

\vec{E} mission

A program with great potential.

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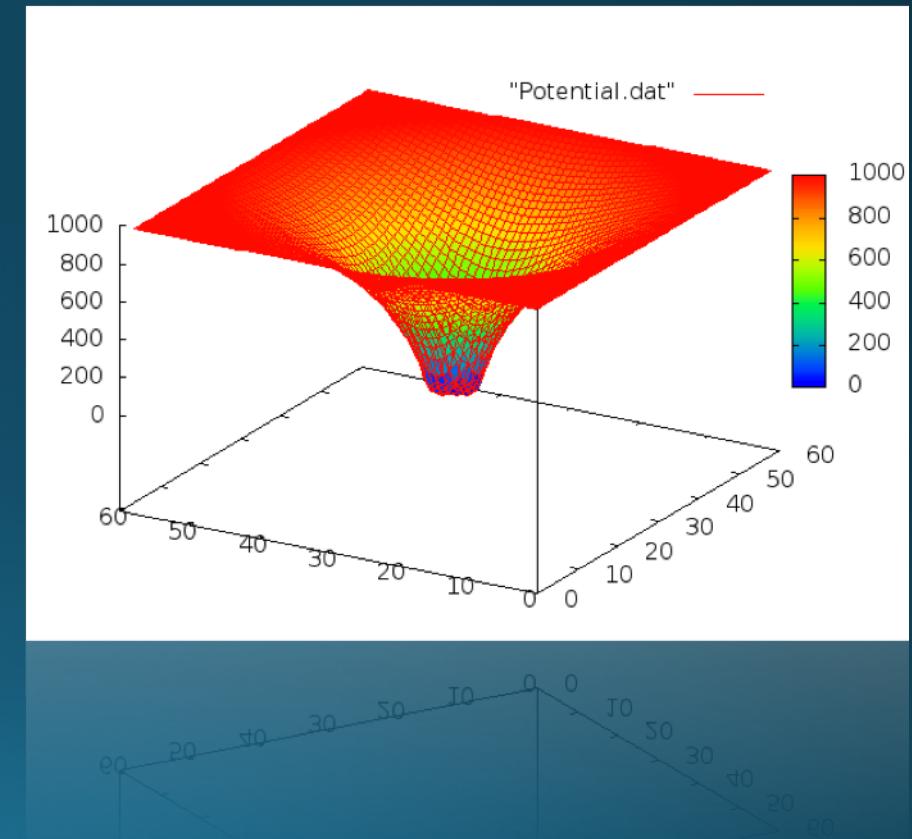
Antonio Smecca

Motivation



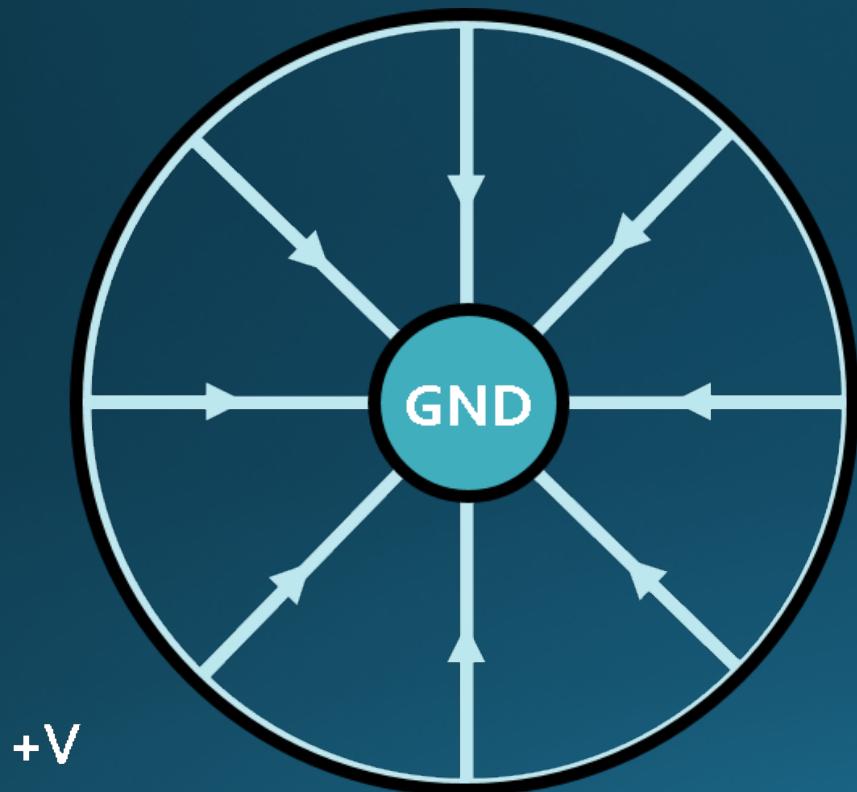
Aims

- Application simulating electric potentials.
- Quick and intuitive numerical solver for general charged geometries.
- User freedom.

