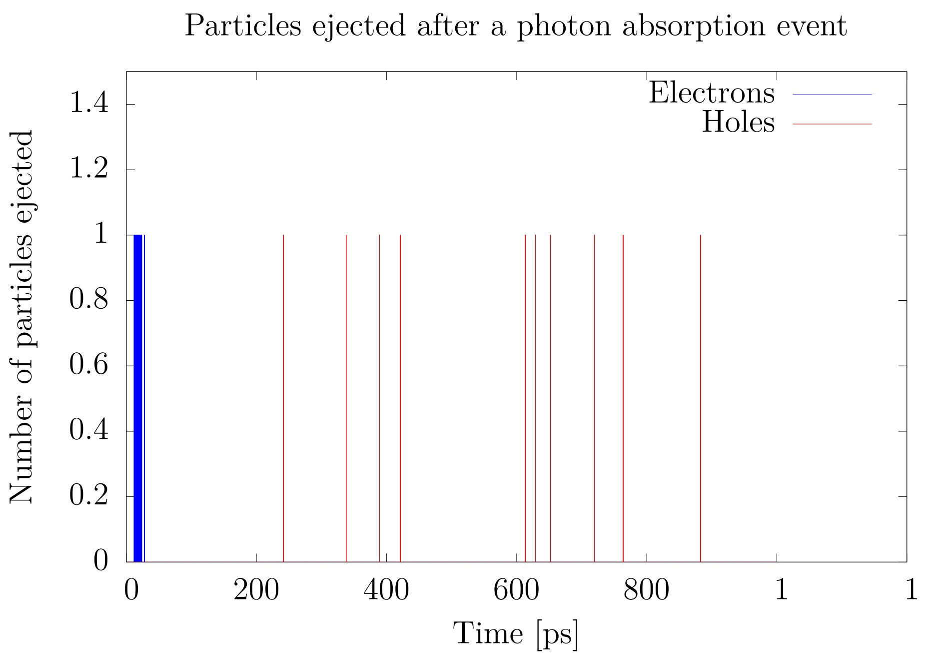

Figure 3.7: Number of ejected electrons and holes per time

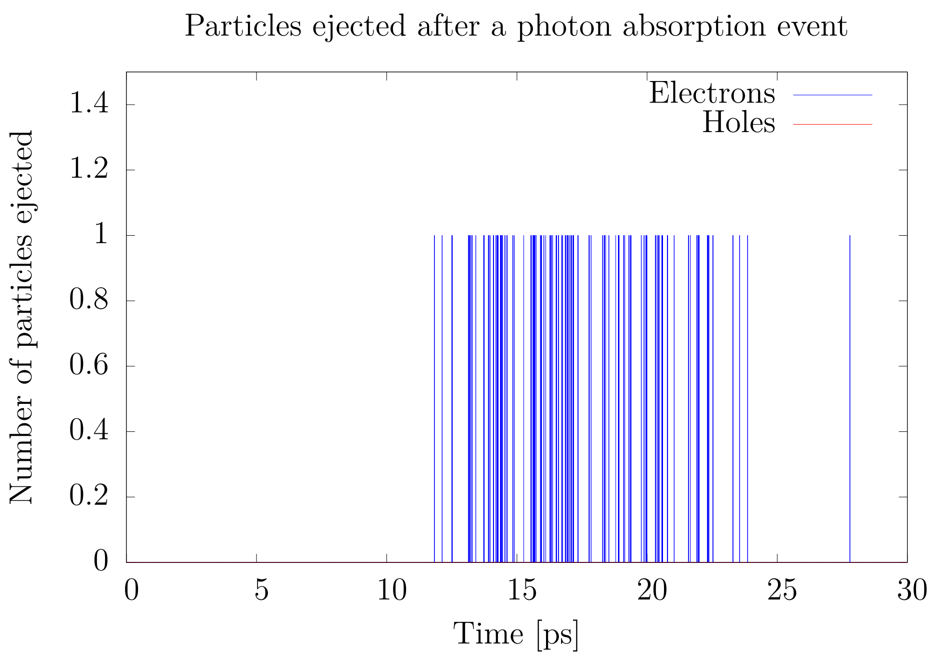

Figure 3.8: Number of ejected electrons per time

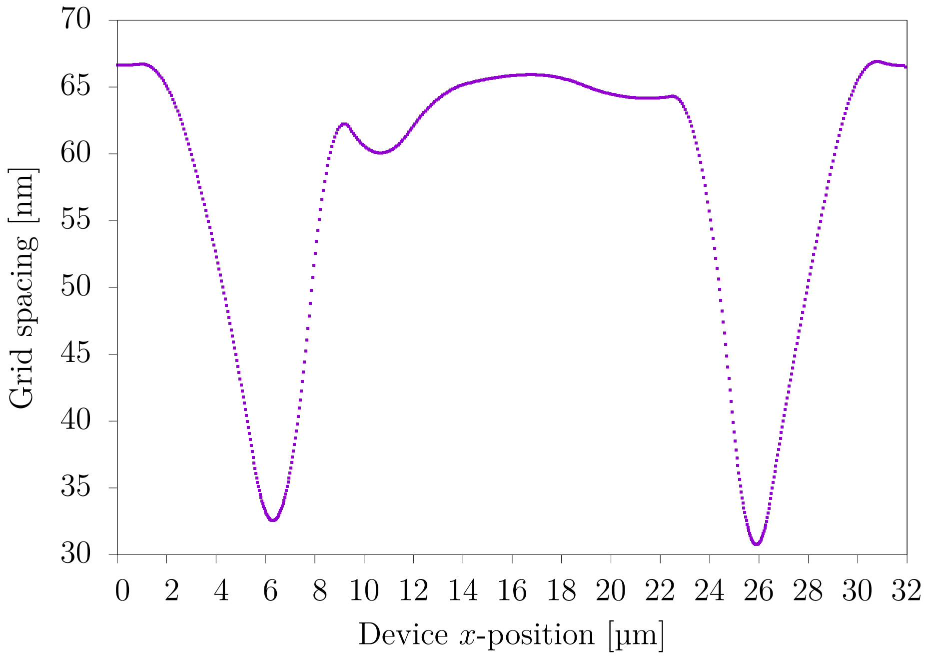

Figure 3.9: Gridspacing in x-direction

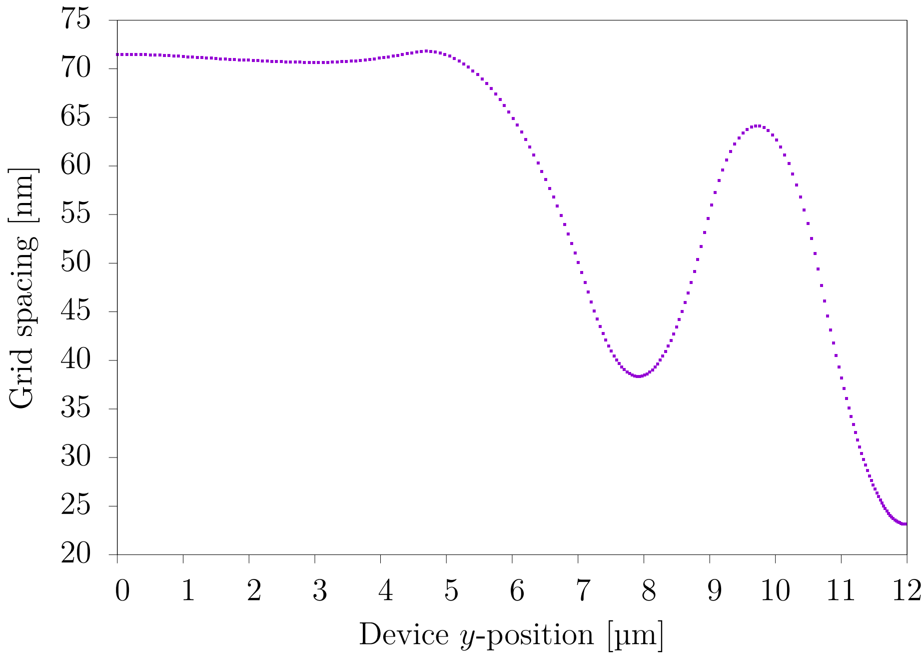

Figure 3.10: Gridspacing in y-direction

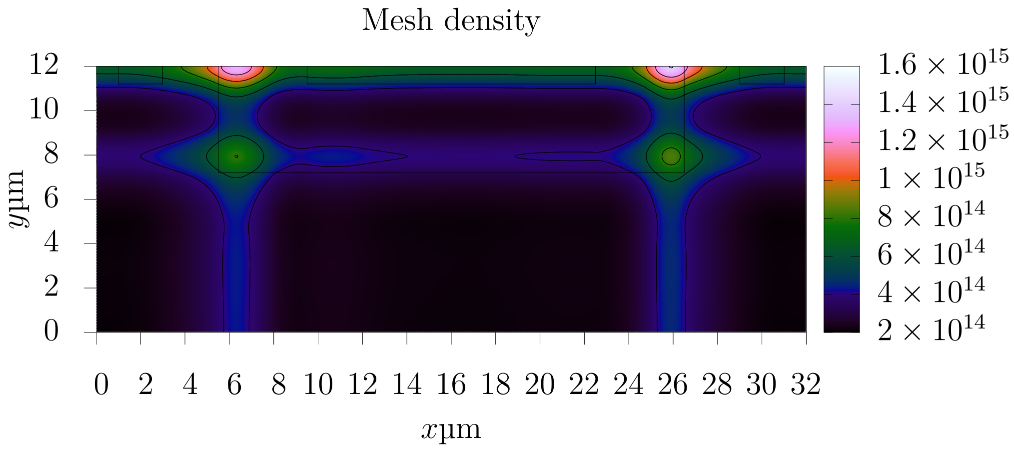

Figure 3.11: Density of meshpoints

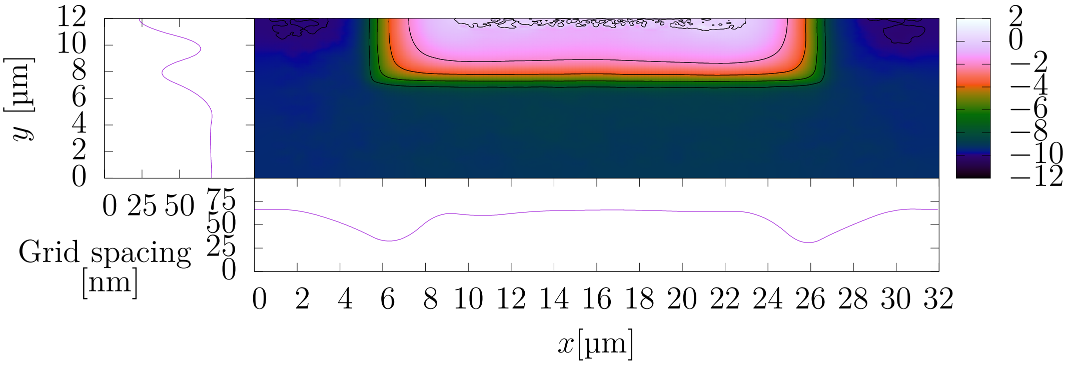

Figure 3.12: Potential and gridpointdistribution in x- and y-direction

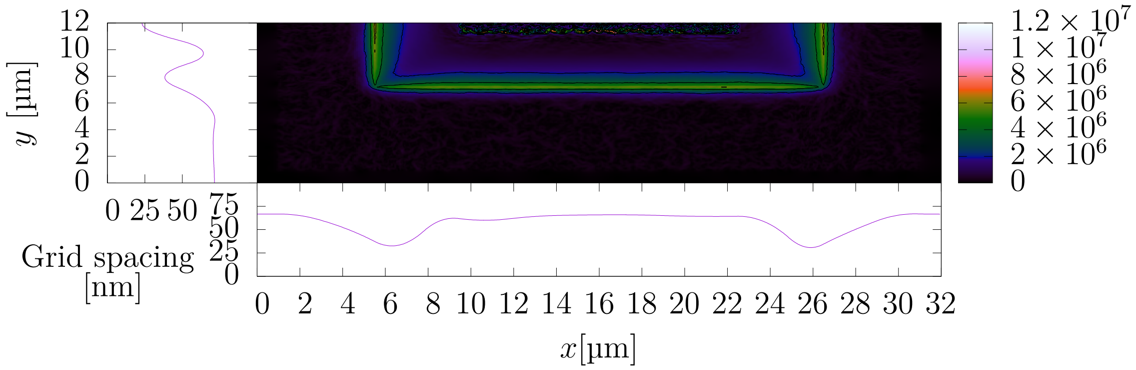

Figure 3.13: Absolute value of electric field, and gridpointdistribution in x- and y-direction

Chapter 4

Discussion

Appendix A

FDM Coefficients

A.1 Uniform Mesh FDs

A.1.1 First derivative for calculation of electric field

For the interior points, a 4th order accurate central difference approximation is used:

$$E_x(i,j) = \frac{-\phi_{i+2,j} + 8\phi_{i+1,j} - 8\phi_{i-1,j} + \phi_{i-2,j}}{12h} + \mathcal{O}(h^4) \qquad \text{(A.1.1)}$$

Forward difference at edges:

$$\phi_{i+1} = \phi_i + h\phi_i' + \frac{h^2}{2}\phi_i'' + \frac{h^3}{3!}\phi_i''' + \frac{h^4}{3!}\phi_i^{(4)} + \mathcal{O}(h^5)$$
$$\phi_{i+2} = \phi_i + 2h\phi_i' + \frac{4h^2}{2}\phi_i'' + \frac{8h^3}{3!}\phi_i''' + \frac{16h^4}{3!}\phi_i^{(4)} + \mathcal{O}(h^5)$$
$$\phi_{i+3} = \phi_i + 3h\phi_i' + \frac{9h^2}{2}\phi_i'' + \frac{27h^3}{3!}\phi_i''' + \frac{81h^4}{3!}\phi_i^{(4)} + \mathcal{O}(h^5)$$
$$\phi_{i+4} = \phi_i + 4h\phi_i' + \frac{16h^2}{2}\phi_i'' + \frac{64h^3}{3!}\phi_i''' + \frac{256h^4}{3!}\phi_i^{(4)} + \mathcal{O}(h^5)$$

Eliminate fouth derivative:

$$\phi_{i+2} - 16\phi_{i+1} = -15\phi_i - 14h\phi_i' - 12\frac{h^2}{2}\phi_i'' - 8\frac{h^3}{3!}\phi_i''' + \mathcal{O}(h^5)$$
$$\phi_{i+3} - 81\phi_{i+1} = -80\phi_i - 78h\phi_i' - 72\frac{h^2}{2}\phi_i'' - 54\frac{h^3}{3!}\phi_i''' + \mathcal{O}(h^5)$$
$$\phi_{i+4} - 256\phi_{i+1} = -255\phi_i - 252\phi_i' - 240\frac{h^2}{2}\phi_i'' - 192\frac{h^3}{3!}\phi_i''' + \mathcal{O}(h^5)$$

Eliminate third derivative:

$$\phi_{i+3} - 81\phi_{i+1} - \frac{54}{8}(\phi_{i+2} - 16\phi_{i+1}) =$$
$$\phi_i(-80 + 15\frac{54}{8}) + h\phi_i'(-78 + 14\frac{54}{8}) + \frac{h^2}{2}\phi_i''(-72 + 12\frac{54}{8}) + \mathcal{O}(h^5)$$
$$\phi_{i+4} - 256\phi_{i+1} - 24(\phi_{i+2} - 16\phi_{i+1}) =$$
$$\phi_i(-255 + 24 \cdot 15) + h\phi_i'(-252 + 24 \cdot 14)$$
$$+ \frac{h^2}{2}\phi_i''(-240 + 24 \cdot 12) + \mathcal{O}(h^5)$$

Tidy up a bit:

$$\phi_{i+3} + 27\phi_{i+1} - \frac{54}{8}\phi_{i+2} = \frac{85}{4}\phi_i + \frac{33}{2}h\phi_i' + 9\frac{h^2}{2}\phi_i'' + \mathcal{O}(h^5)$$
$$\phi_{i+4} + 128\phi_{i+1} - 24\phi_{i+2} = 105\phi_i + 84h\phi_i' + 48\frac{h^2}{2}\phi_i'' + \mathcal{O}(h^5)$$

Eliminate second derivative:

$$\phi_{i+4} + 128\phi_{i+1} - 24\phi_{i+2} - \frac{16}{3}(\phi_{i+3} + 27\phi_{i+1} - \frac{54}{8}\phi_{i+2}) =$$
$$\phi_i(105 - \frac{85 \cdot 16}{12}) + h\phi_i'(84 - \frac{16 \cdot 33}{6}) + \mathcal{O}(h^5)$$

Tidy up again:

$$\phi_{i+4} - 16\phi_{i+1} + 12\phi_{i+2} - \frac{16}{3}\phi_{i+3} = -\frac{100}{12}\phi_i - 4h\phi_i'$$

Finally, this gives the following 4th order accurate forward difference approximation of the first derivative:

$$\phi_i' = \frac{-25\phi_i + 48\phi_{i+1} - 36\phi_{i+2} + 16\phi_{i+3} - 3\phi_{i+4}}{12h} + \mathcal{O}(h^4) \tag{A.1.2}$$

To get the backwards difference formulation, multiply (A.1.2) with -1

The electric field can now be found from:

$$E_x = -\phi_i' \tag{A.1.3}$$

Using forward, backwards or central differences as requiered.

3rd order accuracy forward difference for first derivative

$$\phi_{i+1} = \phi_i + h\phi_i' + \frac{h^2}{2}\phi_i'' + \frac{h^3}{3!}\phi_i''' + \mathcal{O}(h^4) \tag{A.1.4}$$

$$\phi_{i+2} = \phi_i + 2h\phi_i' + \frac{4h^2}{2}\phi_i'' + \frac{8h^3}{3!}\phi_i''' + \mathcal{O}(h^4) \tag{A.1.5}$$

$$\phi_{i+3} = \phi_i + 3h\phi_i' + \frac{9h^2}{2}\phi_i'' + \frac{27h^3}{3!}\phi_i''' + \mathcal{O}(h^4) \tag{A.1.6}$$

Eliminate second derivative terms: $(A.1.5) - 4(A.1.6)$ and $(A.1.6) - 9(A.1.4)$

$$\phi_{i+2} - 4\phi_{i+1} = -3\phi_i - 2h\phi_i' + \frac{4h^3}{3!}\phi_i''' \tag{A.1.7}$$

$$\phi_{i+3} - 9\phi_{i+1} = -8\phi_i - 6h\phi_i' + \frac{18h^3}{3!}\phi_i''' \tag{A.1.8}$$

Eliminate third derivative terms by $(A.1.8) - \frac{9}{2}(A.1.7)$, and solve for ϕ_i'

$$\phi_i' = \frac{-11\phi_i + 18\phi_{i+1} - 9\phi_{i+2} + 2\phi_{i+3}}{6h}$$

Finally:

$$E_x(i,j) = \frac{11\phi_{i,j} - 18\phi_{i+1,j} + 9\phi_{i+2,j} - 2\phi_{i+3,j}}{6h} \tag{A.1.9}$$

This equation holds true for the forward difference edges. At the backwards difference edges, simply flip the sign of the fraction in equation (A.1.9)

A.1.2 FD approximations of second derivatives

Central difference formulation for interior points, with 2nd order accuracy:

$$h^2\phi''(i,j) = \phi(i-1,j) + \phi(i,j-1) - 4\phi(i,j) + \phi(i+1,j) + \phi(i,j+1) \tag{A.1.10}$$

Forward difference approximation of second derivatives 1st order accuracy (edges):

$$\phi_{i+1} = \phi_i + h\phi_i' + \frac{h^2}{2}\phi_i''$$

$$\phi_{i+2} = \phi_i + 2h\phi_i' + \frac{4h^2}{2}\phi_i''$$

$$\phi_{i+2} - 2\phi_{i+1} = -\phi_i + h^2\phi_i''$$

$$h^2\phi_i'' = \phi_i - 2\phi_{i+1} + \phi_{i+2} \tag{A.1.11}$$

Backwards difference approximation of second derivatives 1st order accuracy (edges):

$$
\begin{aligned}
\phi_{i-1} &= \phi_i - h\phi_i' + \frac{h^2}{2}\phi_i'' \\
\phi_{i-2} &= \phi_i - 2h\phi_i' + \frac{4h^2}{2}\phi_i'' \\
\phi_{i-2} - 2\phi_{i-1} &= -\phi_i + h^2\phi_i'' \\
h^2\phi_i'' &= \phi_i - 2\phi_{i+1} + \phi_{i+2}
\end{aligned}
\tag{A.1.12}
$$

Forward and backwards difference are the same for the second derivatives. For the first derivatives one has to change the sign (multiply rhs with -1). This is generally true for the even or odd numbered derivatives (multiply by -1 for odd derivatives).