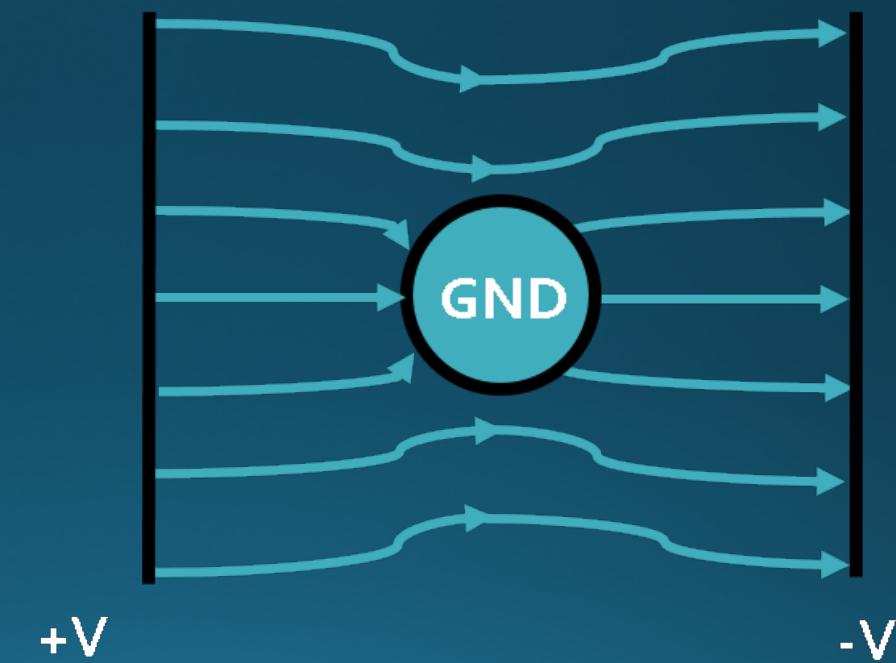


Analytical Problems

$$\nabla^2 V = 0 \quad \text{Laplace's equation}$$

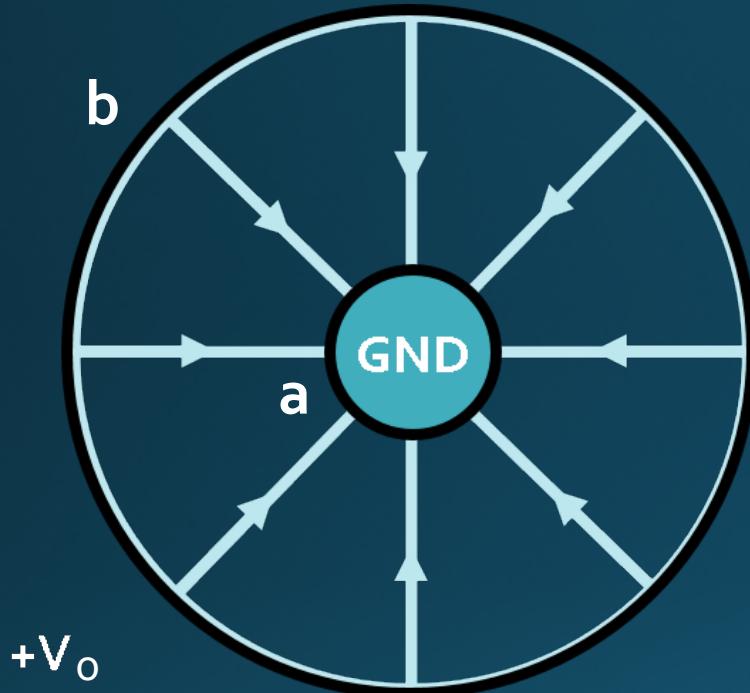


Problem 0



Problem 1

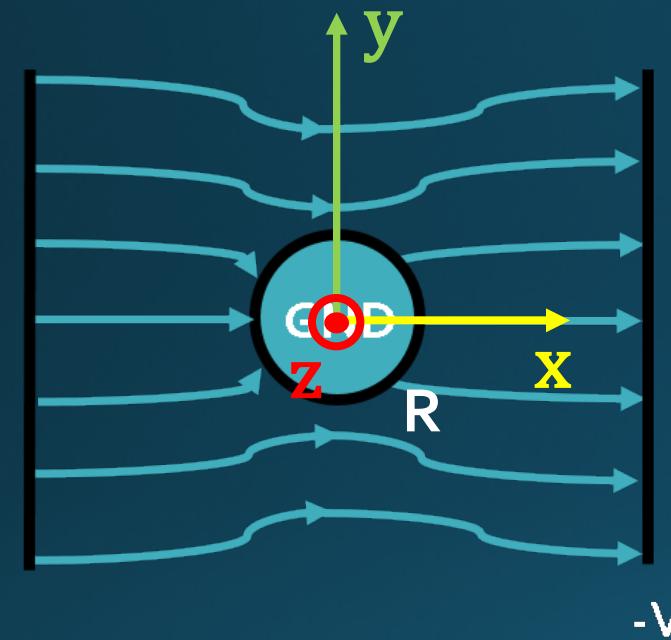
Problem 0



1. Cylindrical form of the Laplace equation
2. Omit the angular coordinate θ and height z
3. Integrate twice
4. Use boundary conditions on surface of conductor and shell

$$V(r) = \frac{V_0}{k} \ln\left(\frac{r}{a}\right) \text{ where } k = \ln\left(\frac{b}{a}\right)$$

Problem 1



Maths:

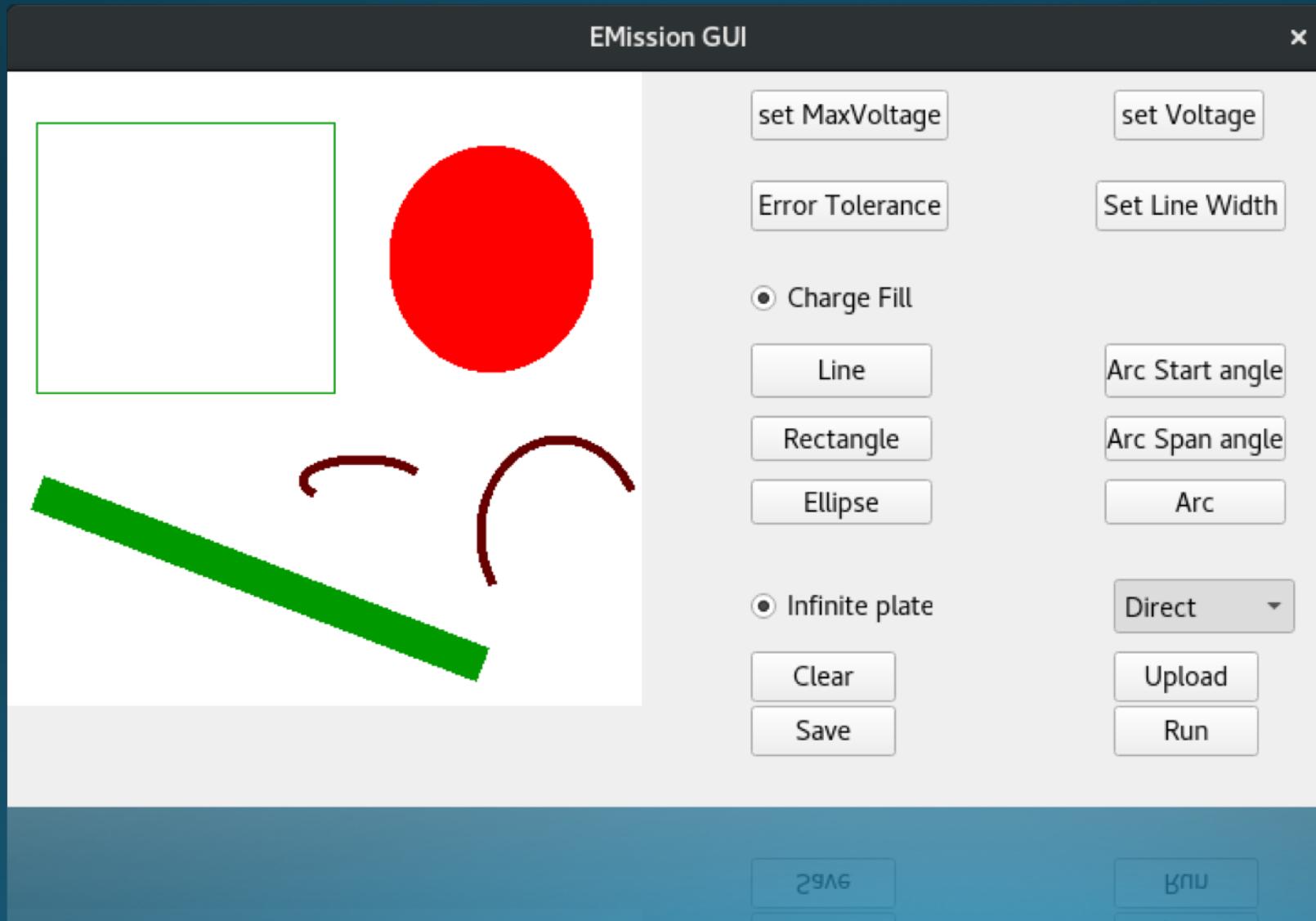
1. Cylindrical form of the Laplace equation
2. Omit the height z
3. Get general solution through separation of variables

Physics:

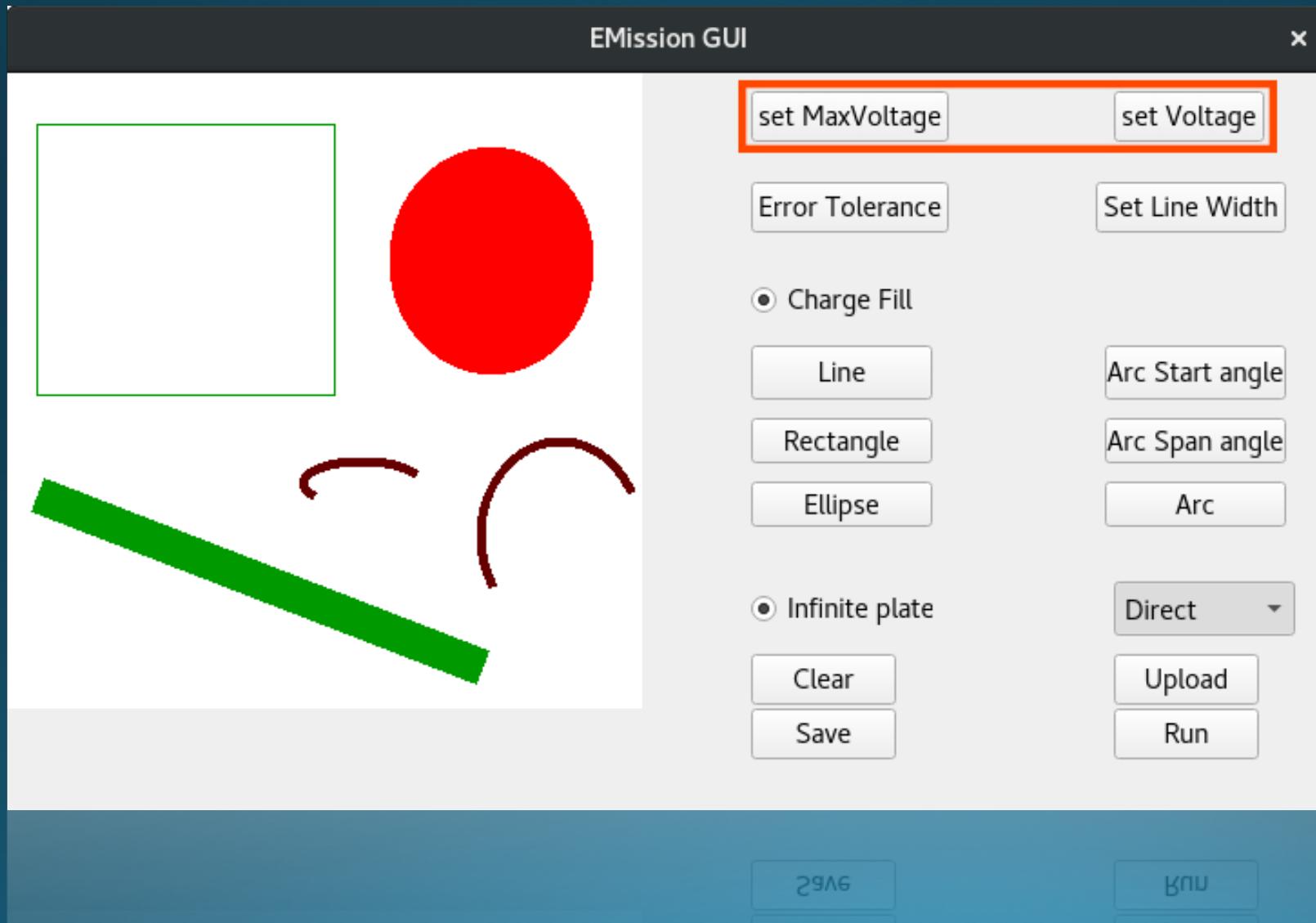
1. Potential at $r \gg R$ unaffected by conductor, $V = -E_0 x + K$
2. No charge on conductor's surface
3. Compare with general solution