Forward difference approximation of second derivatives 2st order accuracy (edges):

$$
\begin{aligned}
\phi_{i+1} &= \phi_i + h\phi' + \frac{h^2}{2}\phi_i'' + \frac{h^3}{3!}\phi_i''' + \mathcal{O}(h^4) \\
\phi_{i+2} &= \phi_i + 2h\phi' + \frac{4h^2}{2}\phi_i'' + \frac{8h^3}{3!}\phi_i''' + \mathcal{O}(h^4) \\
\phi_{i+3} &= \phi_i + 3h\phi' + \frac{9h^2}{2}\phi_i'' + \frac{27h^3}{3!}\phi_i''' + \mathcal{O}(h^4)
\end{aligned}
$$

Eliminate third derivative:

$$
\begin{aligned}
\phi_{i+2} - 8\phi_{i+1} &= -7\phi_i - 6h\phi_i' - 4\frac{h^2}{2}\phi_i'' + \mathcal{O}(h^4) \\
\phi_{i+3} - 27\phi_{i+1} &= -26\phi_i - 24h\phi_i' - 18\frac{h^2}{2}\phi_i'' + \mathcal{O}(h^4)
\end{aligned}
$$

Eliminate first derivative:

$$
\begin{aligned}
\phi_{i+3} - 27\phi_{i+1} - 4(\phi_{i+2} - 8\phi_{i+1}) &= 2\phi_i - 2\frac{h^2}{2}\phi_i'' + \mathcal{O}(h^4) \\
\phi_{i+3} - 27\phi_{i+1} - 4(\phi_{i+2} - 8\phi_{i+1}) &= 2\phi_i - h^2\phi_i'' + \mathcal{O}(h^4) \\
\phi_{i+3} + 5\phi_{i+1} - 4\phi_{i+2} &= 2\phi_i - h^2\phi_i'' + \mathcal{O}(h^4)
\end{aligned}
$$

Finally:

$$
\phi_i'' = \frac{2\phi_i - 5\phi_{i+1} + 4\phi_{i+2} - \phi_{i+3}}{h^2} + \mathcal{O}(h^2) \tag{A.1.13}
$$

Finding an expression for ϕ_i from boundary condition (used to calculate the corner values):

$$\begin{aligned}
\phi_{i+1} &= \phi_i + h\phi_i' + \frac{h^2}{2}\phi_i'' \\
\phi_{i+2} &= \phi_i + 2h\phi_i' + \frac{4h^2}{2}\phi_i'' \\
\phi_{i+2} - 4\phi_{i+1} &= -3\phi_i - 2h\phi_i' \\
\phi_i &= \frac{4\phi_{i+1} - \phi_{i+2} - 2h\phi_i'}{3}
\end{aligned} \tag{A.1.14}$$

When applying von Neumann boundary conditions, we wish to keep the first derivative term. Second Derivative with neumann boundary condition, 1st order accuracy:

$$h^2\phi_i'' = -2\phi_i + 2\phi_{i+1} + 2h\phi_i' \tag{A.1.15}$$

Second Derivative with neumann boundary condition, 2nd order accuracy:

$$\begin{aligned}
\phi_{i+1} &= \phi_i + h\phi_i' + \frac{h^2}{2}\phi_i'' + \frac{h^3}{3!}\phi_i^{(3)} \\
\phi_{i+2} &= \phi_i + 2h\phi_i' + \frac{4h^2}{2}\phi_i'' + \frac{8h^3}{3!}\phi_i^{(3)} \\
\phi_{i+2} - 8\phi_{i+1} &= -7\phi_i - 6h\phi_i' - 2h^2\phi_i'' \\
h^2\phi_i'' &= -\frac{7}{2}\phi_i - 3h\phi' + 4\phi_{i+1} - \frac{1}{2}\phi_{i+2}
\end{aligned} \tag{A.1.16}$$

For the uniform case, 1st order accuracy seems to be good enough. It seems we need to use the 3 point version in the non-uniform case, to have BiCGStab converge correctly, which maybe means it would be a good idea to use 2nd order accuracy for the edges in the uniform case as well. It seems at the very least neat and tidy to be consistent with the order of accuracy in all parts of the domain.

ϕ' is zero at the boundaries. At the corners, ϕ_i is set to the average of the two directional derivatives:

$$2\phi(i,j) = \frac{4\phi(i+1,j) - \phi(i+2,j) + 4\phi(i,j+1) - \phi(i,j+2)}{3} \tag{A.1.17}$$

Simply using equation (A.1.17) for the equation on the corner nodes, results in BiCGStab not converging correctly. Specifically, the potential seems to be spooked up in the corners. If we isolate ϕ' from equation (A.1.16) and

and try to congest what expression makes sense as, for instance, ϕ'_i and ϕ'_j, meet in the lower left corner. Summing ϕ'_i and ϕ'_j and solving for $h^2(\phi''_i + \phi''_j$ leads us to an average expression in the style of (A.1.17) which also enable us to solve poisson's equation on the corners.

$$h^2(\phi''_i + \phi''_j) = -7\phi_i + 4\phi_{i+1} - \frac{1}{2}\phi_{i+2} + 4\phi_{j+1} - \frac{1}{2}\phi_{j+2} \qquad \text{(A.1.18)}$$

Equation (A.1.18) seems to behave correctly

A.1.3 Finite difference scheme for poisson equation

NB! I made some changes to the approach in this section, see Summary for FDM actually used Interior points:

$$h^2\phi''(i,j) = -4\phi(i,j)+\phi(i+1,j)+\phi(i-1,j)+\phi(i,j+1)+\phi(i,j-1) \quad \text{(A.1.19)}$$

Left edge, $i = 1, j = 3, N_y - 2$

$$h^2\phi''(i,j) = -4\phi(i,j) + 2\phi(i+1,j) + \phi(i,j+1) + \phi(i,j-1) \qquad \text{(A.1.20)}$$

bottom edge, $i = 3, N_x - 2, j = 1$

$$h^2\phi''(i,j) = -4\phi(i,j) + \phi(i+1,j) + \phi(i-1,j) + 2\phi(i,j+1) \qquad \text{(A.1.21)}$$

right edge $i = N_x, j = 3, N_y - 2$

$$h^2\phi''(i,j) = -4\phi(i,j) + 2\phi(i-1,j) + \phi(i,j+1) + \phi(i,j-1) \qquad \text{(A.1.22)}$$

top edge, between contacts, $i = 3, N_x - 2, j = N_y$

$$h^2\phi''(i,j) = -4\phi(i,j) + \phi(i+1,j) + \phi(i-1,j) + 2\phi(i,j-1) \qquad \text{(A.1.23)}$$

The corners might as well be left out, but in contrast with the SOR solver, we cannot use the corner values and "update" them between each iteration. We need to use forward and backward differences at the 8 points that otherwise would need the corner values in their FD-equation. Then we can simply use equation (A.1.17) to set the value of the potential at the corners.

For the two points next to the corners, e.g. the lower left corner, we use the following forward difference approximations:

$$h^2\phi''_i = \phi_i - 2\phi_{i+1} + \phi_{i+2} \qquad \text{(A.1.24)}$$
$$h^2\phi''_j = -2\phi_j + 2\phi_{j+1} \qquad \text{(A.1.25)}$$

Here $i = 2$, and $j = 1$. Similar expressions are found for the other points neighbouring a corner, which leads to the following linear equations for the next-to-a-corner-nodes:

$i = 1, j = 2$ and $i = 2, j = 1$:

$$h^2\phi''(i,j) = -\phi(i,j) + 2\phi(i+1,j) - 2\phi(i,j+1) + \phi(i,j+2) \tag{A.1.26}$$

$$h^2\phi''(i,j) = -\phi(i,j) + 2\phi(i,j+1) - 2\phi(i+1,j) + \phi(i+2,j) \tag{A.1.27}$$

$i = N_x, j = 2$ and $i = N_x - 1, j = 1$:

$$h^2\phi''(i,j) = -\phi(i,j) - 2\phi(i,j+1) + \phi(i,j+2) + 2\phi(i-1,j) \tag{A.1.28}$$

$$h^2\phi''(i,j) = -\phi(i,j) - 2\phi(i-1,j) + \phi(i-2,j) + 2\phi(i,j+1) \tag{A.1.29}$$

$i = N_x - 1, j = N_y - 1$ and $i = N_x, j = N_y - 1$:

$$h^2\phi''(i,j) = -\phi(i,j) - 2\phi(i-1,j) + \phi(i-2,j) + 2\phi(i,j-1) \tag{A.1.30}$$

$$h^2\phi''(i,j) = -\phi(i,j) - 2\phi(i,j-1) + \phi(i,j-2) + 2\phi(i-1,j) \tag{A.1.31}$$

$i = 2, j = N_y$ and $i = 1, j = N_y - 1$:

$$h^2\phi''(i,j) = -\phi(i,j) - 2\phi(i+1,j) + \phi(i+2,j) + 2\phi(i,j-1) \tag{A.1.32}$$

$$h^2\phi''(i,j) = -\phi(i,j) - 2\phi(i,j-1) + \phi(i,j-2) + 2\phi(i+1,j) \tag{A.1.33}$$

A.2 Non-uniform Mesh

A.2.1 First derivative approximation for the Electric field

Forward/Backwards Difference on edges

$$\phi_{i+1} = \phi_i + h_i\phi_i' + \frac{h_i^2}{2}\phi'' + \frac{h_i^3}{3!}\phi_i''' + \frac{h_i^4}{4!}\phi_i^{(4)} + \xi \tag{A.2.1}$$

$$\begin{aligned}\phi_{i+2} = \phi_i &+ (h_i + h_{i+1})\phi_i' + \frac{(h_i + h_{i+1})^2}{2}\phi'' + \frac{(h_i + h_{i+1})^3}{3!}\phi_i''' \\ &+ \frac{(h_i + h_{i+1})^4}{4!}\phi_i^{(4)} + \xi\end{aligned} \tag{A.2.2}$$

$$\begin{aligned}\phi_{i+3} = \phi_i &+ (h_i + h_{i+1} + h_{i+2})\phi_i' + \frac{(h_i + h_{i+1} + h_{i+2})^2}{2}\phi'' \\ &+ \frac{(h_i + h_{i+1} + h_{i+2})^3}{3!}\phi_i''' + \frac{(h_i + h_{i+1} + h_{i+2})^4}{4!}\phi_i^{(4)} + \xi\end{aligned} \tag{A.2.3}$$

$$\begin{aligned}\phi_{i+4} = \phi_i &+ (h_i + h_{i+1} + h_{i+2} + h_{i+3})\phi_i' + \frac{(h_i + h_{i+1} + h_{i+2} + h_{i+3})^2}{2}\phi'' \\ &+ \frac{(h_i + h_{i+1} + h_{i+2} + h_{i+3})^3}{3!}\phi_i''' + \frac{(h_i + h_{i+1} + h_{i+2} + h_{i+3})^4}{4!}\phi_i^{(4)} + \xi\end{aligned} \tag{A.2.4}$$

$\xi = \mathcal{O}\left(\left(\sum_{k=i}^{i+4} h_k\right)^5\right)$ Or:

$$\begin{aligned}
24h_1\phi_i' + 12h_1^2\phi_i'' + 4h_1^3\phi_i''' + h_1^4\phi_i^{(4)} &= 24(\phi_{i+1} - \phi_i) \\
24h_2\phi_i' + 12h_2^2\phi_i'' + 4h_2^3\phi_i''' + h_2^4\phi_i^{(4)} &= 24(\phi_{i+2} - \phi_i) \\
24h_3\phi_i' + 12h_3^2\phi_i'' + 4h_3^3\phi_i''' + h_3^4\phi_i^{(4)} &= 24(\phi_{i+3} - \phi_i) \\
24h_4\phi_i' + 12h_4^2\phi_i'' + 4h_4^3\phi_i''' + h_4^4\phi_i^{(4)} &= 24(\phi_{i+4} - \phi_i)
\end{aligned}$$

We now write this as the linear system $Ax = b$:

$$\begin{bmatrix} 24h_1 & 12h_1^2 & 4h_1^3 & h_1^4 \\ 24h_2 & 12h_2^2 & 4h_2^3 & h_2^4 \\ 24h_3 & 12h_3^2 & 4h_3^3 & h_3^4 \\ 24h_4 & 12h_4^2 & 4h_4^3 & h_4^4 \end{bmatrix} \begin{bmatrix} \phi_i' \\ \phi_i'' \\ \phi_i''' \\ \phi_i^{(4)} \end{bmatrix} = \begin{bmatrix} 24(\phi_{i+1} - \phi_i) \\ 24(\phi_{i+2} - \phi_i) \\ 24(\phi_{i+3} - \phi_i) \\ 24(\phi_{i+4} - \phi_i) \end{bmatrix}$$

We make some substitutions to simplify the arithmetics:

$$\begin{bmatrix} a & b & c & d \\ f & g & k & l \\ n & o & p & q \\ s & t & u & v \end{bmatrix} \begin{bmatrix} \phi_i' \\ \phi_i'' \\ \phi_i''' \\ \phi_i^{(4)} \end{bmatrix} = \begin{bmatrix} e \\ m \\ r \\ w \end{bmatrix}$$

Cramer's rule can now give us an expression for ϕ':

$$\phi_i' = \frac{\begin{vmatrix} e & b & c & d \\ m & g & k & l \\ r & o & p & q \\ w & t & u & v \end{vmatrix}}{\begin{vmatrix} a & b & c & d \\ f & g & k & l \\ n & o & p & q \\ s & t & u & v \end{vmatrix}}$$

Note that the factorial factors can be removed. Concentrating on the nominator first:

$$det_t = e\begin{vmatrix} g & k & l \\ o & p & q \\ t & u & v \end{vmatrix} - m\begin{vmatrix} b & c & d \\ o & p & q \\ t & u & v \end{vmatrix} + r\begin{vmatrix} b & c & d \\ g & k & l \\ t & u & v \end{vmatrix} - w\begin{vmatrix} b & c & d \\ g & k & l \\ o & p & q \end{vmatrix}$$

$$= e(g(pv - qu) - k(ov - qt) + l(ou - pt)) - m(b(pv - qu) - c(ov - qt) + d(ou - pt)) \\ + r(b(kv - lu) - c(gv - lt) + d(gu - kt)) - w(b(kq - lp) - c(gq - lo) + d(gp - ko))$$

Then the denominator:

$$det_n = a\begin{vmatrix} g & k & l \\ o & p & q \\ t & u & v \end{vmatrix} - f\begin{vmatrix} b & c & d \\ o & p & q \\ t & u & v \end{vmatrix} + n\begin{vmatrix} b & c & d \\ g & k & l \\ t & u & v \end{vmatrix} - s\begin{vmatrix} b & c & d \\ g & k & l \\ o & p & q \end{vmatrix}$$

$$= a(g(pv - qu) - k(ov - qt) + l(ou - pt)) - f(b(pv - qu) - c(ov - qt) + d(ou - pt)) \\ + n(b(kv - lu) - c(gv - lt) + d(gu - kt)) - s(b(kq - lp) - c(gq - lo) + d(gp - ko))$$

With substitue for the b column vector:

$$(\phi_{i+1} - \phi_i)(g(pv - qu) - k(ov - qt) + l(ou - pt)) - (\phi_{i+2} - \phi_i)(b(pv - qu) - c(ov - qt) + d(ou - \\ + (\phi_{i+3} - \phi_i)(b(kv - lu) - c(gv - lt) + d(gu - kt)) - (\phi_{i+4} - \phi_i)(b(kq - lp) - c(gq - lo) + d(gp$$

We can now kind of see what the finite difference cofactors are gonna be. Let's try to find a_1, the cofactor for ϕ_{i+1}

$$\frac{(g(pv-qu)-k(ov-qt)+l(ou-pt))}{a(g(pv-qu)-k(ov-qt)+l(ou-pt))-f(b(pv-qu)-c(ov-qt)+d(ou-pt))+n(b(kv-lu)-c(gv-lt)+d(gu-kt))-s(b(kq-lp)-c(gq-lo)+d(gp-ko))}$$

Nominator first, susbstitute back the following (the factorial factors are removed, as they eliminate each other in the fraction of cramer's rule)

$$\begin{aligned} a &= h_1 & b &= h_1^2 & c &= h_1^3 & d &= h_1^4 \\ f &= h_2 & g &= h_2^2 & k &= h_2^3 & l &= h_2^4 \\ n &= h_3 & o &= h_3^2 & p &= h_3^3 & q &= h_3^4 \\ s &= h_4 & t &= h_4^2 & u &= h_4^3 & v &= h_4^4 \end{aligned}$$

$$(h_2^2(h_3^3h_4^4 - h_3^4h_4^3) - h_2^3(h_3^2h_4^4 - h_3^4h_4^2) + h_2^4(h_3^2h_4^3 - h_3^3h_4^2))$$

Simplify as best as possible:

$$\begin{aligned} &h_2^2(h_3^3h_4^4 - h_3^4h_4^3) - h_2^3(h_3^2h_4^4 - h_3^4h_4^2) + h_2^4(h_3^2h_4^3 - h_3^3h_4^2) \\ &h_2^2h_3^2h_4^2((h_3h_4^2 - h_3^2h_4) - h_2(h_4^2 - h_3^2) + h_2^2(h_4 - h_3)) \\ &h_2^2h_3^2h_4^2(h_3h_4(h_4 - h_3) - h_2(h_4^2 - h_3^2) + h_2^2(h_4 - h_3)) \\ &h_2^2h_3^2h_4^2((h_3h_4 + h_2^2)(h_4 - h_3) - h_2(h_4^2 - h_3^2)) \\ &h_2^2h_3^2h_4^2((h_3h_4 + h_2^2)(h_4 - h_3) - h_2(h_4 - h_3)(h_4 + h_3)) \\ &h_2^2h_3^2h_4^2(h_4 - h_3)(h_3h_4 + h_2^2 - h_2(h_4 + h_3)) \\ &h_2^2h_3^2h_4^2(h_4 - h_3)(h_3h_4 + h_2^2 - h_2h_4 - h_2h_3)) \\ &h_2^2h_3^2h_4^2(h_4 - h_3)(h_3(h_4 - h_2) - h_2(h_4 - h_2)) \\ &h_2^2h_3^2h_4^2(h_4 - h_3)(h_4 - h_2)(h_3 - h_2) \end{aligned}$$