$$V(r, \theta) = -E_0 \left(r - \frac{R^2}{r} \right) \cos(\theta)$$

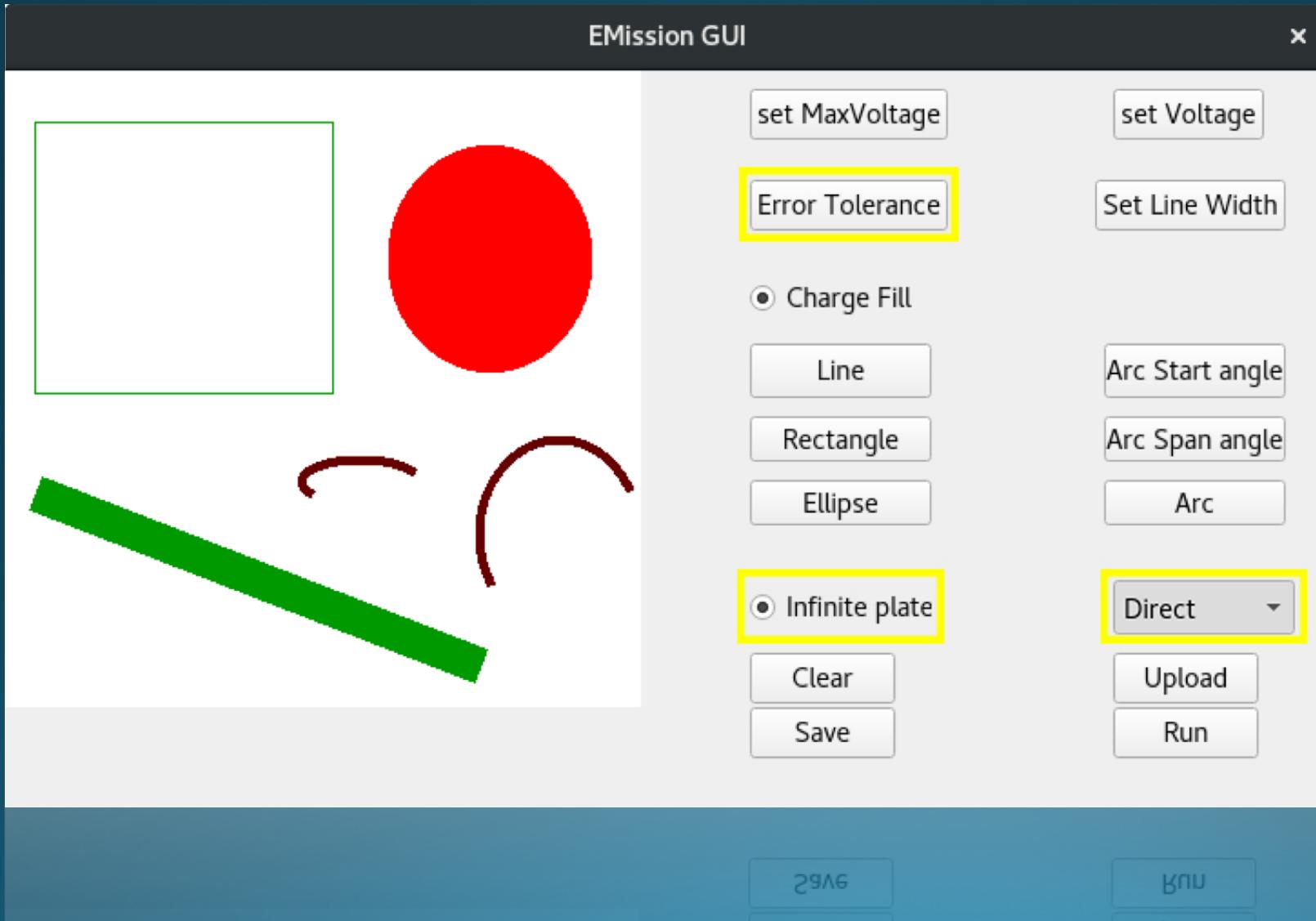
Emission GUI



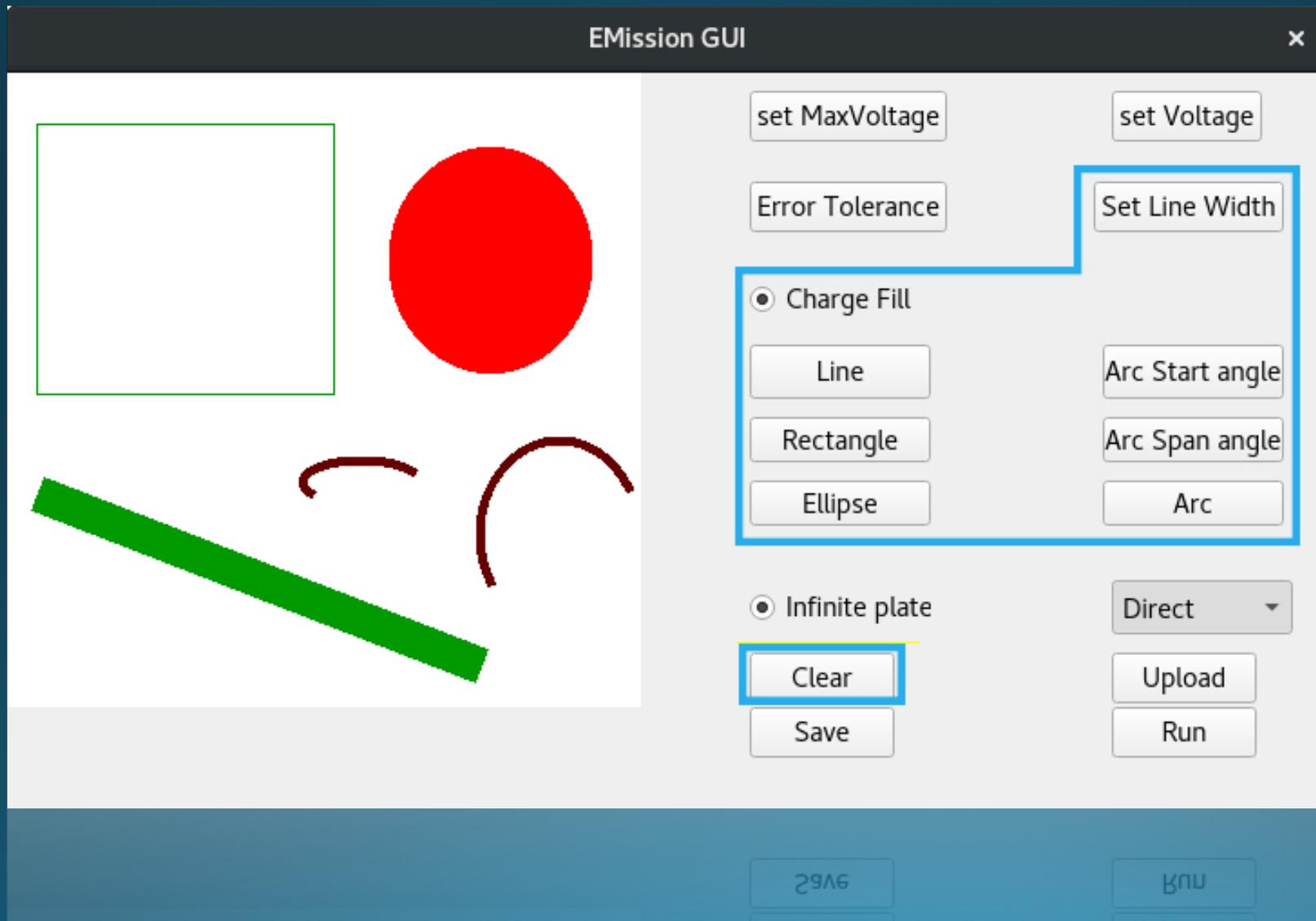
Emission GUI



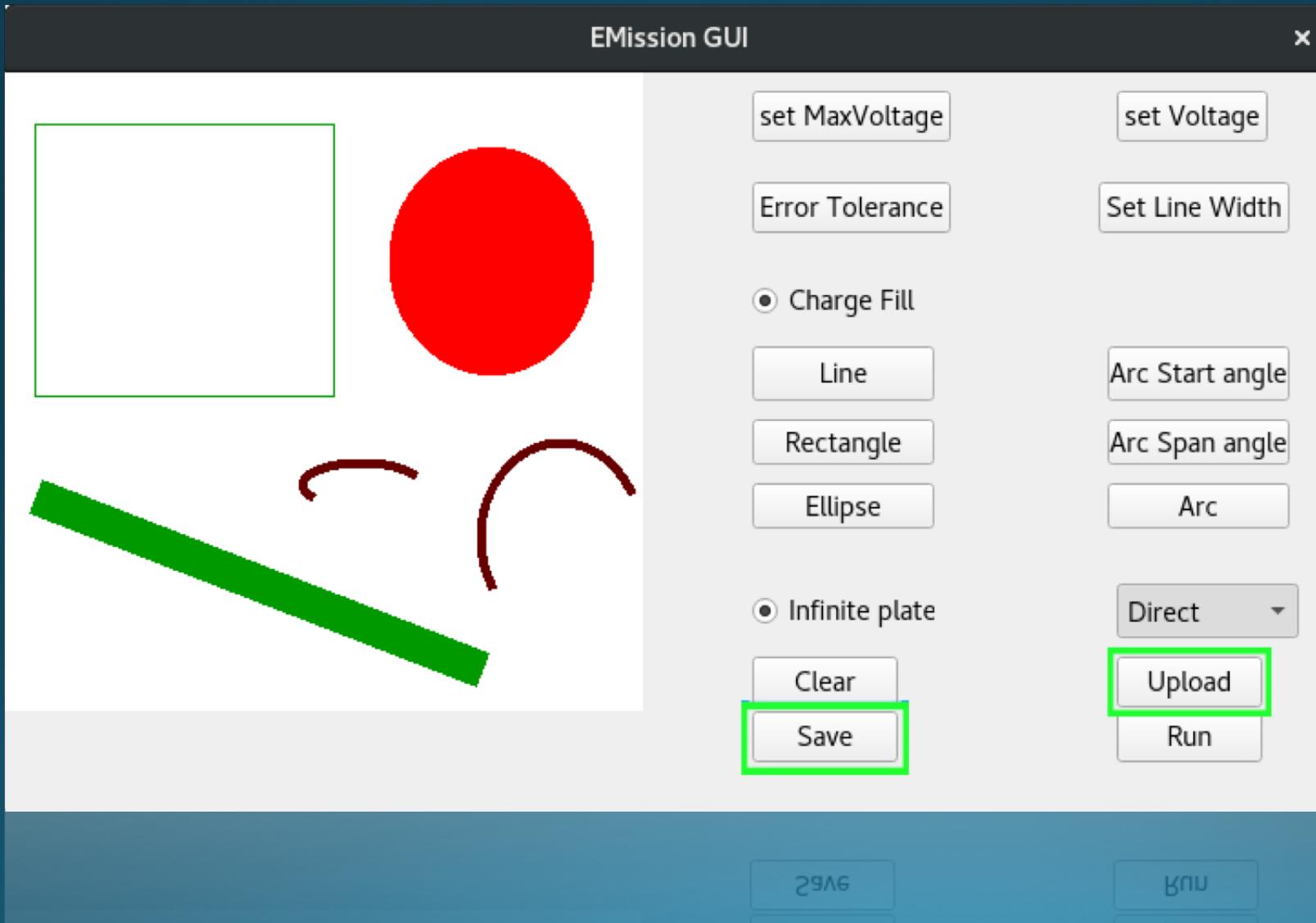
Emission GUI



Emission GUI

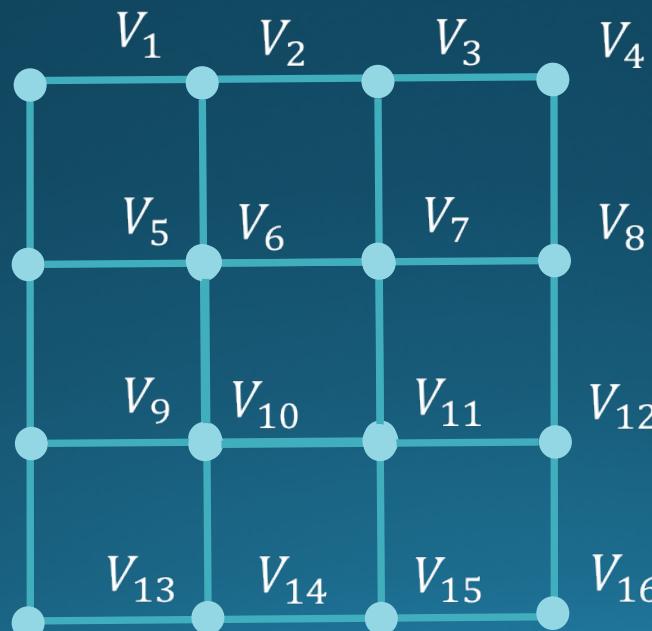


Emission GUI



Outline of the Direct Method:

1. For every point there is an associated equation derived from FPS
2. $N \times N$ grid $\Rightarrow N^2$ simultaneous equations
3. Putting this in a matrix of form $Ax = b$

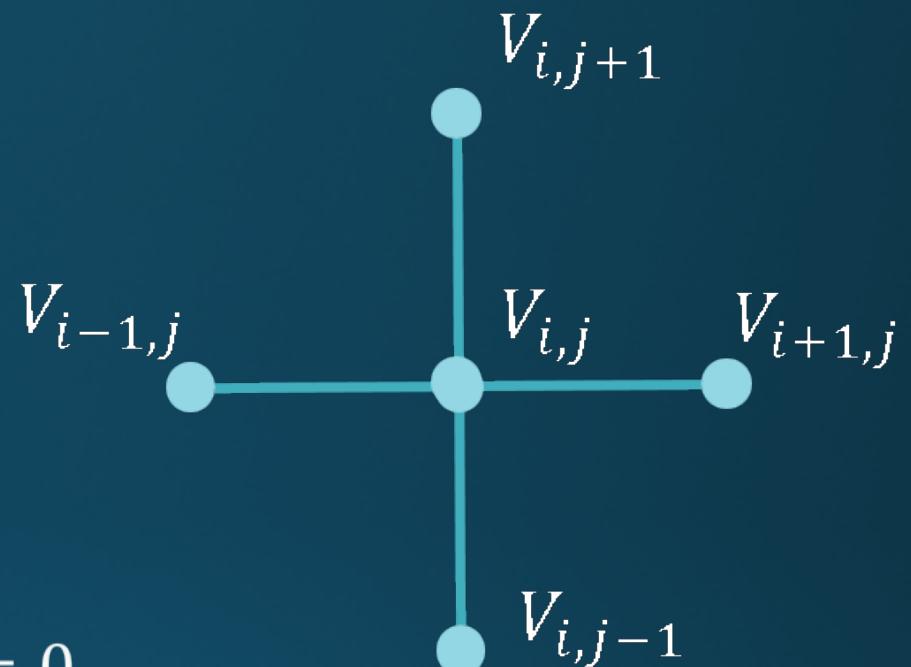


Numerical Approach

$$\nabla^2 V = \frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2} = 0$$

$$\approx \frac{V_{i+1,j} + 2V_{i,j} + V_{i-1,j}}{\delta x^2} + \frac{V_{i,j+1} + 2V_{i,j} + V_{i,j-1}}{\delta y^2} = 0$$
$$\delta x = \delta y \Rightarrow$$