Whip out the magnifying glass, and give the denominator the same treatment:

$$h_1(h_2^2(h_3^3h_4^4 - h_3^4h_4^3) - h_2^3(h_3^2h_4^4 - h_3^4h_4^2) + h_2^4(h_3^2h_4^3 - h_3^3h_4^2)) - h_2(h_1^2(h_3^3h_4^4 - h_3^4h_4^3) - h_1^3(h_3^2h_4^4 - h_3^4h_4^2) + h_1^4(h_3^2h_4^3 - h_3^3h_4^2)) + h_3(h_1^2(h_2^3h_4^4 - h_2^4h_4^3) - h_1^3(h_2^2h_4^4 - h_2^4h_4^2) + h_1^4(h_2^2h_4^3 - h_2^3h_4^2)) - h_4(h_1^2(h_2^3h_3^4 - h_2^4h_3^3) - h_1^3(h_2^2h_3^4 - h_2^4h_3^2) + h_1^4(h_2^2h_3^3 - h_2^3h_3^2))$$

Let's simplify one addend at the time. First addend:

$$\begin{aligned}
&h_1(h_2^2(h_3^3h_4^4 - h_3^4h_4^3) - h_2^3(h_3^2h_4^4 - h_3^4h_4^2) + h_2^4(h_3^2h_4^3 - h_3^3h_4^2))\\
&h_1h_2^2((h_3^3h_4^4 - h_3^4h_4^3) - h_2(h_3^2h_4^4 - h_3^4h_4^2) + h_2^2(h_3^2h_4^3 - h_3^3h_4^2))\\
&h_1h_2^2h_3^2h_4^2((h_3h_4^2 - h_3^2h_4) - h_2(h_4^2 - h_3^2) + h_2^2(h_4 - h_3))\\
&h_1h_2^2h_3^2h_4^2(h_3h_4(h_4 - h_3) - h_2(h_4 - h_3)(h_4 + h_3) + h_2^2(h_4 - h_3))\\
&h_1h_2^2h_3^2h_4^2(h_4 - h_3)(h_3h_4 - h_2(h_4 + h_3) + h_2^2)\\
&h_1h_2^2h_3^2h_4^2(h_4 - h_3)(h_3h_4 - h_2(h_4 + h_3 - h_2))\\
&h_1h_2^2h_3^2h_4^2(h_4 - h_3)(h_4(h_3 - h_2) - h_2(h_3 - h_2))\\
&h_1h_2^2h_3^2h_4^2(h_4 - h_3)(h_4 - h_2)(h_3 - h_2)
\end{aligned}$$

Second addend:

$$\begin{aligned}
&-h_2(h_1^2(h_3^3h_4^4 - h_3^4h_4^3) - h_1^3(h_3^2h_4^4 - h_3^4h_4^2) + h_1^4(h_3^2h_4^3 - h_3^3h_4^2))\\
&-h_2h_1^2h_3^2h_4^2((h_3h_4^2 - h_3^2h_4) - h_1(h_4^2 - h_3^2) + h_1^2(h_4 - h_3))\\
&-h_2h_1^2h_3^2h_4^2(h_3h_4(h_4 - h_3) - h_1(h_4 - h_3)(h_4 + h_3) + h_1^2(h_4 - h_3))\\
&-h_2h_1^2h_3^2h_4^2(h_4 - h_3)(h_3h_4 - h_1(h_4 + h_3) + h_1^2)\\
&-h_2h_1^2h_3^2h_4^2(h_4 - h_3)(h_3h_4 - h_1(h_4 + h_3 - h_1))
\end{aligned}$$

Third addend:

$$
\begin{aligned}
&h_3(h_1^2(h_2^3h_4^4 - h_2^4h_4^3) - h_1^3(h_2^2h_4^4 - h_2^4h_4^2) + h_1^4(h_2^2h_4^3 - h_2^3h_4^2))\\
&h_3h_1^2h_2^2h_4^2((h_2h_4^2 - h_2^2h_4) - h_1(h_4^2 - h_2^2) + h_1^2(h_4 - h_2))\\
&h_3h_1^2h_2^2h_4^2(h_2h_4(h_4 - h_2) - h_1(h_4 - h_2)(h_4 + h_2) + h_1^2(h_4 - h_2))\\
&h_3h_1^2h_2^2h_4^2(h_4 - h_2)(h_2h_4 - h_1(h_4 + h_2) + h_1^2)\\
&h_3h_1^2h_2^2h_4^2(h_4 - h_2)(h_2h_4 - h_1(h_4 + h_2 - h_1))
\end{aligned}
$$

fourth addend:

$$
\begin{aligned}
&- h_4(h_1^2(h_2^3h_3^4 - h_2^4h_3^3) - h_1^3(h_2^2h_3^4 - h_2^4h_3^2) + h_1^4(h_2^2h_3^3 - h_2^3h_3^2))\\
&- h_4h_1^2h_2^2h_3^2((h_2h_3^2 - h_2^2h_3) - h_1(h_3^2 - h_2^2) + h_1^2(h_3 - h_2))\\
&- h_4h_1^2h_2^2h_3^2(h_3 - h_2)(h_2h_3 - h_1(h_3 + h_2 - h_1))
\end{aligned}
$$

The common factor is $h_1h_2h_3h_4$, which gives us the following factor for ϕ':

$$
\frac{h_2h_3h_4(h_4-h_3)(h_3h_4-h_2(h_4+h_3-h_2))}{h_1(h_2h_3h_4(h_4-h_3)(h_3h_4-h_2(h_4+h_3-h_2))-h_1h_3h_4(h_4-h_3)(h_3h_4-h_1(h_4+h_3-h_1))+h_1h_2h_4(h_4-h_2)(h_2h_4-h_1(h_4+h_2-h_1))-h_1h_2h_3(h_3-h_2)(h_2h_3-h_1(h_3+h_2-h_1)))}
$$

Using $h_1 = h, h_2 = 2h, h_3 = 3h, h_4 = 4h$ yields:

$$
a_1 = \frac{4}{h}
$$

Which is what one would expect in the uniform case (ref: wikipedia)

Simplify denominator further: first and second:

$$h_3h_4(h_4-h_3)(h_2h_3h_4-h_2^2(h_4+h_3-h_2)-h_1h_3h_4+h_1^2(h_4+h_3-h_1))$$
$$h_3h_4(h_4-h_3)(h_3h_4(h_2-h_1)-h_2^2(h_4+h_3-h_2)+h_1^2(h_4+h_3-h_1))$$
$$h_3h_4(h_4-h_3)(h_3h_4(h_2-h_1)-h_3(h_2^2-h_1^2)-h_4(h_2^2-h_1^2)+h_2^3-h_1^3)$$
$$h_3h_4(h_4-h_3)(h_3h_4(h_2-h_1)-h_3(h_2-h_1)(h_2+h_1)-h_4(h_2-h_1)(h_2+h_1)+h_2^3-h_1^3)$$
$$h_3h_4(h_4-h_3)(h_3h_4(h_2-h_1)-h_3(h_2-h_1)(h_2+h_1)-h_4(h_2-h_1)(h_2+h_1)+(h_2-h_1)(h_2^2+h_1h_2+h_1^2))$$
$$h_3h_4(h_4-h_3)(h_2-h_1)(h_3h_4-h_3(h_2+h_1)-h_4(h_2+h_1)+(h_2^2+h_2h_1+h_1^2))$$
$$h_3h_4(h_4-h_3)(h_2-h_1)(h_3h_4-h_3(h_2+h_1)-h_4(h_2+h_1)+(h_1+h_2)^2-h_1h_2)$$
$$h_3h_4(h_4-h_3)(h_2-h_1)(h_3h_4-h_1h_2+(h_1+h_2)(h_1+h_2-h_3-h_4))$$

Third and fourth:

$$h_1h_2h_4(h_4-h_2)(h_2h_4-h_1(h_4+h_2-h_1))-h_1h_2h_3(h_3-h_2)(h_2h_3-h_1(h_3+h_2-h_1))$$
$$h_1h_2(h_4(h_4-h_2)(h_2h_4-h_1(h_4+h_2-h_1))-h_3(h_3-h_2)(h_2h_3-h_1(h_3+h_2-h_1)))$$
$$h_1h_2(h_2h_4^2(h_4-h_2)-h_1h_4(h_4-h_2)(h_4+h_2-h_1)-h_2h_3^2(h_3-h_2)+h_1h_3(h_3-h_2)(h_3+h_2-h_1))$$
$$h_1h_2(h_2(h_4^2(h_4-h_2)-h_3^2(h_3-h_2))+h_1(h_3(h_3-h_2)(h_3+h_2-h_1)-h_4(h_4-h_2)(h_4+h_2-h_1)))$$
$$h_1h_2(h_2(h_4^3-h_2h_4^2-h_3^3+h_2h_3^2))+h_1(h_3(h_3-h_2)(h_3+h_2-h_1)-h_4(h_4-h_2)(h_4+h_2-h_1)))$$
$$h_1h_2(h_2((h_4-h_3)(h_4^2+h_4h_3+h_3^2)-h_2(h_4^2-h_3^2))+h_1(h_3(h_3-h_2)(h_3+h_2-h_1)-h_4(h_4-h_2)(h_4+h_2-h_1)))$$
$$h_1h_2(h_2(h_4-h_3)((h_4^2+h_4h_3+h_3^2)-h_2(h_4+h_3))+h_1(h_3(h_3-h_2)(h_3+h_2-h_1)-h_4(h_4-h_2)(h_4+h_2-h_1)))$$
$$h_1h_2(h_2(h_4-h_3)((h_4+h_3)^2-h_4h_3-h_2(h_4+h_3))+h_1(h_3(h_3-h_2)(h_3+h_2-h_1)-h_4(h_4-h_2)(h_4+h_2-h_1)))$$
$$h_1h_2(h_2(h_4-h_3)((h_4+h_3)(h_4+h_3-h_2)-h_4h_3))+h_1(h_3(h_3-h_2)(h_3+h_2-h_1)-h_4(h_4-h_2)(h_4+h_2-h_1)))$$

Second addend of this expression:

$$h_1(h_3(h_3 - h_2)(h_3 + h_2 - h_1) - h_4(h_4 - h_2)(h_4 + h_2 - h_1)))$$
$$h_1((h_3^2 - h_2h_3)(h_3 + h_2 - h_1) - (h_4^2 - h_2h_4)(h_4 + h_2 - h_1)))$$
$$h_1(h_3^3 + h_2h_3^2 - h_1h_3^2 - h_2h_3^2 - h_3h_2^2 + h_2h_3h_1 - h_4^3 - h_2h_4^2 + h_1h_4^2 + h_2h_4^2 + h_2^2h_4 - h_1h_2h_4)$$
$$h_1(h_4 - h_3)(-(h_3^2 + h_4h_3 + h_4^2) + h_1(h_4 + h_3) + h_2^2 - h_2h_1)$$
$$h_1(h_4 - h_3)(-(h_3^2 + h_4h_3 + h_4^2) + h_1(h_4 + h_3) + h_2(h_2 - h_1))$$
$$h_1(h_4 - h_3)(-(h_3 + h_4)^2 + h_3h_4 + h_1(h_4 + h_3) + h_2(h_2 - h_1))$$
$$h_1(h_4 - h_3)((h_3 + h_4)(h_1 - h_3 - h_4) + h_3h_4 + h_2(h_2 - h_1))$$

combined:

$$h_1h_2(h_2(h_4 - h_3)((h_4 + h_3)(h_4 + h_3 - h_2) - h_4h_3) + h_1(h_4 - h_3)((h_3 + h_4)(h_1 - h_3 - h_4) + h_3h_4 + h_2(h_2 - h_1)))$$
$$h_1h_2(h_4 - h_3)(h_2((h_4 + h_3)(h_4 + h_3 - h_2) - h_4h_3) + h_1((h_3 + h_4)(h_1 - h_3 - h_4) + h_3h_4 + h_2(h_2 - h_1)))$$
$$h_1h_2(h_4 - h_3)((h_4 + h_3)(h_2(h_4 + h_3 - h_2) + h_1(h_1 - h_3 - h_4)) - h_3h_4(h_2 - h_1) + h_1h_2(h_2 - h_1)))$$
$$h_1h_2(h_4 - h_3)((h_4 + h_3)(h_2h_4 + h_3h_2 - h_2^2 + h_1^2 - h_1h_3 - h_1h_4) + (h_2 - h_1)(h_1h_2 - h_3h_4))$$
$$h_1h_2(h_4 - h_3)((h_4 + h_3)(h_4(h_2 - h_1) + h_3(h_2 - h_1) - (h_2^2 - h_1^2)) + (h_2 - h_1)(h_1h_2 - h_3h_4))$$
$$h_1h_2(h_4 - h_3)((h_4 + h_3)(h_4(h_2 - h_1) + h_3(h_2 - h_1) - (h_2 - h_1)(h_2 + h_1)) + (h_2 - h_1)(h_1h_2 - h_3h_4))$$
$$h_1h_2(h_4 - h_3)(h_2 - h_1)((h_4 + h_3)(h_4 + h_3 - (h_2 + h_1)) + (h_1h_2 - h_3h_4))$$
$$h_1h_2(h_4 - h_3)(h_2 - h_1)(h_1h_2 - h_3h_4 + (h_4 + h_3)(h_4 + h_3 - h_2 - h_1))$$

denominator, total

$$h_1h_2h_3h_4(h_3h_4(h_4 - h_3)(h_2 - h_1)(h_3h_4 - h_1h_2 + (h_1 + h_2)(h_1 + h_2 - h_3 - h_4)) + h_1h_2(h_4 - h_3)(h_2 - h_1)(h_1h_2 - h_3h_4 + (h_4 + h_3)(h_4 + h_3 - h_2 - h_1)))$$
$$h_1h_2h_3h_4(h_4 - h_3)(h_2 - h_1)(h_3h_4(h_3h_4 - h_1h_2 + (h_1 + h_2)(h_1 + h_2 - h_3 - h_4)) + h_1h_2(h_1h_2 - h_3h_4 + (h_4 + h_3)(h_4 + h_3 - h_2 - h_1)))$$

Leave out the common factors

$$h_3h_4(h_3h_4 - h_1h_2 + (h_1+h_2)(h_1+h_2-h_3-h_4)) + h_1h_2(h_1h_2 - h_3h_4 + (h_4+h_3)(h_4+h_3-h_2-h_1))$$
$$(h_1+h_2-h_3-h_4)(h_3h_4(h_1+h_2) - h_1h_2(h_4+h_3)) + h_3^2h_4^2 + h_1^2h_2^2 - 2h_1h_2h_3h_4$$
$$(h_1+h_2-h_3-h_4)(h_3h_4(h_1+h_2) - h_1h_2(h_4+h_3)) + (h_3h_4 - h_1h_2)^2$$
$$(h_1+h_2-h_3-h_4)(h_1h_3h_4 + h_2h_3h_4 - h_1h_2h_4 - h_1h_2h_3) + (h_3h_4 - h_1h_2)^2$$
$$h_1^2h_3h_4 - h_1^2h_2h_4 - h_1^2h_2h_3 + h_2^2h_3h_4 - h_1h_2^2h_4 - h_1h_2^2h_3 - h_1h_3^2h_4 - h_2h_3^2h_4 + h_1h_2h_3^2 - h_1h_3h_4^2 - h_2h_3h_4^2 + h_1h_2h_4^2 + h_3^2h_4^2 + h_1^2h_2^2 + 2h_1h_2h_3h_4$$
$$h_1^2(h_3h_4 - h_2h_4 - h_2h_3) + h_2^2(h_3h_4 - h_1h_4 - h_1h_3) + h_3^2(-h_1h_4 - h_2h_4 + h_1h_2) + h_4^2(-h_1h_3 - h_2h_3 + h_1h_2) + h_3^2h_4^2 + h_1^2h_2^2 + 2h_1h_2h_3h_4$$
$$h_1^2(h_4(h_3-h_2) - h_2h_3) + h_2^2(h_3(h_4-h_1) - h_1h_4) + h_3^2(h_2(h_1-h_4) - h_1h_4) + h_4^2(h_1(h_2-h_3) - h_2h_3) + h_3^2h_4^2 + h_1^2h_2^2 + 2h_1h_2h_3h_4$$
$$h_1^2(h_4(h_3-h_2) - h_2h_3) + h_2^2(h_3(h_4-h_1) - h_1h_4) - h_3^2(h_2(h_4-h_1) + h_1h_4) - h_4^2(h_1(h_3-h_2) + h_2h_3) + h_3^2h_4^2 + h_1^2h_2^2 + 2h_1h_2h_3h_4$$
$$(h_3-h_2)(h_1^2h_4 - h_4^2h_1) + (h_4-h_1)(h_2^2h_3 - h_3^2h_2) - h_1^2h_2h_3 - h_2^2h_1h_4 - h_3^2h_1h_4 - h_4^2h_2h_3 + h_3^2h_4^2 + h_1^2h_2^2 + 2h_1h_2h_3h_4$$
$$(h_3-h_2)(h_1h_4(h_1-h_4)) + (h_4-h_1)(h_2h_3(h_2-h_3)) - h_2h_3(h_1^2+h_4^2) - h_1h_4(h_2^2+h_3^2) + h_3^2h_4^2 + h_1^2h_2^2 + 2h_1h_2h_3h_4$$
$$-h_1h_4(h_3-h_2)(h_4-h_1) - h_2h_3(h_4-h_1)(h_3-h_2) - h_2h_3(h_1^2+h_4^2) - h_1h_4(h_2^2+h_3^2) + h_3^2h_4^2 + h_1^2h_2^2 + 2h_1h_2h_3h_4$$
$$-(h_3-h_2)(h_4-h_1)(h_1h_4 + h_2h_3) - h_2h_3(h_1^2+h_4^2) - h_1h_4(h_2^2+h_3^2) + h_3^2h_4^2 + h_1^2h_2^2 + 2h_1h_2h_3h_4$$
$$-(h_3-h_2)(h_4-h_1)(h_1h_4 + h_2h_3) - h_2h_3(h_1^2+h_4^2) - h_1h_4(h_2^2+h_3^2) + h_3^2h_4^2 + h_1^2h_2^2 + 2h_1h_2h_3h_4$$
$$-(h_3-h_2)(h_4-h_1)(h_1h_4 + h_2h_3) + h_2(-h_1^2h_3 - h_3h_4^2) + h_4(-h_1h_2^2 - h_1h_3^2) + h_3^2h_4^2 + h_1^2h_2^2 + 2h_1h_2h_3h_4$$
$$-(h_3-h_2)(h_4-h_1)(h_1h_4 + h_2h_3) + h_2(-h_1^2h_3 - h_3h_4^2 + h_1^2h_2) + h_4(-h_1h_2^2 - h_1h_3^2 + h_3^2h_4 + 2h_1h_2h_3)$$
$$-(h_3-h_2)(h_4-h_1)(h_1h_4 + h_2h_3) + h_2(-h_1^2(h_3-h_2) - h_3h_4^2) + h_4(-h_1h_2^2 + h_3^2(h_4-h_1) + 2h_1h_2h_3)$$
$$-(h_3-h_2)(h_4-h_1)(h_1h_4 + h_2h_3) - h_2h_1^2(h_3-h_2) - h_2h_3h_4^2 - h_4h_1h_2^2 + h_4h_3^2(h_4-h_1) + 2h_1h_2h_3h_4$$
$$-(h_3-h_2)(h_4-h_1)(h_1h_4 + h_2h_3) - h_2h_1(h_1(h_3-h_2) + h_4h_2) + h_4h_3(h_3h_4 - h_3h_1 - h_2h_4) + 2h_1h_2h_3h_4$$
$$-(h_3-h_2)(h_4-h_1)(h_1h_4 + h_2h_3) - h_2h_1(h_1(h_3-h_2) + h_4h_2) + h_4h_3(h_4(h_3-h_2) - h_3h_1 + 2h_1h_2h_3h_4$$
$$-(h_3-h_2)(h_4-h_1)(h_1h_4 + h_2h_3) - h_2h_1^2(h_3-h_2) - h_1h_4h_2^2 + h_4^2h_3(h_3-h_2) - h_3^2h_4h_1 + 2h_1h_2h_3h_4$$
$$-(h_3-h_2)(h_4-h_1)(h_1h_4 + h_2h_3) - (h_3-h_2)(h_2h_1^2 - h_4^2h_3) - h_1h_4(h_2^2 + h_3^2 + 2h_2h_3)$$
$$-(h_3-h_2)(h_4-h_1)(h_1h_4 + h_2h_3) - (h_3-h_2)(h_2h_1^2 - h_4^2h_3) - h_1h_4(h_3-h_2)^2$$
$$-(h_3-h_2)(h_4-h_1)(h_1h_4 + h_2h_3) - (h_3-h_2)(h_2h_1^2 - h_4^2h_3 - h_1h_4(h_3-h_2))$$
$$-(h_3-h_2)(h_4-h_1)(h_1h_4 + h_2h_3) - (h_3-h_2)(-h_4h_3(h_4-h_1) + h_2h_1^2 - h_1h_4h_2))$$
$$-(h_3-h_2)(h_4-h_1)(h_1h_4 + h_2h_3) - (h_3-h_2)(-h_4h_3(h_4-h_1) - h_1h_2(h_4-h_1)))$$
$$-(h_3-h_2)(h_4-h_1)(h_1h_4 + h_2h_3) - (h_3-h_2)(-h_4h_3(h_4-h_1) - h_1h_2(h_4-h_1)))$$
$$-(h_3-h_2)(h_4-h_1)(h_1h_4 + h_2h_3) - (h_3-h_2)(h_4-h_1)(-h_4h_3 - h_1h_2))$$

$$
\begin{aligned}
&-(h_3-h_2)(h_4-h_1)(h_1h_4+h_2h_3-h_4h_3-h_1h_2)\\
&-(h_3-h_2)(h_4-h_1)(h_1(h_4-h_2)+h_3(h_2-h_4))\\
&-(h_3-h_2)(h_4-h_1)(h_1(h_4-h_2)-h_3(h_4-h_2))\\
&(h_4-h_1)(h_4-h_2)(h_3-h_2)(h_3-h_1)
\end{aligned}
$$

Finally; The factorized denominator of our finite difference coefficients are:

$$h_1h_2h_3h_4(h_4-h_3)(h_4-h_2)(h_4-h_1)(h_3-h_2)(h_3-h_1)(h_2-h_1) \tag{A.2.5}$$

The coefficient a_1 is now:

$$\frac{h_2h_3h_4}{h_1(h_4-h_1)(h_3-h_1)(h_2-h_1)}$$

Let's examine the rest of the coefficients, concentrating on the nominators:

$$\begin{aligned}
a'_0 &= -(a'_1 + a'_2 + a'_3 + a'_4) \\
a'_2 &= -(b(pv - qu) - c(ov - qt) + d(ou - pt)) \\
a'_3 &= b(kv - lu) - c(gv - lt) + d(gu - kt) \\
a'_4 &= -(b(kq - lp) - c(gq - lo) + d(gp - ko))
\end{aligned}$$

Remembering that:

$$\begin{aligned}
a =& h_1 & b =& h_1^2 & c =& h_1^3 & d =& h_1^4 \\
f =& h_2 & g =& h_2^2 & k =& h_2^3 & l =& h_2^4 \\
n =& h_3 & o =& h_3^2 & p =& h_3^3 & q =& h_3^4 \\
s =& h_4 & t =& h_4^2 & u =& h_4^3 & v =& h_4^4
\end{aligned}$$

$$\begin{aligned}
a'_2 &= -(h_1^2(h_3^3h_4^4 - h_3^4h_4^3) - h_1^3(h_3^2h_4^4 - h_3^4h_4^2) + h_1^4(h_3^2h_4^3 - h_3^3h_4^2)) \\
a'_3 &= h_1^2(h_2^3h_4^4 - h_2^4h_4^3) - h_1^3(h_2^2h_4^4 - h_2^4h_4^2) + h_1^4(h_2^2h_4^3 - h_2^3h_4^2) \\
a'_4 &= -(h_1^2(h_2^3h_3^4 - h_2^4h_3^3) - h_1^3(h_2^2h_3^4 - h_2^4h_3^2) + h_1^4(h_2^2h_3^3 - h_2^3h_3^2))
\end{aligned}$$

for a'_2:

$$\begin{aligned}
&-(h_1^2(h_3^3h_4^4 - h_3^4h_4^3) - h_1^3(h_3^2h_4^4 - h_3^4h_4^2) + h_1^4(h_3^2h_4^3 - h_3^3h_4^2)) \\
&-h_1^2h_3^2h_4^2((h_3h_4^2 - h_3^2h_4) - h_1(h_4 - h_3)(h_4 + h_3) + h_1^2(h_4 - h_3)) \\
&-h_1^2h_3^2h_4^2(h_3h_4(h_4 - h_3) - h_1(h_4 - h_3)(h_4 + h_3) + h_1^2(h_4 - h_3)) \\
&-h_1^2h_3^2h_4^2(h_4 - h_3)(h_3h_4 - h_1(h_4 + h_3) + h_1^2) \\
&-h_1^2h_3^2h_4^2(h_4 - h_3)(h_3(h_4 - h_1) - h_1(h_4 - h_1)) \\
&-h_1^2h_3^2h_4^2(h_4 - h_3)(h_4 - h_1)(h_3 - h_1) \\
a_2 =& \frac{-h_1^2h_3^2h_4^2(h_4 - h_3)(h_4 - h_1)(h_3 - h_1)}{h_1h_2h_3h_4(h_4 - h_3)(h_4 - h_2)(h_4 - h_1)(h_3 - h_2)(h_3 - h_1)(h_2 - h_1)}
\end{aligned}$$

$$a_2 = \frac{-h_1h_3h_4}{h_2(h_4 - h_2)(h_3 - h_2)(h_2 - h_1)}$$

for a_3':

$$\begin{aligned}
a_3' &= h_1^2(h_2^3h_4^4 - h_2^4h_4^3) - h_1^3(h_2^2h_4^4 - h_2^4h_4^2) + h_1^4(h_2^2h_4^3 - h_2^3h_4^2)\\
a_3' &= h_1^2(h_2^3h_4^4 - h_2^4h_4^3 - h_1(h_2^2h_4^4 - h_2^4h_4^2) + h_1^2(h_2^2h_4^3 - h_2^3h_4^2))\\
a_3' &= h_1^2h_2^2h_4^2(h_2h_4^2 - h_2^2h_4 - h_1(h_4^2 - h_2^2) + h_1^2(h_4 - h_2))\\
a_3' &= h_1^2h_2^2h_4^2(h_2h_4(h_4 - h_2) - h_1(h_4 - h_2)(h_4 + h_2) + h_1^2(h_4 - h_2))\\
a_3' &= h_1^2h_2^2h_4^2(h_4 - h_2)(h_2h_4 - h_1(h_4 + h_2) + h_1^2)\\
a_3' &= h_1^2h_2^2h_4^2(h_4 - h_2)(h_4(h_2 - h_1) - h_1(h_2 - h_1))\\
a_3' &= h_1^2h_2^2h_4^2(h_4 - h_2)(h_4 - h_1)(h_2 - h_1)\\
a_3 &= \frac{h_1^2h_2^2h_4^2(h_4 - h_2)(h_4 - h_1)(h_2 - h_1)}{h_1h_2h_3h_4(h_4 - h_3)(h_4 - h_2)(h_4 - h_1)(h_3 - h_2)(h_3 - h_1)(h_2 - h_1)}
\end{aligned}$$

$$a_3 = \frac{h_1h_2h_4}{h_3(h_4 - h_3)(h_3 - h_2)(h_3 - h_1)}$$

for a_4':

$$\begin{aligned}
&- (h_1^2(h_2^3h_3^4 - h_2^4h_3^3) - h_1^3(h_2^2h_3^4 - h_2^4h_3^2) + h_1^4(h_2^2h_3^3 - h_2^3h_3^2))\\
&- h_1^2((h_2^3h_3^4 - h_2^4h_3^3) - h_1(h_2^2h_3^4 - h_2^4h_3^2) + h_1^2(h_2^2h_3^3 - h_2^3h_3^2))\\
&- h_1^2h_2^2h_3^2(h_2h_3(h_3 - h_2) - h_1(h_3 - h_2)(h_3 + h_2) + h_1^2(h_3 - h_2))\\
&- h_1^2h_2^2h_3^2(h_3 - h_2)(h_2h_3 - h_1(h_3 + h_2) + h_1^2)\\
&- h_1^2h_2^2h_3^2(h_3 - h_2)(h_3 - h_1)(h_2 - h_1)\\
a_4 =& \frac{-h_1^2h_2^2h_3^2(h_3 - h_2)(h_3 - h_1)(h_2 - h_1)}{h_1h_2h_3h_4(h_4 - h_3)(h_4 - h_2)(h_4 - h_1)(h_3 - h_2)(h_3 - h_1)(h_2 - h_1)}
\end{aligned}$$

$$a_4 = \frac{-h_1h_2h_3}{h_4(h_4 - h_3)(h_4 - h_2)(h_4 - h_1)}$$

and a_0:

$$\begin{aligned}
a_0 =& -\frac{h_2h_3h_4}{h_1(h_4 - h_1)(h_3 - h_1)(h_2 - h_1)} + \frac{h_1h_3h_4}{h_2(h_4 - h_2)(h_3 - h_2)(h_2 - h_1)}\\
&- \frac{h_1h_2h_4}{h_3(h_4 - h_3)(h_3 - h_2)(h_3 - h_1)} + \frac{h_1h_2h_3}{h_4(h_4 - h_3)(h_4 - h_2)(h_4 - h_1)}
\end{aligned}$$

This finally gives the forward difference approximation for the first derivative:

$$\phi_i' = a_0\phi_i + a_1\phi_{i+1} + a_2\phi_{i+2} + a_3\phi_{i+3} + a_4\phi_{i+4}$$

Central difference - interior

THe central difference taylor series formulation:

$$\phi_{i+1} = \phi_i + h_i\phi' + \frac{h_i^2}{2}\phi_i'' + \frac{h_i^3}{3!}\phi_i''' + \frac{h_i^4}{4!}\phi_i^{(4)} + \xi_{i+1}$$
$$\phi_{i-1} = \phi_i - h_{i-1}\phi' + \frac{h_{i-1}^2}{2}\phi_i'' - \frac{h_{i-1}^3}{3!}\phi_i''' + \frac{h_{i-1}^4}{4!}\phi_i^{(4)} + \xi_{i-1}$$
$$\phi_{i+2} = \phi_i + (h_i + h_{i+1})\phi' + \frac{(h_i + h_{i+1})^2}{2}\phi_i'' + \frac{(h_i + h_{i+1})^3}{3!}\phi_i''' + \frac{(h_i + h_{i+1})^4}{4!}\phi_i^{(4)} + \xi_{i+2}$$
$$\phi_{i-2} = \phi_i - (h_{i-1} - h_{i-2})\phi' + \frac{(h_{i-1} + h_{i-2})^2}{2}\phi_i'' - \frac{(h_{i-1} + h_{i-2})^3}{3!}\phi_i''' + \frac{(h_{i-1} + h_{i-2})^4}{4!}\phi_i^{(4)} + \xi_{i-2}$$

Rewrite as:

$$\begin{aligned}
\phi_{i+1} &= \phi_i + h_1\phi' + \frac{h_1^2}{2}\phi_i'' + \frac{h_1^3}{3!}\phi_i''' + \frac{h_1^4}{4!}\phi_i^{(4)} + \xi_{i+1} \\
\phi_{i-1} &= \phi_i - h_{-1}\phi' + \frac{h_{-1}^2}{2}\phi_i'' - \frac{h_{-1}^3}{3!}\phi_i''' + \frac{h_{-1}^4}{4!}\phi_i^{(4)} + \xi_{i-1} \\
\phi_{i+2} &= \phi_i + h_2\phi' + \frac{h_2^2}{2}\phi_i'' + \frac{h_2^3}{3!}\phi_i''' + \frac{h_2^4}{4!}\phi_i^{(4)} + \xi_{i+2} \\
\phi_{i-2} &= \phi_i - h_{-2}\phi' + \frac{h_{-2}^2}{2}\phi_i'' - \frac{h_{-2}^3}{3!}\phi_i''' + \frac{h_{-2}^4}{4!}\phi_i^{(4)} + \xi_{i-2}
\end{aligned}$$

$$\begin{bmatrix} 24h_1 & 12h_1^2 & 4h_1^3 & h_1^4 \\ -24h_{-1} & 12h_{-1}^2 & -4h_{-1}^3 & h_{-1}^4 \\ 24h_2 & 12h_2^2 & 4h_2^3 & h_2^4 \\ -24h_{-2} & 12h_{-2}^2 & -4h_{-2}^3 & h_{-2}^4 \end{bmatrix} \begin{bmatrix} \phi_i' \\ \phi_i'' \\ \phi_i''' \\ \phi_i^{(4)} \end{bmatrix} = \begin{bmatrix} 24(\phi_{i+1} - \phi_i) \\ 24(\phi_{i-1} - \phi_i) \\ 24(\phi_{i+2} - \phi_i) \\ 24(\phi_{i-2} - \phi_i) \end{bmatrix}$$

This is the same form as the previous section, where we got:

$$\phi_i' = \frac{\begin{array}{c} e(g(pv - qu) - k(ov - qt) + l(ou - pt)) - m(b(pv - qu) - c(ov - qt) + d(ou - pt)) \\ + r(b(kv - lu) - c(gv - lt) + d(gu - kt)) - w(b(kq - lp) - c(gq - lo) + d(gp - ko)) \end{array}}{\begin{array}{c} a(g(pv - qu) - k(ov - qt) + l(ou - pt)) - f(b(pv - qu) - c(ov - qt) + d(ou - pt)) \\ + n(b(kv - lu) - c(gv - lt) + d(gu - kt)) - s(b(kq - lp) - c(gq - lo) + d(gp - ko)) \end{array}}$$

Here, however, the substitutions are:

$$\begin{aligned}
a &= h_1 & b &= h_1^2 & c &= h_1^3 & d &= h_1^4 \\
f &= -h_{-1} & g &= h_{-1}^2 & k &= -h_{-1}^3 & l &= h_{-1}^4 \\
n &= h_2 & o &= h_2^2 & p &= h_2^3 & q &= h_2^4 \\
s &= -h_{-2} & t &= h_{-2}^2 & u &= -h_{-2}^3 & v &= h_{-2}^4
\end{aligned}$$

Let's deal with the denominator first:

$$a(g(pv-qu)-k(ov-qt)+l(ou-pt))-f(b(pv-qu)-c(ov-qt)+d(ou-pt))$$
$$+n(b(kv-lu)-c(gv-lt)+d(gu-kt))-s(b(kq-lp)-c(gq-lo)+d(gp-ko))$$
$$=$$
$$h_1(h_{-1}^2(h_2^3h_{-2}^4+h_2^4h_{-2}^3)+h_{-1}^3(h_2^2h_{-2}^4-h_2^4h_{-2}^2)-h_{-1}^4(h_2^2h_{-2}^3+h_2^3h_{-2}^2))$$
$$+h_{-1}(h_1^2(h_2^3h_{-2}^4+h_2^4h_{-2}^3)-h_1^3(h_2^2h_{-2}^4-h_2^4h_{-2}^2)-h_1^4(h_2^2h_{-2}^3+h_2^3h_{-2}^2))$$
$$+h_2(h_1^2(h_{-1}^4h_{-2}^3-h_{-1}^3h_{-2}^4)-h_1^3(h_{-1}^2h_{-2}^4-h_{-1}^4h_{-2}^2)+h_1^4(h_{-1}^3h_{-2}^2-h_{-1}^2h_{-2}^3))$$
$$+h_{-2}(-h_1^2(h_{-1}^3h_2^4+h_{-1}^4h_2^3)-h_1^3(h_{-1}^2h_2^4-h_{-1}^4h_2^2)+h_1^4(h_{-1}^2h_2^3+h_{-1}^3h_2^2))$$

Simplify one addend at a time.

First addend:

$$h_1(h_{-1}^2(h_2^3h_{-2}^4+h_2^4h_{-2}^3)+h_{-1}^3(h_2^2h_{-2}^4-h_2^4h_{-2}^2)-h_{-1}^4(h_2^2h_{-2}^3+h_2^3h_{-2}^2))$$
$$h_1h_{-1}^2((h_2^3h_{-2}^4+h_2^4h_{-2}^3)+h_{-1}(h_2^2h_{-2}^4-h_2^4h_{-2}^2)-h_{-1}^2(h_2^2h_{-2}^3+h_2^3h_{-2}^2))$$
$$h_2^2h_1h_{-1}^2h_{-2}^2((h_2h_{-2}^2+h_2^2h_{-2})+h_{-1}(h_{-2}^2-h_2^2)-h_{-1}^2(h_{-2}+h_2))$$
$$h_2^2h_1h_{-1}^2h_{-2}^2(h_2h_{-2}(h_{-2}+h_2)+h_{-1}(h_{-2}-h_2)(h_{-2}+h_2)-h_{-1}^2(h_{-2}+h_2))$$
$$h_2^2h_1h_{-1}^2h_{-2}^2(h_{-2}+h_2)(h_2h_{-2}+h_{-1}(h_{-2}-h_2)-h_{-1}^2)$$
$$h_2^2h_1h_{-1}^2h_{-2}^2(h_2+h_{-2})(h_2+h_{-1})(h_{-2}-h_{-1})$$

Second addend:

$$+h_{-1}(h_1^2(h_2^3h_{-2}^4+h_2^4h_{-2}^3)-h_1^3(h_2^2h_{-2}^4-h_2^4h_{-2}^2)-h_1^4(h_2^2h_{-2}^3+h_2^3h_{-2}^2))$$
$$+h_{-1}h_1^2h_2^2h_{-2}^2(h_2h_{-2}^2+h_2^2h_{-2}-h_1(h_{-2}^2-h_2^2)-h_1^2(h_{-2}+h_2))$$
$$+h_{-1}h_1^2h_2^2h_{-2}^2(h_2h_{-2}(h_{-2}+h_2)-h_1(h_{-2}-h_2)(h_{-2}+h_2)-h_1^2(h_{-2}+h_2))$$
$$+h_{-1}h_1^2h_2^2h_{-2}^2(h_{-2}+h_2)(h_2h_{-2}-h_1(h_{-2}-h_2)-h_1^2)$$
$$+h_{-1}h_1^2h_2^2h_{-2}^2(h_{-2}+h_2)(h_{-2}(h_2-h_1)+h_1(h_2-h_1))$$
$$+h_{-1}h_1^2h_2^2h_{-2}^2(h_{-2}+h_2)(h_2-h_1)(h_{-2}+h_1)$$

Third addend:

$$+h_2(h_1^2(h_{-1}^4h_{-2}^3-h_{-1}^3h_{-2}^4)-h_1^3(h_{-1}^2h_{-2}^4-h_{-1}^4h_{-2}^2)+h_1^4(h_{-1}^3h_{-2}^2-h_{-1}^2h_{-2}^3))$$
$$+h_2h_1^2((h_{-1}^4h_{-2}^3-h_{-1}^3h_{-2}^4)-h_1(h_{-1}^2h_{-2}^4-h_{-1}^4h_{-2}^2)+h_1^2(h_{-1}^3h_{-2}^2-h_{-1}^2h_{-2}^3))$$
$$+h_2h_1^2h_{-1}^2h_{-2}^2(h_{-1}^2h_{-2}-h_{-1}h_{-2}^2-h_1(h_{-2}^2-h_{-1}^2)+h_1^2(h_{-1}-h_{-2}))$$
$$+h_2h_1^2h_{-1}^2h_{-2}^2(h_{-1}h_{-2}(h_{-1}-h_{-2})-h_1(h_{-2}-h_{-1})(h_{-2}+h_{-1})+h_1^2(h_{-1}-h_{-2}))$$
$$+h_2h_1^2h_{-1}^2h_{-2}^2(h_{-1}-h_{-2})(h_{-1}h_{-2}+h_1(h_{-2}+h_{-1})+h_1^2)$$
$$+h_2h_1^2h_{-1}^2h_{-2}^2(h_{-1}-h_{-2})(h_{-1}h_{-2}+h_1(h_{-2}+h_{-1})+h_1^2)$$
$$+h_2h_1^2h_{-1}^2h_{-2}^2(h_{-1}-h_{-2})(h_{-2}(h_{-1}+h_1)+h_1(h_{-1}+h_1))$$
$$+h_2h_1^2h_{-1}^2h_{-2}^2(h_{-1}-h_{-2})(h_{-1}+h_1)(h_{-2}+h_1)$$

Fourth addend:

$$+\,h_{-2}(-h_1^2(h_{-1}^3h_2^4 + h_{-1}^4h_2^3) - h_1^3(h_{-1}^2h_2^4 - h_{-1}^4h_2^2) + h_1^4(h_{-1}^2h_2^3 + h_{-1}^3h_2^2))$$
$$+\,h_{-2}h_1^2(-(h_{-1}^3h_2^4 + h_{-1}^4h_2^3) - h_1(h_{-1}^2h_2^4 - h_{-1}^4h_2^2) + h_1^2(h_{-1}^2h_2^3 + h_{-1}^3h_2^2))$$
$$+\,h_{-2}h_1^2h_{-1}^2h_2^2(-(h_{-1}h_2^2 + h_{-1}^2h_2) - h_1(h_2^2 - h_{-1}^2) + h_1^2(h_2 + h_{-1}))$$
$$+\,h_{-2}h_1^2h_{-1}^2h_2^2(-h_{-1}h_2(h_2 + h_{-1}) - h_1(h_2 - h_{-1})(h_2 + h_{-1}) + h_1^2(h_2 + h_{-1}))$$
$$+\,h_{-2}h_1^2h_{-1}^2h_2^2(h_2 + h_{-1})(-h_{-1}h_2 - h_1(h_2 - h_{-1}) + h_1^2)$$
$$+\,h_{-2}h_1^2h_{-1}^2h_2^2(h_2 + h_{-1})(-h_2(h_{-1} + h_1) + h_1(h_{-1} + h_1))$$
$$+\,h_{-2}h_1^2h_{-1}^2h_2^2(h_2 + h_{-1})(h_{-1} + h_1)(h_1 - h_2)$$

Common factor:

$$h_2h_1h_{-1}h_{-2}$$

First and second addend (common factor left out):

$$h_2h_{-1}h_{-2}(h_2 + h_{-2})(h_2 + h_{-1})(h_{-2} - h_{-1}) + h_1h_2h_{-2}(h_{-2} + h_2)(h_2 - h_1)(h_{-2} + h_1)$$
$$h_2h_{-2}(h_2 + h_{-2})(h_{-1}(h_2 + h_{-1})(h_{-2} - h_{-1}) + h_1(h_2 - h_1)(h_{-2} + h_1))$$
$$h_2h_{-2}(h_2 + h_{-2})(h_{-1}(h_2 + h_{-1})(h_{-2} - h_{-1}) + h_1(h_2 - h_1)(h_{-2} + h_1))$$
$$h_2h_{-2}(h_2 + h_{-2})(h_2h_{-1}h_{-2} - h_2h_{-1}^2 + h_{-2}h_{-1}^2 - h_{-1}^3 + h_2h_1h_{-2} + h_2h_1^2 - h_1^2h_{-2} - h_1^3)$$
$$h_2h_{-2}(h_2 + h_{-2})(h_2h_{-2}(h_{-1} + h_1) + h_2(h_1^2 - h_{-1}^2) + h_{-2}(h_{-1}^2 - h_1^2) - (h_{-1}^3 + h_1^3))$$
$$h_2h_{-2}(h_2 + h_{-2})((h_{-1} + h_1)(h_2h_{-2} + h_2(h_1 - h_{-1}) + h_{-2}(h_{-1} - h_1)) - (h_{-1} + h_1)(h_{-1}^2 - h_{-1}h_1 +$$
$$h_2h_{-2}(h_2 + h_{-2})(h_{-1} + h_1)(h_2h_{-2} + h_2(h_1 - h_{-1}) + h_{-2}(h_{-1} - h_1) - h_{-1}^2 + h_{-1}h_1 - h_1^2)$$
$$h_2h_{-2}(h_2 + h_{-2})(h_{-1} + h_1)(h_2h_{-2} + h_2(h_1 - h_{-1}) + h_{-2}(h_{-1} - h_1) - h_{-1}^2 - h_1^2 + h_{-1}h_1)$$
$$h_2h_{-2}(h_2 + h_{-2})(h_{-1} + h_1)(h_2h_{-2} + h_2(h_1 - h_{-1}) - h_{-2}(h_1 - h_{-1}) - (h_1 - h_{-1})^2 - h_1h_{-1})$$
$$h_2h_{-2}(h_2 + h_{-2})(h_{-1} + h_1)(h_2h_{-2} - h_1h_{-1} + (h_1 - h_{-1})(h_2 - h_{-2} - h_1 + h_{-1}))$$

Third and fourth addend (common factor left out):

$$h_1h_{-1}h_{-2}(h_{-1} - h_{-2})(h_{-1} + h_1)(h_{-2} + h_1) + h_1h_{-1}h_2(h_2 + h_{-1})(h_{-1} + h_1)(h_1 - h_2)$$
$$h_1h_{-1}(h_{-1} + h_1)(h_{-2}(h_{-1} - h_{-2})(h_{-2} + h_1) + h_2(h_2 + h_{-1})(h_1 - h_2))$$
$$h_1h_{-1}(h_{-1} + h_1)(h_{-1}h_{-2}^2 + h_1h_{-1}h_{-2} - h_{-2}^3 - h_1h_{-2}^2 + h_2h_1h_{-1} - h_2^2h_{-1} + h_1h_2^2 - h_2^3)$$
$$h_1h_{-1}(h_{-1} + h_1)(-h_{-1}(h_2^2 - h_{-2}^2) + h_1(h_2^2 - h_{-2}^2) + h_1h_{-1}(h_2 + h_{-2}) - (h_2^3 + h_{-2}^3))$$
$$h_1h_{-1}(h_{-1} + h_1)(-h_{-1}(h_2 - h_{-2})(h_2 + h_{-2}) + h_1(h_2 - h_{-2})(h_2 + h_{-2})$$
$$\quad + h_1h_{-1}(h_2 + h_{-2}) - (h_2 + h_{-2})(h_2^2 + h_{-2}^2 - h_2h_{-2}))$$
$$h_1h_{-1}(h_{-1} + h_1)(h_2 + h_{-2})(-h_{-1}(h_2 - h_{-2}) + h_1(h_2 - h_{-2}) + h_1h_{-1} - h_2^2 - h_{-2}^2 + h_2h_{-2})$$
$$h_1h_{-1}(h_{-1} + h_1)(h_2 + h_{-2})(-h_{-1}(h_2 - h_{-2}) + h_1(h_2 - h_{-2}) + h_1h_{-1} - (h_2 - h_{-2})^2 - h_2h_{-2})$$
$$h_1h_{-1}(h_{-1} + h_1)(h_2 + h_{-2})(-h_{-1}(h_2 - h_{-2}) + h_1(h_2 - h_{-2}) + h_1h_{-1} - (h_2 - h_{-2})^2 - h_2h_{-2})$$
$$h_1h_{-1}(h_{-1} + h_1)(h_2 + h_{-2})(h_1h_{-1} - h_2h_{-2} + (h_2 - h_{-2})(-h_{-1} + h_1 - h_2 + h_{-2})$$

Common factor (total expression):

$$h_2 h_1 h_{-1} h_{-2} (h_{-1} + h_1)(h_2 + h_{-2})$$

Factorize further, without common factor

$$h_2h_{-2}(h_2h_{-2} - h_1h_{-1} + (h_1 - h_{-1})(h_2 - h_{-2} - h_1 + h_{-1})) + h_1h_{-1}(h_1h_{-1} - h_2h_{-2} + (h_2 - h_{-2})(-h_{-1} + h_1 - h_2 + h_{-2}))$$

$$h_2^2h_{-2}^2 - h_2h_{-2}h_1h_{-1} + h_2h_{-2}(h_1 - h_{-1})(h_2 - h_{-2} - h_1 + h_{-1}) + h_1^2h_{-1}^2 - h_1h_{-1}h_2h_{-2} + h_1h_{-1}(h_2 - h_{-2})(-h_{-1} + h_1 - h_2 + h_{-2})$$

$$h_2h_{-2}(h_1 - h_{-1})(h_2 - h_{-2} - h_1 + h_{-1}) + h_1h_{-1}(h_2 - h_{-2})(-h_{-1} + h_1 - h_2 + h_{-2}) + h_2^2h_{-2}^2 + h_1^2h_{-1}^2 - 2h_1h_{-1}h_2h_{-2}$$

$$h_2h_{-2}(h_2h_1 - h_1h_{-2} - h_1^2 + h_1h_{-1} - h_2h_{-1} + h_{-1}h_{-2} + h_1h_{-1} - h_{-1}^2)$$
$$\quad + h_1h_{-1}(-h_2h_{-1} + h_2h_1 - h_2^2 + h_2h_{-2} + h_{-1}h_{-2} - h_1h_{-2} + h_2h_{-2} - h_{-2}^2) + h_2^2h_{-2}^2 + h_1^2h_{-1}^2 - 2h_1h_{-1}h_2h_{-2}$$

$$h_2^2h_1h_{-2} - h_2h_1h_{-2}^2 - h_2h_1^2h_{-2} + h_2h_1h_{-1}h_{-2} - h_2^2h_{-1}h_{-2} + h_2h_{-1}h_{-2}^2 + h_2h_1h_{-1}h_{-2} - h_2h_{-1}^2h_{-2}$$
$$\quad - h_2h_1h_{-1}^2 + h_2h_1^2h_{-1} - h_2^2h_1h_{-1} + h_2h_{-2}h_1h_{-1} + h_1h_{-1}^2h_{-2} - h_1^2h_{-1}h_{-2} + h_2h_1h_{-1}h_{-2} - h_1h_{-1}h_{-2}^2 + h_2^2h_{-2}^2 + h_1^2h_{-1}^2 - 2h_1h_{-1}h_2h_{-2}$$

$$h_2^2h_1h_{-2} - h_2h_1h_{-2}^2 - h_2h_1^2h_{-2} - h_2^2h_{-1}h_{-2} + h_2h_{-1}h_{-2}^2 - h_2h_{-1}^2h_{-2}$$
$$\quad - h_2h_1h_{-1}^2 + h_2h_1^2h_{-1} - h_2^2h_1h_{-1} + h_1h_{-1}^2h_{-2} - h_1^2h_{-1}h_{-2} - h_1h_{-1}h_{-2}^2 + h_2^2h_{-2}^2 + h_1^2h_{-1}^2 + 2h_1h_{-1}h_2h_{-2}$$

$$h_2^2(h_1h_{-2} - h_{-1}h_{-2} - h_1h_{-1}) + h_{-2}^2(h_2h_{-1} - h_2h_1 - h_1h_{-1}) + h_1^2(h_2h_{-1} - h_2h_{-2} - h_{-1}h_{-2})$$
$$\quad + h_{-1}^2(h_1h_{-2} - h_2h_{-2} - h_2h_1) + h_2^2h_{-2}^2 + h_1^2h_{-1}^2 + 2h_1h_{-1}h_2h_{-2}$$

$$h_2^2(h_1(h_{-2} - h_{-1}) - h_{-1}h_{-2}) + h_{-2}^2(h_{-1}(h_2 - h_1) - h_2h_1) + h_1^2(-h_2(h_{-2} - h_{-1}) - h_{-1}h_{-2})$$
$$\quad + h_{-1}^2(-h_{-2}(h_2 - h_1) - h_2h_1) + h_2^2h_{-2}^2 + h_1^2h_{-1}^2 + 2h_1h_{-1}h_2h_{-2}$$

$$h_2^2h_1(h_{-2} - h_{-1}) - h_2^2h_{-1}h_{-2} + h_{-1}h_{-2}^2(h_2 - h_1) - h_2h_1h_{-2}^2 - h_2h_1^2(h_{-2} - h_{-1}) - h_1^2h_{-1}h_{-2}$$
$$\quad - h_{-1}^2h_{-2}(h_2 - h_1) - h_2h_1h_{-1}^2 + h_2^2h_{-2}^2 + h_1^2h_{-1}^2 + 2h_1h_{-1}h_2h_{-2}$$

$$
\begin{aligned}
&(h_{-2}-h_{-1})(h_2^2h_1-h_2h_1^2)+(h_2-h_1)(h_{-1}h_{-2}^2-h_{-1}^2h_{-2})-h_2h_1h_{-2}^2-h_1^2h_{-1}h_{-2}\\
&\quad -h_2h_1h_{-1}^2-h_2^2h_{-1}h_{-2}+h_2^2h_{-2}^2+h_1^2h_{-1}^2+2h_1h_{-1}h_2h_{-2}
\end{aligned}
$$

$$
\begin{aligned}
&(h_{-2}-h_{-1})(h_2h_1(h_2-h_1))+(h_2-h_1)(h_{-1}h_{-2}(h_{-2}-h_{-1}))-h_2h_1h_{-2}^2-h_1^2h_{-1}h_{-2}\\
&\quad -h_2h_1h_{-1}^2-h_2^2h_{-1}h_{-2}+h_2^2h_{-2}^2+h_1^2h_{-1}^2+2h_1h_{-1}h_2h_{-2}
\end{aligned}
$$

$$
\begin{aligned}
&(h_{-2}-h_{-1})(h_2-h_1)(h_2h_1+h_{-1}h_{-2})-h_2h_1h_{-2}^2-h_1^2h_{-1}h_{-2}\\
&\quad -h_2h_1h_{-1}^2-h_2^2h_{-1}h_{-2}+h_2^2h_{-2}^2+h_1^2h_{-1}^2+2h_1h_{-1}h_2h_{-2}\\
&(h_{-2}-h_{-1})(h_2-h_1)(h_2h_1+h_{-1}h_{-2})-h_2h_1h_{-2}^2-h_1^2h_{-1}h_{-2}-h_2h_1h_{-1}^2-h_2^2h_{-1}h_{-2}+h_2^2h_{-2}^2+h_1^2h_{-1}^2+2h_1h_{-1}h_2h_{-2}\\
&(h_{-2}-h_{-1})(h_2-h_1)(h_2h_1+h_{-1}h_{-2})-h_2h_{-2}(h_1h_{-2}-h_2h_{-2})-h_{-1}(h_1^2h_{-2}-h_1^2h_{-1}+h_2h_1h_{-1}+h_2^2h_{-2}-2h_1h_2h_{-2})\\
&(h_{-2}-h_{-1})(h_2-h_1)(h_2h_1+h_{-1}h_{-2})+h_2h_{-2}(h_{-2}(h_2-h_1))-h_{-1}(h_1^2h_{-2}-h_1^2h_{-1}+h_2h_1h_{-1}+h_2^2h_{-2}-2h_1h_2h_{-2})\\
&(h_{-2}-h_{-1})(h_2-h_1)(h_2h_1+h_{-1}h_{-2})+h_2h_{-2}(h_{-2}(h_2-h_1))-h_{-1}(h_{-2}(h_1^2+h_2^2-2h_1h_2)-h_1h_{-1}(h_1-h_2))\\
&(h_{-2}-h_{-1})(h_2-h_1)(h_2h_1+h_{-1}h_{-2})+h_2h_{-2}(h_{-2}(h_2-h_1))-h_{-1}(h_{-2}(h_2-h_1)^2+h_1h_{-1}(h_2-h_1))\\
&(h_{-2}-h_{-1})(h_2-h_1)(h_2h_1+h_{-1}h_{-2})+(h_2-h_1)(h_2h_{-2}^2)-h_{-1}h_{-2}(h_2-h_1)^2-h_1h_{-1}^2(h_2-h_1))\\
&(h_{-2}-h_{-1})(h_2-h_1)(h_2h_1+h_{-1}h_{-2})+(h_2-h_1)(h_2h_{-2}^2-h_{-1}h_{-2}(h_2-h_1)-h_1h_{-1}^2)\\
&(h_{-2}-h_{-1})(h_2-h_1)(h_2h_1+h_{-1}h_{-2})+(h_2-h_1)(h_2h_{-2}^2-h_2h_{-1}h_{-2}+h_1h_{-1}h_{-2}-h_1h_{-1}^2)\\
&(h_{-2}-h_{-1})(h_2-h_1)(h_2h_1+h_{-1}h_{-2})+(h_2-h_1)(h_2h_{-2}(h_{-2}-h_{-1})+h_1h_{-1}(h_{-2}-h_{-1}))\\
&(h_{-2}-h_{-1})(h_2-h_1)(h_2h_1+h_{-1}h_{-2})+(h_2-h_1)(h_{-2}-h_{-1})(h_2h_{-2}+h_1h_{-1})\\
&(h_{-2}-h_{-1})(h_2-h_1)(h_2h_1+h_{-1}h_{-2}+h_2h_{-2}+h_1h_{-1})\\
&(h_{-2}-h_{-1})(h_2-h_1)(h_2h_1+h_{-1}h_{-2}+h_2h_{-2}+h_1h_{-1})\\
&(h_{-2}-h_{-1})(h_2-h_1)(h_1(h_2+h_{-1})+h_{-2}(h_2+h_{-1}))\\
&(h_{-2}-h_{-1})(h_2-h_1)(h_2+h_{-1})(h_1+h_{-2})
\end{aligned}
$$

Factorized denominator:

$$h_2 h_1 h_{-1} h_{-2}(h_{-1}+h_1)(h_2+h_{-2})(h_{-2}-h_{-1})(h_2-h_1)(h_2+h_{-1})(h_1+h_{-2})$$

Now for the numerator.

$$\begin{aligned} e(g(pv-qu)-k(ov-qt)+l(ou-pt))\\ -m(b(pv-qu)-c(ov-qt)+d(ou-pt))\\ +r(b(kv-lu)-c(gv-lt)+d(gu-kt))\\ -w(b(kq-lp)-c(gq-lo)+d(gp-ko)) \end{aligned}$$

Substitutions:

$$\begin{aligned} b &= h_1^2 & c &= h_1^3 & d &= h_1^4 & e &= (\phi_{i+1}-\phi_i)\\ g &= h_{-1}^2 & k &= -h_{-1}^3 & l &= h_{-1}^4 & m &= (\phi_{i-1}-\phi_i)\\ o &= h_2^2 & p &= h_2^3 & q &= h_2^4 & r &= (\phi_{i+2}-\phi_i)\\ t &= h_{-2}^2 & u &= -h_{-2}^3 & v &= h_{-2}^4 & w &= (\phi_{i-2}-\phi_i) \end{aligned}$$

$$\begin{aligned} &(\phi_{i+1}-\phi_i)(h_{-1}^2(h_2^3h_{-2}^4+h_2^4h_{-2}^3)+h_{-1}^3(h_2^2h_{-2}^4-h_2^4h_{-2}^2)-h_{-1}^4(h_2^2h_{-2}^3+h_2^3h_{-2}^2))\\ &\quad-(\phi_{i-1}-\phi_i)(h_1^2(h_2^3h_{-2}^4+h_2^4h_{-2}^3)-h_1^3(h_2^2h_{-2}^4-h_2^4h_{-2}^2)-h_1^4(h_2^2h_{-2}^3+h_2^3h_{-2}^2))\\ &\quad+(\phi_{i+2}-\phi_i)(h_1^2(-h_{-1}^3h_{-2}^4+h_{-1}^4h_{-2}^3)-h_1^3(h_{-1}^2h_{-2}^4-h_{-1}^4h_{-2}^2)+h_1^4(-h_{-1}^2h_{-2}^3+h_{-1}^3h_{-2}^2))\\ &\quad-(\phi_{i-2}-\phi_i)(h_1^2(-h_{-1}^3h_2^4-h_{-1}^4h_2^3)-h_1^3(h_{-1}^2h_2^4-h_{-1}^4h_2^2)+h_1^4(h_{-1}^2h_2^3+h_{-1}^3h_2^2)) \end{aligned}$$

We can now see what the finite difference coefficients will be:

$$
\begin{aligned}
a_1' =&\\
&h_{-1}^2(h_2^3h_{-2}^4 + h_2^4h_{-2}^3) + h_{-1}^3(h_2^2h_{-2}^4 - h_2^4h_{-2}^2) - h_{-1}^4(h_2^2h_{-2}^3 + h_2^3h_{-2}^2)\\
&h_2^2h_{-1}^2h_{-2}^2(h_2h_{-2}^2 + h_2^2h_{-2} + h_{-1}(h_{-2}^2 - h_2^2) - h_{-1}^2(h_{-2} + h_2))\\
&h_2^2h_{-1}^2h_{-2}^2(h_2h_{-2}(h_{-2} + h_2) + h_{-1}(h_{-2} - h_2)(h_{-2} + h_3) - h_{-1}^2(h_{-2} + h_2))\\
&h_2^2h_{-1}^2h_{-2}^2(h_{-2} + h_2)(h_2h_{-2} + h_{-1}(h_{-2} - h_2) - h_{-1}^2)\\
&h_2^2h_{-1}^2h_{-2}^2(h_{-2} + h_2)(h_{-2}(h_2 + h_{-1}) - h_{-1}(h_2 + h_{-1}))\\
&h_2^2h_{-1}^2h_{-2}^2(h_{-2} + h_2)(h_2 + h_{-1})(h_{-2} - h_{-1})\\
a_1 =&\frac{h_2^2h_{-1}^2h_{-2}^2(h_{-2} + h_2)(h_2 + h_{-1})(h_{-2} - h_{-1})}{h_2h_1h_{-1}h_{-2}(h_{-1} + h_1)(h_2 + h_{-2})(h_{-2} - h_{-1})(h_2 - h_1)(h_2 + h_{-1})(h_1 + h_{-2})}\\
a_1 =&\frac{h_2h_{-1}h_{-2}}{h_1(h_{-1} + h_1)(h_2 - h_1)(h_1 + h_{-2})}
\end{aligned}
$$

$$
\begin{aligned}
a_{-1}' =&\\
&-h_1^2(h_2^3h_{-2}^4 + h_2^4h_{-2}^3) + h_1^3(h_2^2h_{-2}^4 - h_2^4h_{-2}^2) + h_1^4(h_2^2h_{-2}^3 + h_2^3h_{-2}^2))\\
&h_2^2h_1^2h_{-2}^2(-h_2h_{-2}^2 - h_2^2h_{-2} + h_1(h_{-2}^2 - h_2^2) + h_1^2(h_{-2} + h_2))\\
&h_2^2h_1^2h_{-2}^2(-h_2h_{-2}^2 - h_2^2h_{-2} + h_1(h_{-2}^2 - h_2^2) + h_1^2(h_{-2} + h_2))\\
&h_2^2h_1^2h_{-2}^2(-h_2h_{-2}(h_{-2} + h_2) + h_1(h_{-2} - h_2)(h_{-2} + h_2) + h_1^2(h_{-2} + h_2))\\
&h_2^2h_1^2h_{-2}^2(h_{-2} + h_2)(-h_2h_{-2} + h_1(h_{-2} - h_2) + h_1^2)\\
&h_2^2h_1^2h_{-2}^2(h_{-2} + h_2)(-h_{-2}(h_2 - h_1) - h_1(h_2 - h_1))\\
&-h_2^2h_1^2h_{-2}^2(h_{-2} + h_2)(h_2 - h_1)(h_{-2} + h_1)\\
a_{-1} =&-\frac{h_2^2h_1^2h_{-2}^2(h_{-2} + h_2)(h_2 - h_1)(h_{-2} + h_1)}{h_2h_1h_{-1}h_{-2}(h_{-1} + h_1)(h_2 + h_{-2})(h_{-2} - h_{-1})(h_2 - h_1)(h_2 + h_{-1})(h_1 + h_{-2})}
\end{aligned}
$$

$$
a_{-1} = -\frac{h_2h_1h_{-2}}{h_{-1}(h_{-1} + h_1)(h_{-2} - h_{-1})(h_2 + h_{-1})}
$$

$$
\begin{aligned}
a_2' =&\\
&(h_1^2(-h_{-1}^3h_{-2}^4 + h_{-1}^4h_{-2}^3) - h_1^3(h_{-1}^2h_{-2}^4 - h_{-1}^4h_{-2}^2) + h_1^4(-h_{-1}^2h_{-2}^3 + h_{-1}^3h_{-2}^2))\\
&h_1^2h_{-1}^2h_{-2}^2(-h_{-1}h_{-2}(h_{-2} - h_{-1}) - h_1(h_{-2}^2 - h_{-1}^2) + h_1^2(-h_{-2} + h_{-1}))\\
&h_1^2h_{-1}^2h_{-2}^2(-h_{-1}h_{-2}(h_{-2} - h_{-1}) - h_1(h_{-2} - h_{-1})(h_{-2} + h_{-1}) - h_1^2(h_{-2} - h_{-1}))\\
&h_1^2h_{-1}^2h_{-2}^2(h_{-2} - h_{-1})(-h_{-1}h_{-2} - h_1(h_{-2} + h_{-1}) - h_1^2)\\
&h_1^2h_{-1}^2h_{-2}^2(h_{-2} - h_{-1})(-h_{-2}(h_{-1} + h_1) - h_1(h_{-1} + h_1))\\
&-h_1^2h_{-1}^2h_{-2}^2(h_{-2} - h_{-1})(h_{-1} + h_1)(h_{-2} + h_1)\\
a_2 =&-\frac{h_1^2h_{-1}^2h_{-2}^2(h_{-2} - h_{-1})(h_{-1} + h_1)(h_{-2} + h_1)}{h_2h_1h_{-1}h_{-2}(h_{-1} + h_1)(h_2 + h_{-2})(h_{-2} - h_{-1})(h_2 - h_1)(h_2 + h_{-1})(h_1 + h_{-2})}\\
a_2 =&-\frac{h_1h_{-1}h_{-2}}{h_2(h_2 + h_{-2})(h_2 - h_1)(h_2 + h_{-1})}
\end{aligned}
$$

$$
\begin{aligned}
a_{-2} =& \\
&-(-h_1^2(h_{-1}^3h_2^4 + h_{-1}^4h_2^3) - h_1^3(h_{-1}^2h_2^4 - h_{-1}^4h_2^2) + h_1^4(h_{-1}^2h_2^3 + h_{-1}^3h_2^2)) \\
&h_1^2(h_{-1}^3h_2^4 + h_{-1}^4h_2^3 + h_1(h_{-1}^2h_2^4 - h_{-1}^4h_2^2) - h_1^2(h_{-1}^2h_2^3 + h_{-1}^3h_2^2)) \\
&h_1^2h_{-1}^2h_2^2(h_{-1}h_2^2 + h_{-1}^2h_2 + h_1(h_2^2 - h_{-1}^2) - h_1^2(h_2 + h_{-1})) \\
&h_1^2h_{-1}^2h_2^2(h_{-1}h_2(h_2 + h_{-1}) + h_1(h_2 - h_{-1})(h_2 + h_{-1}) - h_1^2(h_2 + h_{-1})) \\
&h_1^2h_{-1}^2h_2^2(h_2 + h_{-1})(h_2(h_{-1} + h_1) + h_1(-h_{-1}) - h_1^2) \\
&h_1^2h_{-1}^2h_2^2(h_2 + h_{-1})(h_{-1} + h_1)(h_2 - h_1) \\
a_{-2} =& \frac{h_1^2h_{-1}^2h_2^2(h_2 + h_{-1})(h_{-1} + h_1)(h_2 - h_1)}{h_2h_1h_{-1}h_{-2}(h_{-1} + h_1)(h_2 + h_{-2})(h_{-2} - h_{-1})(h_2 - h_1)(h_2 + h_{-1})(h_1 + h_{-2})} \\
a_{-2} =& \frac{h_1h_{-1}h_2}{h_{-2}(h_2 + h_{-2})(h_{-2} - h_{-1})(h_1 + h_{-2})}
\end{aligned}
$$

$$
a_0 = -(a_{-2} + a_{-1} + a_1 + a_2)
$$

A.2.2 FD approximations of 2nd derivative

Central difference, interior points

$$
\begin{aligned}
\phi_{i+1} =& \phi_i + h_i\phi_i' + \frac{h_i^2}{2}\phi_i'' + \frac{h_i^3}{3!}\phi_i''' + \mathcal{O}(h^4) \\
\phi_{i-1} =& \phi_i - h_{i-1}\phi_i' + \frac{h_{i-1}^2}{2}\phi_i'' - \frac{h_{i-1}^3}{3!}\phi_i''' + \mathcal{O}(h^4)
\end{aligned}
$$

Eliminate first derivative:

$$
\begin{aligned}
\phi_{i+1} + \frac{h_i}{h_{i-1}}\phi_{i-1} &= \phi_i\left(1 + \frac{h_i}{h_{i-1}}\right) + \phi_i''\left(\frac{h_i^2}{2} + \frac{h_i}{h_{i-1}}\frac{h_{i-1}^2}{2}\right) \\
&\quad + \phi_i'''\left(\frac{h_i^3}{3!} - \frac{h_i}{h_{i-1}}\frac{h_{i-1}^3}{3!}\right) + \mathcal{O}(h^4) \\
h_{i-1}\phi_{i+1} + h_i\phi_{i-1} &= \phi_i(h_{i-1} + h_i) + \phi_i''\left(\frac{h_{i-1}h_i^2 + h_ih_{i-1}^2}{2}\right) + \phi_i'''\left(\frac{h_{i-1}h_i^3 - h_ih_{i-1}^3}{3!}\right) + \mathcal{O}(h^5) \\
2h_{i-1}\phi_{i+1} + 2h_i\phi_{i-1} &= 2\phi_i(h_{i-1} + h_i) + \phi_i''\left(h_{i-1}h_i(h_i + h_{i-1})\right) + 2\phi_i'''\left(\frac{h_{i-1}h_i(h_i^2 - h_{i-1}^2)}{3!}\right) + \mathcal{O}(h^5) \\
\phi_i''\left(h_{i-1}h_i(h_i + h_{i-1})\right) &= 2\left(h_{i-1}\phi_{i+1} + h_i\phi_{i-1} - \phi_i(h_{i-1} + h_i)\right) - 2\phi_i'''\left(\frac{h_{i-1}h_i(h_i^2 - h_{i-1}^2)}{3!}\right) + \mathcal{O}(h^5) \\
\phi_i'' &= 2\left(\frac{h_{i-1}\phi_{i+1} + h_i\phi_{i-1} - \phi_i(h_{i-1} + h_i)}{h_{i-1}h_i(h_i + h_{i-1})}\right) - 2\phi_i'''\left(\frac{(h_i - h_{i-1})}{3!}\right) + \mathcal{O}(h^2))
\end{aligned}
$$

Second order accuracy for $h_i \approx h_{i-1}$. The $\mathcal{O}$-notation is sloppy in this instance; it kind of assumes approximately uniform grid.

$$\frac{1}{2}\phi_i'' = \frac{h_{i-1}\phi_{i+1} + h_i\phi_{i-1} - \phi_i(h_{i-1} + h_i)}{h_{i-1}h_i(h_i + h_{i-1})}$$
$$\frac{1}{2}\phi_i'' = \frac{h_{i-1}\phi_{i+1}}{h_{i-1}h_i(h_i + h_{i-1})} + \frac{h_i\phi_{i-1}}{h_{i-1}h_i(h_i + h_{i-1})} - \frac{-\phi_i(h_{i-1} + h_i)}{h_{i-1}h_i(h_i + h_{i-1})}$$
$$\frac{1}{2}\phi_i'' = \phi_{i+1}\frac{1}{h_i(h_i + h_{i-1})} + \phi_{i-1}\frac{1}{h_{i-1}(h_i + h_{i-1})} - \phi_i\left(\frac{1}{h_i(h_i + h_{i-1})} + \frac{1}{h_{i-1}(h_i + h_{i-1})}\right) \tag{A.2.6}$$

Forward/backwards difference, edges

$$\phi_{i+1} = \phi_i + h_i\phi_i' + \frac{h_i^2}{2}\phi_i'' + \frac{h_i^3}{3!}\phi_i''' + \mathcal{O}(h^4)$$
$$\phi_{i+2} = \phi_i + (h_i + h_{i+1})\phi_i' + \frac{(h_i + h_{i+1})^2}{2}\phi_i'' + \frac{(h_i + h_{i+1})^3}{3!}\phi_i''' + \mathcal{O}(h^4)$$

Eliminate third derivative:

$$\phi_{i+2} - \frac{(h_i+h_{i+1})^3}{h_i^3}\phi_{i+1} = \phi_i\left(1 - \frac{(h_i+h_{i+1})^3}{h_i^3}\right) + \phi_i'\left((h_i+h_{i+1}) - \frac{(h_i+h_{i+1})^3}{h_i^3}\right)$$
$$+ \frac{\phi_i''}{2}\left((h_i+h_{i+1})^2 - \frac{h_i^2(h_i+h_{i+1})^3}{h_i^3}\right) + \mathcal{O}(h^4)$$

$$h_i^3\phi_{i+2} - (h_i+h_{i+1})^3\phi_{i+1} = \phi_i\left(h_i^3 - (h_i+h_{i+1})^3\right) + \phi_i'\left(h_i^3(h_i+h_{i+1}) - (h_i+h_{i+1})^3\right)$$
$$+ \frac{\phi_i''}{2}\left(h_i^3(h_i+h_{i+1})^2 - h_i^2(h_i+h_{i+1})^3\right) + \mathcal{O}(h^7)$$

$$h_i^3\phi_{i+2} - (h_i+h_{i+1})^3\phi_{i+1} = \phi_i\left(h_i^3 - (h_i+h_{i+1})^3\right)$$
$$+ \phi_i'\left((h_i+h_{i+1})(h_i^3 - (h_i+h_{i+1})^2)\right) + \frac{\phi_i''}{2}\left((h_i+h_{i+1})^2h_i^2(h_i - (h_i+h_{i+1}))\right) + \mathcal{O}(h^7)$$

$$h_i^3\phi_{i+2} - (h_i+h_{i+1})^3\phi_{i+1} = \phi_i\left(h_i^3 - (h_i+h_{i+1})^3\right)$$
$$+ \phi_i'\left((h_i+h_{i+1})(h_i^3 - (h_i+h_{i+1})^2)\right) - \frac{\phi_i''}{2}\left((h_i+h_{i+1})^2h_i^2h_{i+1}\right) + \mathcal{O}(h^7)$$

$$\frac{\phi_i''}{2} - \phi_i'\left(\frac{(h_i+h_{i+1})(h_i^3 - (h_i+h_{i+1})^2)}{(h_i+h_{i+1})^2h_i^2h_{i+1}}\right) =$$
$$\phi_i\left(\frac{h_i^3 - (h_i+h_{i+1})^3}{(h_i+h_{i+1})^2h_i^2h_{i+1}}\right) + \phi_{i+1}\left(\frac{(h_i+h_{i+1})^3}{(h_i+h_{i+1})^2h_i^2h_{i+1}}\right)$$
$$- \phi_{i+2}\left(\frac{h_i^3}{(h_i+h_{i+1})^2h_i^2h_{i+1}}\right) + \mathcal{O}(h^2)$$

$$\frac{\phi_i''}{2} + \phi_i'\left(\frac{(h_i+h_{i+1})(h_i^3 - (h_i+h_{i+1})^2)}{(h_i+h_{i+1})^2h_i^2h_{i+1}}\right) =$$
$$+ \phi_i\left(\frac{h_i^3 - (h_i+h_{i+1})^3}{(h_i+h_{i+1})^2h_i^2h_{i+1}}\right) + \phi_{i+1}\left(\frac{h_i+h_{i+1}}{h_i^2h_{i+1}}\right)$$
$$- \phi_{i+2}\left(\frac{h_i}{(h_i+h_{i+1})^2h_{i+1}}\right) + \mathcal{O}(h^2)$$

For the Neumann boundary condition $\phi' = 0$, we have the following expression for the points on the edges:

$$\begin{aligned}\frac{\phi_i''}{2} &= \phi_i\left(\frac{h_i^3-(h_i+h_{i+1})^3}{(h_i+h_{i+1})^2h_i^2h_{i+1}}\right)+\phi_{i+1}\left(\frac{h_i+h_{i+1}}{h_i^2h_{i+1}}\right)\\ &-\phi_{i+2}\left(\frac{h_i}{(h_i+h_{i+1})^2h_{i+1}}\right)+\mathcal{O}(h^2)\end{aligned} \tag{A.2.7}$$

A second order forward difference approximation with no Neumann boundary condition have been useful earlier:

$$\begin{aligned}\phi_{i+1} =&\phi_i + h_i\phi_i' + \frac{h_i^2}{2}\phi_i'' + \frac{h_i^3}{3!}\phi_i''' + \mathcal{O}(h^4)\\ \phi_{i+2} =&\phi_i + (h_i+h_{i+1})\phi_i' + \frac{(h_i+h_{i+1})^2}{2}\phi_i'' + \frac{(h_i+h_{i+1})^3}{3!}\phi_i''' + \mathcal{O}(h^4)\\ \phi_{i+3} =&\phi_i + (h_i+h_{i+1}+h_{i+2})\phi_i' + \frac{(h_i+h_{i+1}+h_{i+2})^2}{2}\phi_i'' + \frac{(h_i+h_{i+1}+h_{i+2})^3}{3!}\phi_i''' + \mathcal{O}(h^4)\end{aligned}$$

Or:

$$\begin{aligned}\phi_{i+1} =&\phi_i + h_1\phi_i' + \frac{h_i^2}{2}\phi_i'' + \frac{h_1^3}{3!}\phi_i''' + \mathcal{O}(h^4)\\ \phi_{i+2} =&\phi_i + h_2\phi_i' + \frac{h_2^2}{2}\phi_i'' + \frac{h_2^3}{3!}\phi_i''' + \mathcal{O}(h^4)\\ \phi_{i+3} =&\phi_i + h_3\phi_i' + \frac{h_3^2}{2}\phi_i'' + \frac{h_3^3}{3!}\phi_i''' + \mathcal{O}(h^4)\end{aligned}$$

This constitutes the linear system:

$$\begin{bmatrix}6h_1 & 3h_1^2 & h_1^3\\ 6h_2 & 3h_2^2 & h_2^3\\ 6h_3 & 3h_3^2 & h_3^3\end{bmatrix}\begin{bmatrix}\phi_i'\\ \phi_i''\\ \phi_i'''\end{bmatrix} = \begin{bmatrix}6(\phi_{i+1}-\phi_i)\\ 6(\phi_{i+2}-\phi_i)\\ 6(\phi_{i+3}-\phi_i)\end{bmatrix}$$

Make some substitutions:

$$\begin{bmatrix}6a & 3b & c\\ 6d & 3e & f\\ 6g & 3k & l\end{bmatrix}\begin{bmatrix}\phi_i'\\ \phi_i''\\ \phi_i'''\end{bmatrix} = \begin{bmatrix}6m\\ 6n\\ 6o\end{bmatrix}$$

Cramer's rule:

$$\phi_i'' = \frac{\begin{vmatrix}6a & 6m & c\\ 6d & 6n & f\\ 6g & 6o & l\end{vmatrix}}{\begin{vmatrix}6a & 3b & c\\ 6d & 3e & f\\ 6g & 3k & l\end{vmatrix}}$$

$$\begin{aligned}
\phi_i'' &= \frac{-6m(6dl-6fg)+6n(6al-6cg)-6o(6af-6cd)}{-3b(6dl-6fg)+3e(6al-6cg)-3k(6af-6cd)} \\
&= \frac{6\cdot 6}{3\cdot 6}\frac{-m(dl-fg)+n(al-cg)-o(af-cd)}{-b(dl-fg)+e(al-cg)-k(af-cd)} \\
&= 2\cdot\frac{-m(dl-fg)+n(al-cg)-o(af-cd)}{-b(dl-fg)+e(al-cg)-k(af-cd)} \\
\frac{1}{2}\phi_i'' &= \frac{-m(dl-fg)+n(al-cg)-o(af-cd)}{-b(dl-fg)+e(al-cg)-k(af-cd)}
\end{aligned}$$

substitute back:

$$\begin{aligned}
a &= h_1 & b &= h_1^2 & c &= h_1^3 & m &= (\phi_{i+1}-\phi_i) \\
d &= h_2 & e &= h_2^2 & f &= h_2^3 & n &= (\phi_{i+2}-\phi_i) \\
g &= h_3 & k &= h_3^2 & l &= h_3^3 & o &= (\phi_{i+3}-\phi_i)
\end{aligned}$$

$$\frac{1}{2}\phi_i'' = \frac{-(\phi_{i+1}-\phi_i)(h_2h_3^3-h_2^3h_3)+(\phi_{i+2}-\phi_i)(h_1h_3^3-h_1^3h_3)-(\phi_{i+3}-\phi_i)(h_1h_2^3-h_1^3h_2)}{-h_1^2(h_2h_3^3-h_2^3h_3)+h_2^2(h_1h_3^3-h_1^3h_3)-h_3^2(h_1h_2^3-h_1^3h_2)}$$

Simplify denominator:

$$\begin{aligned}
&-h_1^2(h_2h_3^3-h_2^3h_3)+h_2^2(h_1h_3^3-h_1^3h_3)-h_3^2(h_1h_2^3-h_1^3h_2) \\
&h_1h_2h_3(-h_1(h_3^2-h_2^2)+h_2(h_3^2-h_1^2)-h_3(h_2^2-h_1^2)) \\
&h_1h_2h_3(-h_1h_3^2+h_1h_2^2+h_2h_3^2-h_2h_1^2-h_3(h_2^2-h_1^2)) \\
&h_1h_2h_3(h_2(h_1h_2-h_1^2)+h_3^2(h_2-h_1)-h_3(h_2^2-h_1^2)) \\
&h_1h_2h_3(h_2(h_1(h_2-h_1))+h_3^2(h_2-h_1)-h_3(h_2-h_1)(h_2+h_1)) \\
&h_1h_2h_3(h_2-h_1)(h_2h_1+h_3^2-h_3(h_2+h_1)) \\
&h_1h_2h_3(h_2-h_1)(-h_2(h_3-h_1)+h_3(h_3-h_1)) \\
&h_1h_2h_3(h_2-h_1)(h_3-h_1)(h_3-h_2)
\end{aligned}$$

Our finite difference coefficients are now:

$$\begin{aligned}
a_1 =& \frac{h_2^3 h_3 - h_2 h_3^3}{h_1 h_2 h_3 (h_2 - h_1)(h_3 - h_1)(h_3 - h_2)} \\
=& \frac{h_2 h_3 (h_2 - h_3)(h_2 + h_3)}{h_1 h_2 h_3 (h_2 - h_1)(h_3 - h_1)(h_3 - h_2)} \\
=& - \frac{h_2 + h_3}{h_1 (h_2 - h_1)(h_3 - h_1)} \\
=& - \frac{2h_i + 2h_{i+1} + h_{i+2}}{h_i h_{i+1} (h_{i+2} + h_{i+1})}
\end{aligned}$$

$$\begin{aligned}
a_2 =& \frac{h_1 h_3^3 - h_1^3 h_3}{h_1 h_2 h_3 (h_2 - h_1)(h_3 - h_1)(h_3 - h_2)} \\
a_2 =& \frac{h_1 h_3 (h_3 - h_1)(h_3 + h_1)}{h_1 h_2 h_3 (h_2 - h_1)(h_3 - h_1)(h_3 - h_2)} \\
a_2 =& \frac{h_3 + h_1}{h_2 (h_2 - h_1)(h_3 - h_2)} \\
a_2 =& \frac{2h_i + h_{i+1} + h_{i+2}}{h_{i+1} h_{i+2} (h_i + h_{i+1})}
\end{aligned}$$

$$\begin{aligned}
a_3 =& - \frac{h_1 h_2^3 - h_1^3 h_2}{h_1 h_2 h_3 (h_2 - h_1)(h_3 - h_1)(h_3 - h_2)} \\
a_3 =& - \frac{h_1 h_2 (h_2 - h_1)(h_2 + h_1)}{h_1 h_2 h_3 (h_2 - h_1)(h_3 - h_1)(h_3 - h_2)} \\
a_3 =& - \frac{h_2 + h_1}{h_3 (h_3 - h_1)(h_3 - h_2)} \\
a_3 =& - \frac{2h_i + h_{i+1}}{h_i (h_i + h_{i+1} + h_{i+2})(h_{i+1} + h_{i+2})} \\
a_0 =& - (a_1 + a_2 + a_3)
\end{aligned}$$

The same type of equation is used on the corner as in the uniform case, for instance in the lower left corner, $i = 1$, $j = 1$:

$$\frac{1}{2}(\phi_i'' + \phi_j'') = \phi_i \left(\frac{h_i^3 - (h_i + h_{i+1})^3}{(h_i + h_{i+1})^2 h_i^2 h_{i+1}} + \frac{h_j^3 - (h_j + h_{j+1})^3}{(h_j + h_{j+1})^2 h_j^2 h_{j+1}} \right) + \phi_{i+1} \left(\frac{h_i + h_{i+1}}{h_i^2 h_{i+1}} \right) - \phi_{i+2} \left(\frac{h_i}{(h_i + h_{i+1})^2 h_{i+1}} \right) + \phi_{j+1} \left(\frac{h_j + h_{j+1}}{h_j^2 h_{j+1}} \right) - \phi_{j+2} \left(\frac{h_j}{(h_j + h_{j+1})^2 h_{j+1}} \right) + \mathcal{O}(h^2) \quad \text{(A.2.8)}$$

A.3 Finite Difference Approximations for Poisson's Equation and Calculation of Electric Field - Summary

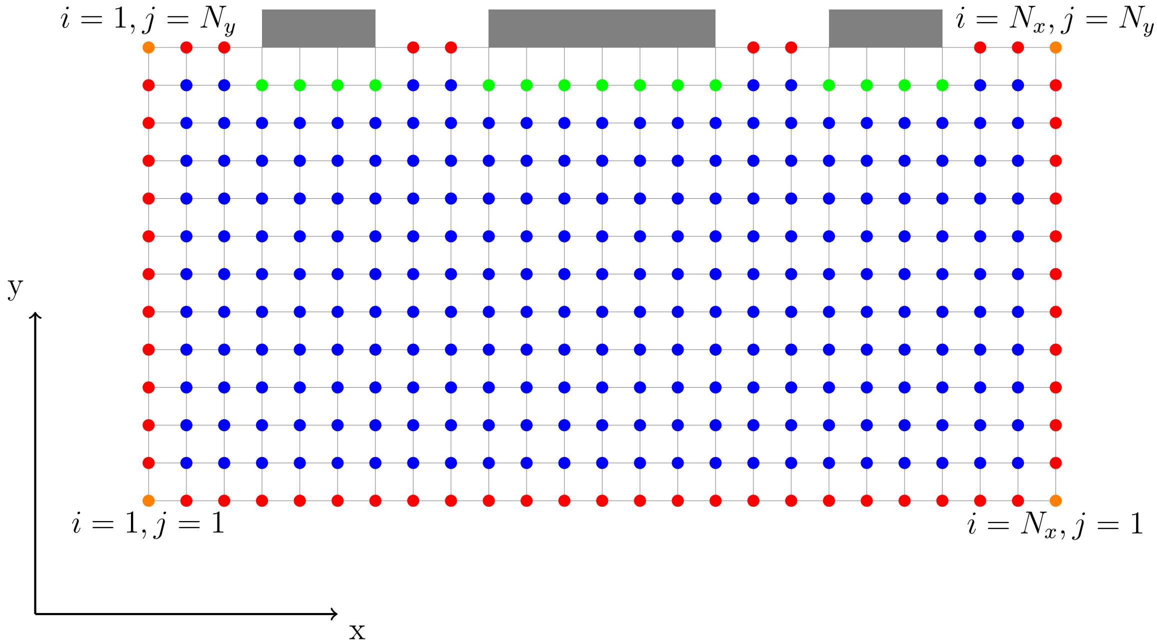

Figure A.1: Discretized device with colors corresponding to appropriate FD-approximation of poisson's equation at that point

A.3.1 Uniform Grid Spacing

BLUE interior points:

$$-\frac{h^2}{\epsilon}\rho(i,j) = \phi(i-1,j) + \phi(i,j-1) - 4\phi(i,j) + \phi(i+1,j) + \phi(i,j+1)$$

RED Neumann boundary (zero flux through surface):
left

$$-\frac{h^2}{\epsilon}\rho(i,j) = \phi(i,j-1) - \frac{11}{2}\phi(i,j) + \phi(i,j+1) + 4\phi(i+1,j) - \frac{1}{2}\phi(i+2,j)$$

right

$$-\frac{h^2}{\epsilon}\rho(i,j) = \phi(i,j-1) + 4\phi(i-1,j) - \frac{1}{2}\phi(i-2,j) - \frac{11}{2}\phi(i,j) + \phi(i,j+1)$$

bottom

$$-\frac{h^2}{\epsilon}\rho(i,j) = \phi(i-1,j) - \frac{11}{2}\phi(i,j) + \phi(i+1,j) + 4\phi(i,j+1) - \frac{1}{2}\phi(i,j+2)$$

top

$$-\frac{h^2}{\epsilon}\rho(i,j) = \phi(i-1,j) + 4\phi(i,j-1) - \frac{1}{2}\phi(i,j-2) - \frac{11}{2}\phi(i,j) + \phi(i+1,j)$$

GREEN points directly below contacts:

$$-\frac{h^2}{\epsilon}\rho(i,j) - \phi(i,j+1) = \phi(i-1,j) + \phi(i,j-1) - 4\phi(i,j) + \phi(i+1,j)$$

ORANGE corner points, calculated after BiCGStab is finished:
bottom left, $i = 1, j = 1$

$$-\frac{h^2}{\epsilon}\rho(i,j) = -7\phi(i,j) + 4\phi(i+1,j) - \frac{1}{2}\phi(i+2,j) + 4\phi(i,j+1) - \frac{1}{2}\phi(i,j+2)$$

bottom right, $i = N_x, j = 1$

$$-\frac{h^2}{\epsilon}\rho(i,j) = -7\phi(i,j) + 4\phi(i-1,j) - \frac{1}{2}\phi(i-2,j) + 4\phi(i,j+1) - \frac{1}{2}\phi(i,j+2)$$

top left, $i = 1, j = N_y$

$$-\frac{h^2}{\epsilon}\rho(i,j) = -7\phi(i,j) + 4\phi(i+1,j) - \frac{1}{2}\phi(i+2,j) + 4\phi(i,j-1) - \frac{1}{2}\phi(i,j-2)$$

top right, $i = N_x, j = N_y$

$$-\frac{h^2}{\epsilon}\rho(i,j) = -7\phi(i,j) + 4\phi(i-1,j) - \frac{1}{2}\phi(i-2,j) + 4\phi(i,j-1) - \frac{1}{2}\phi(i,j-2)$$

A.3.2 Non-uniform Grid Spacing

We still refer to figure A.1, but imagine that the grid spacing is not uniform. $h_x(i)$ and $h_y(j)$ is the grid spacing between points i, j and $i+1, j+1$, i.e. $h_x(i) = x_{i+1} - x_i$.

BLUE interior points (from equation (A.2.6)):

$$
\begin{aligned}
-\frac{1}{2\epsilon}\rho(i,j) = & \frac{\phi(i+1,j)}{h_x(i)(h_x(i)+h_x(i-1))} + \frac{\phi(i-1,j)}{h_x(i-1)(h_x(i)+h_x(i-1))} \\
& - \phi(i,j)\left(\frac{h_x(i-1)+h_x(i)}{h_x(i)h_x(i-1)(h_x(i)+h_x(i-1))} + \frac{h_y(j-1)+h_y(j)}{h_y(j)h_y(j-1)(h_y(j)+h_y(j-1))}\right) \\
& + \frac{\phi(i,j+1))}{h_y(j)(h_y(j)+h_y(j-1))} + \frac{\phi(i,j-1)}{h_y(j-1)(h_y(j)+h_y(j-1))}
\end{aligned}
$$

RED Neumann boundary (from equation (A.2.6) and (A.2.7), zero flux through surface):

left

$$
\begin{aligned}
-\frac{1}{2\epsilon}\rho(i,j) = & -\phi(i+1,j)\left(\frac{(h_x(i)+h_x(i+1))}{h_x(i)^3-(h_x(i)+h_x(i+1))}\right) \\
& + \phi(i+2,j)\left(\frac{h_x(i)^3}{(h_x(i)+h_x(i+1))^2(h_x(i)^3-(h_x(i)+h_x(i+1)))}\right) \\
& - \phi(i,j)\left(\frac{h_x(i)^3-(h_x(i)+h_x(i+1))^3}{(h_x(i)+h_x(i+1))^2(h_x(i)^3-(h_x(i)+h_x(i+1)))} + \frac{h_y(j-1)+h_y(j)}{h_y(j)h_y(j-1)(h_y(j)+h_y(j-1}\right. \\
& + \frac{\phi(i,j+1)}{h_y(j)(h_y(j)+h_y(j-1))} + \frac{\phi(i,j-1)}{h_y(j-1)(h_y(j)+h_y(j-1))}
\end{aligned}
$$

right

$$
\begin{aligned}
-\frac{1}{2\epsilon}\rho(i,j) = & -\phi(i-1,j)\left(\frac{(h_x(i-1)+h_x(i-2))}{h_x(i-1)^3-(h_x(i-1)+h_x(i-2))}\right) \\
& + \phi(i-2,j)\left(\frac{h_x(i-1)^3}{(h_x(i-1)+h_x(i-2))^2(h_x(i-1)^3-(h_x(i-1)+h_x(i-2)))}\right) \\
& - \phi(i,j)\left(\frac{h_x(i-1)^3-(h_x(i-1)+h_x(i-2))^3}{(h_x(i-1)+h_x(i-2))^2(h_x(i-1)^3-(h_x(i-1)+h_x(i-2)))}\right. \\
& \left. + \frac{h_y(j-1)+h_y(j)}{h_y(j)h_y(j-1)(h_y(j)+h_y(j-1))}\right) \\
& + \frac{\phi(i,j+1)}{h_y(j)(h_y(j)+h_y(j-1))} + \frac{\phi(i,j-1)}{h_y(j-1)(h_y(j)+h_y(j-1))}
\end{aligned}
$$

bottom

$$
\begin{aligned}
-\frac{1}{2\epsilon}\rho(i,j) = &-\phi(i,j+1)\left(\frac{(h_y(j)+h_y(j+1))}{h_y(j)^3-(h_y(j)+h_y(j+1))}\right)\\
&+\phi(i,j+2)\left(\frac{h_y(j)^3}{(h_y(j)+h_y(j+1))^2(h_y(j)^3-(h_y(j)+h_y(j+1)))}\right)\\
&-\phi(i,j)\left(\frac{h_y(j)^3-(h_y(j)+h_y(j+1))^3}{(h_y(j)+h_y(j+1))^2(h_y(j)^3-(h_y(j)+h_y(j+1)))}+\frac{h_x(i-1)+h_x(i)}{h_x(i)h_x(i-1)(h_x(i)+h_x(i-1}\right.\\
&+\frac{\phi(i+1,j)}{h_x(i)(h_x(i)+h_x(i-1))}+\frac{\phi(i-1,j)}{h_x(i-1)(h_x(i)+h_x(i-1))}
\end{aligned}
$$

top

$$
\begin{aligned}
-\frac{1}{2\epsilon}\rho(i,j) = &-\phi(i,j-1)\left(\frac{(h_y(j-1)+h_y(j-2))}{h_y(j-1)^3-(h_y(j-1)+h_y(j-2))}\right)\\
&+\phi(i,j-2)\left(\frac{h_y(j-1)^3}{(h_y(j-1)+h_y(j-2))^2(h_y(j-1)^3-(h_y(j-1)+h_y(j-2)))}\right)\\
&-\phi(i,j)\left(\frac{h_y(j-1)^3-(h_y(j-1)+h_y(j-2))^3}{(h_y(j-1)+h_y(j-2))^2(h_y(j-1)^3-(h_y(j-1)+h_y(j-2)))}\right.\\
&\left.+\frac{h_x(i-1)+h_x(i)}{h_x(i)h_x(i-1)(h_x(i)+h_x(i-1))}\right)\\
&+\frac{\phi(i,j+1)}{h_x(i)(h_x(i)+h_x(i-1))}+\frac{\phi(i,i-1)}{h_x(i-1)(h_x(i)+h_x(i-1))}
\end{aligned}
$$

GREEN points directly below contacts:

$$
\begin{aligned}
-\frac{1}{2\epsilon}\rho(i,j)-\frac{\phi(i,j+1))}{h_y(j)(h_y(j)+h_y(j-1))} = &\frac{\phi(i+1,j)}{h_x(i)(h_x(i)+h_x(i-1))}+\frac{\phi(i-1,j)}{h_x(i-1)(h_x(i)+h_x(i-1))}\\
&-\phi(i,j)\left(\frac{h_x(i-1)+h_x(i)}{h_x(i)h_x(i-1)(h_x(i)+h_x(i-1))}+\frac{h_y(j-1)+h_y(j)}{h_y(j)h_y(j-1)(h_y(j)+h_y(j-1))}\right)\\
&+\frac{\phi(i,j-1)}{h_y(j-1)(h_y(j)+h_y(j-1))}
\end{aligned}
$$

ORANGE corner points, calculated after BiCGStab is finished:

bottom left, $i = 1, j = 1$

$$
\begin{aligned}
-\frac{1}{2\epsilon}\rho(i,j) = -\phi(i+1,j)&\left(\frac{(h_x(i)+h_x(i+1))}{h_x(i)^3-(h_x(i)+h_x(i+1))}\right)\\
+\phi(i+2,j)&\left(\frac{h_x(i)^3}{(h_x(i)+h_x(i+1))^2(h_x(i)^3-(h_x(i)+h_x(i+1)))}\right)\\
-\phi(i,j)&\left(\frac{h_x(i)^3-(h_x(i)+h_x(i+1))^3}{(h_x(i)+h_x(i+1))^2(h_x(i)^3-(h_x(i)+h_x(i+1)))}\right.\\
&+\left.\frac{h_y(j)^3-(h_y(j)+h_y(j+1))^3}{(h_y(j)+h_y(j+1))^2(h_y(j)^3-(h_y(j)+h_y(j+1)))}\right)\\
-\phi(i,j+1)&\left(\frac{(h_y(j)+h_y(j+1))}{h_y(j)^3-(h_y(j)+h_y(j+1))}\right)\\
+\phi(i,j+2)&\left(\frac{h_y(j)^3}{(h_y(j)+h_y(j+1))^2(h_y(j)^3-(h_y(j)+h_y(j+1)))}\right)
\end{aligned}
$$

bottom right, $i = N_x, j = 1$

$$
\begin{aligned}
-\frac{1}{2\epsilon}\rho(i,j) = -\phi(i-1,j)&\left(\frac{(h_x(i-1)+h_x(i-2))}{h_x(i-1)^3-(h_x(i-1)+h_x(i-2))}\right)\\
+\phi(i-2,j)&\left(\frac{h_x(i-1)^3}{(h_x(i-1)+h_x(i-2))^2(h_x(i-1)^3-(h_x(i-1)+h_x(i-2)))}\right)\\
-\phi(i,j)&\left(\frac{h_x(i-1)^3-(h_x(i-1)+h_x(i-2))^3}{(h_x(i-1)+h_x(i-2))^2(h_x(i-1)^3-(h_x(i-1)+h_x(i-2)))}\right.\\
&+\left.\frac{h_y(j)^3-(h_y(j)+h_y(j+1))^3}{(h_y(j)+h_y(j+1))^2(h_y(j)^3-(h_y(j)+h_y(j+1)))}\right)\\
-\phi(i,j+1)&\left(\frac{(h_y(j)+h_y(j+1))}{h_y(j)^3-(h_y(j)+h_y(j+1))}\right)\\
+\phi(i,j+2)&\left(\frac{h_y(j)^3}{(h_y(j)+h_y(j+1))^2(h_y(j)^3-(h_y(j)+h_y(j+1)))}\right)
\end{aligned}
$$

top left, $i = 1, j = N_y$

$$
\begin{aligned}
-\frac{1}{2\epsilon}\rho(i,j) = &-\phi(i+1,j)\left(\frac{(h_x(i)+h_x(i+1))}{h_x(i)^3-(h_x(i)+h_x(i+1))}\right)\\
&+\phi(i+2,j)\left(\frac{h_x(i)^3}{(h_x(i)+h_x(i+1))^2(h_x(i)^3-(h_x(i)+h_x(i+1)))}\right)\\
&-\phi(i,j)\left(\frac{h_x(i)^3-(h_x(i)+h_x(i+1))^3}{(h_x(i)+h_x(i+1))^2(h_x(i)^3-(h_x(i)+h_x(i+1)))}\right.\\
&\left.+\frac{h_y(j-1)^3-(h_y(j-1)+h_y(j-2))^3}{(h_y(j-1)+h_y(j-2))^2(h_y(j-1)^3-(h_y(j-1)+h_y(j-2)))}\right)\\
&-\phi(i,j-1)\left(\frac{(h_y(j-1)+h_y(j-2))}{h_y(j-1)^3-(h_y(j-1)+h_y(j-2))}\right)\\
&+\phi(i,j-2)\left(\frac{h_y(j-1)^3}{(h_y(j-1)+h_y(j-2))^2(h_y(j-1)^3-(h_y(j-1)+h_y(j-2)))}\right)
\end{aligned}
$$

top right, $i = N_x, j = N_y$

$$
\begin{aligned}
-\frac{1}{2\epsilon}\rho(i,j) = &-\phi(i-1,j)\left(\frac{(h_x(i-1)+h_x(i-2))}{h_x(i-1)^3-(h_x(i-1)+h_x(i-2))}\right)\\
&+\phi(i-2,j)\left(\frac{h_x(i-1)^3}{(h_x(i-1)+h_x(i-2))^2(h_x(i-1)^3-(h_x(i-1)+h_x(i-2)))}\right)\\
&-\phi(i,j)\left(\frac{h_x(i-1)^3-(h_x(i-1)+h_x(i-2))^3}{(h_x(i-1)+h_x(i-2))^2(h_x(i-1)^3-(h_x(i-1)+h_x(i-2)))}\right.\\
&\left.+\frac{h_y(j-1)^3-(h_y(j-1)+h_y(j-2))^3}{(h_y(j-1)+h_y(j-2))^2(h_y(j-1)^3-(h_y(j-1)+h_y(j-2)))}\right)\\
&-\phi(i,j-1)\left(\frac{(h_y(j-1)+h_y(j-2))}{h_y(j-1)^3-(h_y(j-1)+h_y(j-2))}\right)\\
&+\phi(i,j-2)\left(\frac{h_y(j-1)^3}{(h_y(j-1)+h_y(j-2))^2(h_y(j-1)^3-(h_y(j-1)+h_y(j-2)))}\right)
\end{aligned}
$$

Appendix B

Solving for NUM

```
SUBROUTINE updateGridSpacing(Ex, Ey, init)

   IMPLICIT NONE
   LOGICAL, INTENT(IN) :: init
   REAL(KIND=dbl), DIMENSION(:,:), INTENT(IN) :: Ex
   REAL(KIND=dbl), DIMENSION(:), ALLOCATABLE :: fracx, nk, gridhits
   REAL(KIND=dbl), DIMENSION(:), ALLOCATABLE :: Lk, Lk0
   INTEGER :: i, j, ii, ip, ib, ie, hn, LNx, corr, iimax, first
   INTEGER :: hits, hiti, done, mininfrac, minin0, signfh0, restart
   REAL(KIND=dbl) :: xpos, fac, acl, acr
   REAL(KIND=dbl) :: xposprev, xL, ak0, h0, h0next, hfrac
   REAL(KIND =DBL) :: Exjsum, Exijsum, Exrest
   REAL(KIND=DBL) :: tmp, smoothL, h1, ac, aprev
   REAL(KIND=DBL) :: maxin, maxin1, sec
   REAL(KIND=DBL) :: h0l, h0r, fach0l, fach0r, h0prev

   IF (allocated(xgridNew)) DEALLOCATE(xgridNew)

   ALLOCATE(xgridNew(Nx))

   hits = 9 !Number of x-positions we want to fit a gridpoint exactly
   mininfrac = 10 !Minimum number of grid points in a given interval

   !maxin0, biggest ratio of number of gridpoints total of interval
   maxin0 = (1.01_dbl**REAL(Ny/mininfrac))/(0.99**REAL(Ny/mininfrac))

   smoothL = Lx/(mininfrac*2_dbl) !Length of intervals
   LNx = int(Lx/smoothL) !Number of intervals
```

```
ALLOCATE(fracx(Nx), nk(LNx), gridhits(hits))
corr = 0
minin=0
minin0 = 10

LNx = int(Lx*2_dbl/smoothL)
IF (allocated(Lk0)) DEALLOCATE(Lk0)
ALLOCATE(Lk0(LNx))

!Positions WHERE one wants a gridpoint
gridhits(1) = LRim
gridhits(2) = LRim+Lxcrp
gridhits(3) = x1N
gridhits(4) = x1Np
gridhits(5) = x2Np
gridhits(6) = x2N
gridhits(7) = Lx-LRim-Lxcrp
gridhits(8) = Lx-LRim
gridhits(9) = Lx


!Find the length of the intervals
done = 0
DO WHILE (done == 0)

   hiti = 1 !Gridpoint position number to look for
   LNx = 1 !Number of intervals
   i=1
   xpos = smoothL  !current position
   xposprev = 0_dbl !previous position

   DO WHILE (xpos<Lx)

      !If position is bigger or equal to a position that's beging looked
      !THEN adjust the length of interval to hit position exactly
      IF (xpos>=gridhits(hiti)) THEN
         IF (xpos==gridhits(hiti)) THEN
            Lk0(i) = xpos-xposprev
           xposprev=xpos
           xpos = xpos+smoothL
           i=i+1
```

```
          hiti=hiti+1
       ELSE IF (xpos-gridhits(hiti) <= smoothL/2_dbl) THEN
           xpos=gridhits(hiti)
          Lk0(i) = xpos-xposprev
          xposprev=xpos
          xpos = xpos+smoothL
          i=i+1
          hiti=hiti+1
       ELSE IF (i>1) THEN
           IF (xposprev == gridhits(hiti-1)) THEN
              xpos=gridhits(hiti)
             Lk0(i) = xpos-xposprev
             xposprev=xpos
             xpos = xpos+smoothL
             i=i+1
             hiti=hiti+1
          ELSE
              i=i-1
             xpos = gridhits(hiti)
             Lk0(i) = Lk0(i)+(xpos-xposprev)
             xposprev = xpos
             xpos = xpos +smoothL
             i=i+1
             hiti=hiti+1
          END IF
        ELSE IF (i==1) THEN
           xpos=gridhits(hiti)
          Lk0(i) = xpos-xposprev
          xposprev=xpos
          xpos=xpos+smoothL
          i=i+1
          hiti=hiti+1
       END IF
    ELSE ! Interval doesn't contain any positions to be hit exactly
       Lk0(i) = xpos-xposprev
       xposprev=xpos
       xpos = xpos+smoothL
       i=i+1
    END IF

    IF (xpos >= Lx) THEN
```

```
         IF (xpos==Lx) THEN
            Lk0(i) = ypos-yposprev
            i=i+1
         ELSE IF (xpos-Lx < smoothL/2_dbl) THEN
            xpos = Lx
            Lk0(i) = xpos-xposprev
            i=i+1
         ELSE IF (xposprev == gridhits(hiti-1)) THEN
            xpos = Lx
            Lk0(i) = xpos-xposprev
            i=i+1
         ELSE
            i=i-1
            xpos = Lx
            Lk0(i) = Lk0(i) + xpos-xposprev
            i=i+1
         END IF
         xpos = xpos+smoothL
      END IF

   END DO

   LNx = i-1
   IF (LNx > mininfrac) THEN
      smoothL = smoothL*1.01_dbl
   ELSE
      done = 1
   END IF

END DO



ALLOCATE(Lk(LNx))
Lk = 1_dbl
DO i=1,LNx
   Lk(i)=Lk0(i)
END DO

DEALLOCATE(Lk0)
DEALLOCATE(nk)
```

```
ALLOCATE(nk(LNx))

IF (init) THEN

   DO i=1, LNx
      nk(i) = REAL(Nx-1)*Lk(i)/Lx
   END DO
   nk=nint(nk)
   tmp = REAL(Nx-1)-sum(nk)
   IF (abs(tmp)>0) THEN
      ii=maxloc(nk,1)
      nk(ii) = nk(ii)+tmp
   END IF

ELSE
   fracx = 0_dbl
   DO i=1,Nx
      tmp = 0_dbl
      ExjSum = 0_dbl
      Exrest = 0_dbl
      DO j=1,Ny
         tmp = ExjSum+Exrest+abs(Ex(i,j))
         Exrest = (abs(Ex(i,j))+Exrest)-(tmp-ExjSum)
         ExjSum = tmp
      END DO
      fracx(i) = ExjSum
   END DO


   fracx=fracx/sum(fracx)
   corr = 0
   minin = 0

   DO WHILE ((minin < minin0).or.(maxin > maxin0))


      tmp = sum(fracx)/size(fracx)
      IF (corr>0) THEN
         fracx = fracx + REAL(corr)*tmp/100_dbl
         fracx=fracx/sum(fracx)
      END IF
```

```
 IF (corr == 1000) THEN
    fracx = 1_dbl
   fracx=fracx/sum(fracx)
END IF

 ip=1
tmp = 0_dbl
DO i=1, LNx-1

   tmp = tmp+Lk(i)
   call NECindx(tmp, j)
   nk(i) = sum(fracx(ip:j))
   ip = j+1

END DO

 nk(LNx) = sum(fracx(ip+1:Nx))
nk = nk/sum(nk)
fracsmooth = real(Nx-1)*fracsmooth
nk = NINT(nk)


tmp = REAL(Nx-1)-sum(nk)
IF (abs(tmp)>0) THEN
    ii=maxloc(nk,1)
   nk(ii) = nk(ii)+tmp
END IF

 minin = nk(1)/Lk(1)
maxin = 0_dbl
DO i=1, LNx
  tmp = nk(i)/Lk(i)
  if(tmp<minin)THEN
     minin=tmp
  END IF
   IF(tmp>maxin) maxin=tmp
END DO
 maxin = maxin/minin
minin = minval(nk)
```

```
            IF (corr>=1000) EXIT

            corr=corr+1


         END DO
      END IF

      tmp = REAL(Nx-1)-sum(nk)
      IF (abs(tmp)>0) THEN
         ii=maxloc(nk,1)
         nk(ii) = nk(ii)+tmp
      END IF

!_____________________________________________
!
!     Fit xgrid
!_____________________________________________

      ii=1
      hn = nk(ii)
      xL = Lk(ii)
      done = 0
      h0 = h0sx
      hfrac = 1.1_dbl
      first = 1
      h0Next = h0
      sec = 0
      restart = 0
      iimax = 0
      h0prev=0_dbl

      DO WHILE (done==0)

         ii=1
         ak0 = 1_dbl
         hn = nk(ii)
         xL = Lk(ii)
         h1=h0
         acl = 0_dbl
         facl = xL-h1
```

```
fac = facl

IF (h0>h0ex) then
  h0=h0next
  hfrac=1_dbl+(hfrac-1_dbl)/5_dbl
END IF

DO WHILE (fac>=0_dbl)
   ac = acl+0.1_dbl
   aprev = ak0
   fac = h1
   tmp = h1
   DO i=2, hn
      tmp=tmp*aprev
      fac = fac+tmp
      aprev=aprev*ac
   END DO

   fac = xL-fac

   IF (fac>=0_dbl) THEN
      acl = ac
      facl =fac
   END IF
END DO

acr = ac
facr = fac
tmp = h1
fac = 1_dbl
corr=0_dbl

DO WHILE (abs(fac) > tmp*1.D-10)
   ac = (acl+acr)/2_dbl
   tmp = h1
   fac = h1
   aprev = ak0
   DO i=2, hn
      tmp = tmp*aprev
      fac = fac+tmp
      aprev = aprev*ac
```

```
   END DO
   fac = xL - fac

   IF (fac > 0_dbl) THEN
      acl = ac
      facl = fac
   ELSE
      acr = ac
      facr = ac
   END IF
   IF (corr>1000) exit
   corr=corr+1

END DO



ib = 1
ie = ib+hn-1
hgx(ib) = h1
xgridNew(ib) = 0_dbl
xgridNew(ib+1) = xgridNew(ib)+hgx(ib)
aprev = ak0
DO i=2, ie
   hgx(i) = hgx(i-1)*aprev
   xgridNew(i+1) = xgridNew(i) + hgx(i)
   aprev=aprev*ac
END DO
xgridNew(ie+1) = xL
hgx(ie) = xgridNew(ie+1)-xgridNew(ie)
ak0 = aprev


DO ii=2, LNx-1

   IF (ak0>1.2_dbl.or.ak0<0.8_dbl) then
      restart=1
      exit
   END IF
   IF (ii>=iimax) then
      IF (ii>iimax) then
```

```
      iimax = ii
      h0next = h0/(hfrac**2)
   ELSE IF (first==1 .and. sec == 0) then
      h0next = h0/(hfrac**2)
   END IF
END IF

hn = nk(ii)
xL = Lk(ii)
h1 = hgx(ie)*ak0

acl = 0_dbl
facl = xL-h1
fac = facl

DO WHILE (fac>=0_dbl)

   ac = acl+0.001_dbl
   aprev = ak0
   tmp = h1
   fac = h1
   DO i=2, hn
      aprev = aprev*ac
      tmp = tmp*aprev
      fac = fac + tmp
   END DO

   fac = xL-fac

   IF (fac>=0_dbl) THEN
      acl = ac
      facl = fac
   END IF

END DO

acr = ac
facr = fac

corr = 0
fac=1_dbl
```

```
tmp=1_dbl
DO WHILE (abs(fac)>tmp*1.D-20)
   ac = (acl+acr)/2_dbl
   tmp = h1
   aprev = ak0
   fac = h1
   DO i=2, hn
      aprev=aprev*ac
      tmp = tmp*aprev
      fac = fac+ tmp
   END DO
   fac = xL - fac

   IF (fac>0_dbl) THEN
      acl = ac
      facl = fac
   ELSE
      acr = ac
      facr = fac
   END IF
   corr = corr +1

   IF (corr>1000) EXIT

END DO

ib=ie+1
ie =ib+hn-1

hgx(ib) = h1
xgridNew(ib+1) = xgridNew(ib)+hgx(ib)
aprev = ak0
DO i=ib+1, ie
   aprev=aprev*ac
   hgx(i) = hgx(i-1)*aprev
   xgridNew(i+1) = xgridNew(i)+hgx(i)
END DO
xgridNew(ie+1) = xgridNew(ib)+xL
hgx(ie) = xgridNew(ie+1)-xgridNew(ie)
ak0 = aprev
```

```
   ak0 = aprev


END DO

IF (restart == 1.or.(ak0>1000_dbl .or. ak0<0.001)) then
   restart = 0
   h0=h0*hfrac
   cycle
END IF

ii=LNx
iimax = ii
hn = nk(ii)
xL = Lk(ii)
h1 = hgx(ie)*ak0
ac = ak0**real(1_dbl/real(1_dbl-REAL(hn)))

ib = ie+1
ie = ib+hn-1
hgx(ib) = h1
xgridNew(ib+1) = xgridNew(ib) + hgx(ib)
aprev = ak0

DO i=ib+1, ie
   aprev=aprev*ac
   hgx(i) = hgx(i-1)*aprev
   xgridNew(i+1) = xgridNew(i) + hgx(i)
END DO

fac = Lx-xgridNew(ie+1)


IF (first == 1) then
   signfh0 = int(fac/abs(fac))
   h0sx = 0.85_dbl*h0
   IF (init) h0sx  = 0.6_dbl*h0
   h0next = h0/(hfrac**2)

   first = 0
   sec = 1
```

```
         h0l = h0
         fach0l = fac
         h0=h0*hfrac
      ELSE IF (sec == 1) then
         IF (signfh0 == int(fac/abs(fac))) then
            h0=h0*hfrac
         ELSE
            sec = 0
            h0ex = 1.2_dbl*h0
            IF (init) h0ex =h0*1.5_dbl
            h0r = h0
            fach0r = fac
         END IF
      ELSE IF (abs(fac)<1.D-10) then
         done = 1
      ELSE
         IF (int(fac/abs(fac)) == signfh0) then
            h0l = h0
            fach0l = fac
         ELSE
            h0r = h0
            fach0r = fac
         END IF
         h0 = (h0l+h0r)/2_dbl
         IF (h0==h0prev) done = 1
         h0prev=h0

      END IF

   open(10, file="hgxn.dat", ACTION="WRITE", status="replace")
   DO i=1, Nx-1
     WRITE(10,*) i, hgx(i)
   END DO
   CLOSE (10)

   END DO

      xgridNew(Nx) = Lx
      hgx(Nx-1) = Lx-xgridNew(Nx-1)

END SUBROUTINE updateGridSpacing
```

Bibliography

[1] C. Jacoboni and P. Lubli, *The Monte Carlo Method for Semiconductor Device Simulation*, 1st ed. (Springer-Verlag, Wien - New York, 1989).