$$V_{i,j} = \frac{1}{4} (V_{i+1,j} + V_{i-1,j} + V_{i,j+1} + V_{i,j-1})$$



Five Point Stencil

Equations for the Grid

- The equations for the whole grid:
- $-4V_1 + V_2 + 0V_3 + 0V_4 + V_5 + \cdots + 0V_{16} = 0$
- $V_1 - 4V_2 + V_3 + 0V_4 + 0V_5 + V_6 + \cdots + 0V_{16} = 0$
- \vdots *13 more equations*
- $0V_1 + \cdots + V_{12} + 0V_{13} + 0V_{14} + V_{15} - 4V_{16} = 0$
- How can we express this as a matrix?

$$\begin{pmatrix} -4 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & -4 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & -4 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & -4 & 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & -4 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 & -4 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & -4 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & -4 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & -4 \end{pmatrix}$$

Matrix Formulation

$$\begin{pmatrix} -4 & 1 & 0 & \dots & 0 & 0 & 0 \\ 1 & -4 & 1 & \dots & 0 & 0 & 0 \\ 0 & 1 & -4 & \ddots & 0 & 0 & 0 \\ \vdots & & & \ddots & \vdots & & \\ 0 & 0 & 0 & \dots & -4 & 1 & 0 \\ 0 & 0 & 0 & \dots & 1 & -4 & 1 \\ 0 & 0 & 0 & \dots & 0 & 1 & -4 \end{pmatrix} \begin{pmatrix} V_1 \\ V_2 \\ V_3 \\ \vdots \\ V_{14} \\ V_{15} \\ V_{16} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

This matrix equation is now of the form $Ax = b$ but is not quite complete. We need to tailor it to our specific geometry.

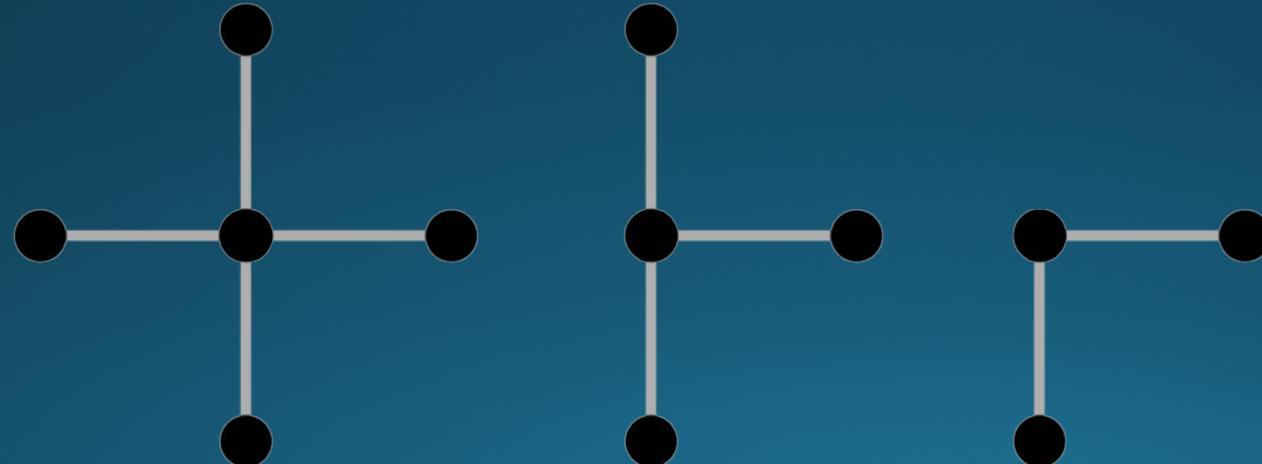
Tailoring the Matrix

Say V_2 is known to be 25V. We can then edit our system to reflect this:

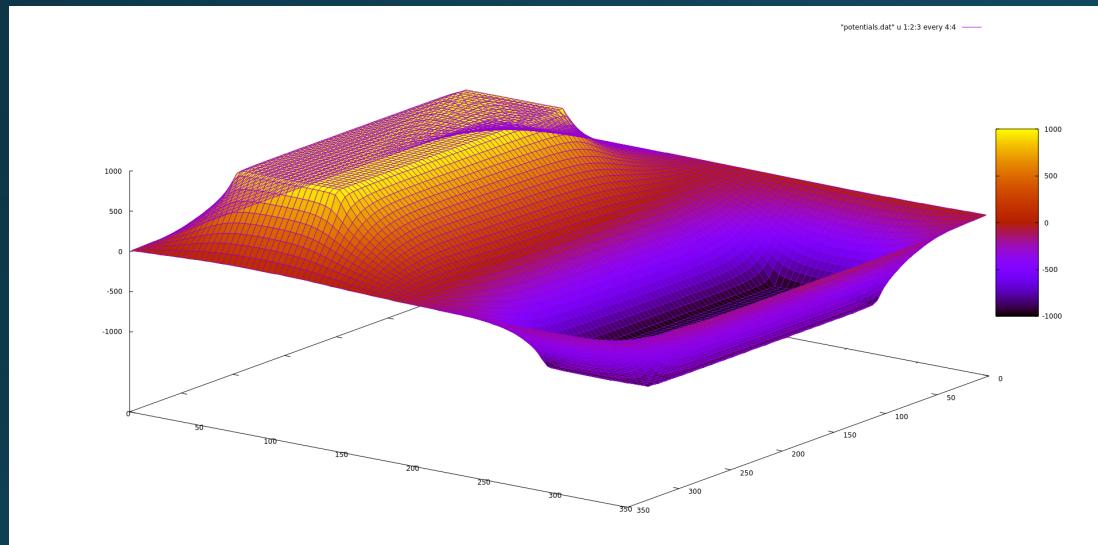
$$\begin{pmatrix} -4 & 1 & 0 & & 0 & 0 & 0 \\ 0 & \textcolor{red}{1} & 0 & \cdots & 0 & 0 & 0 \\ 0 & 1 & -4 & & 0 & 0 & 0 \\ \vdots & & & \ddots & & \vdots & \\ 0 & 0 & 0 & & -4 & 1 & 0 \\ 0 & 0 & 0 & \cdots & 1 & -4 & 1 \\ 0 & 0 & 0 & & 0 & 1 & -4 \end{pmatrix} \begin{pmatrix} V_1 \\ V_2 \\ V_3 \\ \vdots \\ V_{14} \\ V_{15} \\ V_{16} \end{pmatrix} = \begin{pmatrix} 0 \\ \textcolor{red}{25} \\ 0 \\ \vdots \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

Adaptive Stencilling

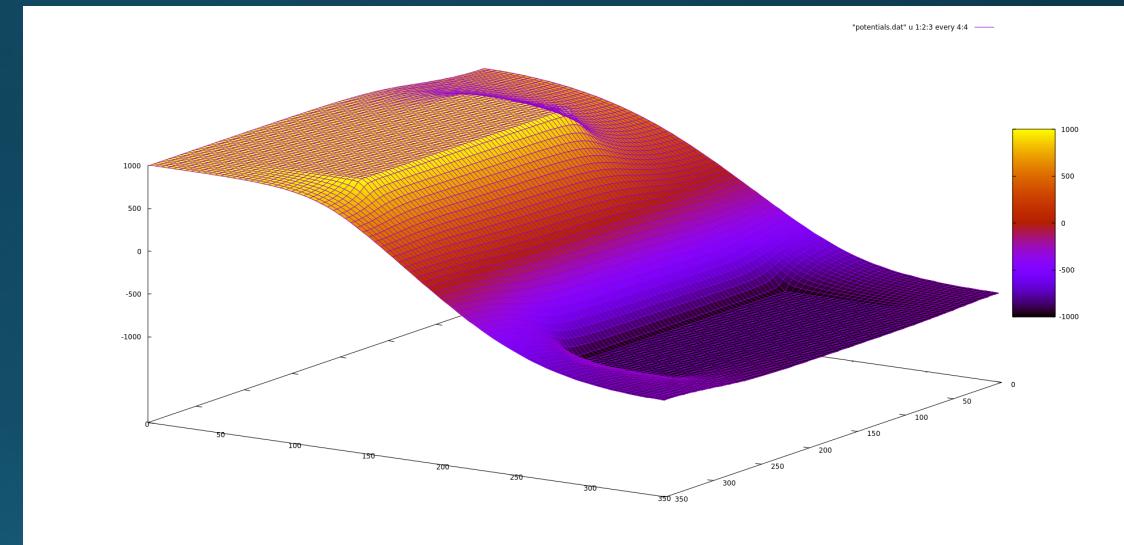
- Adaptive Stencilling is a method where the number of *legs* in the stencil is modified depending on where we are on the grid.
- This avoids the problem of artificially depressing the boundaries.



Adaptive Stencilling



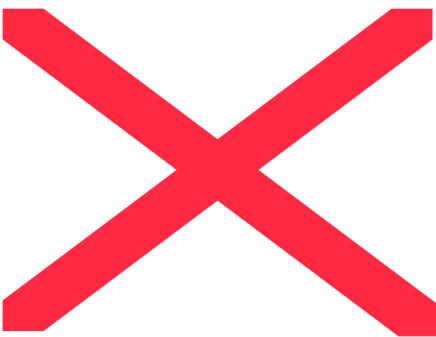
Before



After

Sparse Storage Systems

Assuming an integer is stored in 4 bytes this would imply the matrix A associated with a 400×400 problem would require around 95 GB to store!



Sparse Triplet Format

1	1	-4
1	2	1
1	5	1
:	:	:

Sparse triplet storage cuts the storage size of A from $O(N^4)$ to $O(N^2)$.

Compressed Column Storage

These column offsets tell us where the next column starts in the row array.

nz values	-4	1	1	1	-4	1	...
row index	1	2	4	1	2	3	...
col shift	1	4	...				

Solving the System

- A can never be stored in all its uncompressed glory.
- For maximum efficiency we use the SuperLU package linked with the ATLAS library.
- SuperLU accepts matrices in CCS but it is easier to generate them in sparse triplet so we use the CSparse package to handle the conversion.

LU Decomposition

- The basic idea is to factorise the matrix A into lower and upper triangular matrices L and U .

- The system $Ax = b$ then becomes $LUX = b$

- Letting $Ux = y$ we get the system

$$\begin{aligned}Ly &= b \\ Ux &= y\end{aligned}$$

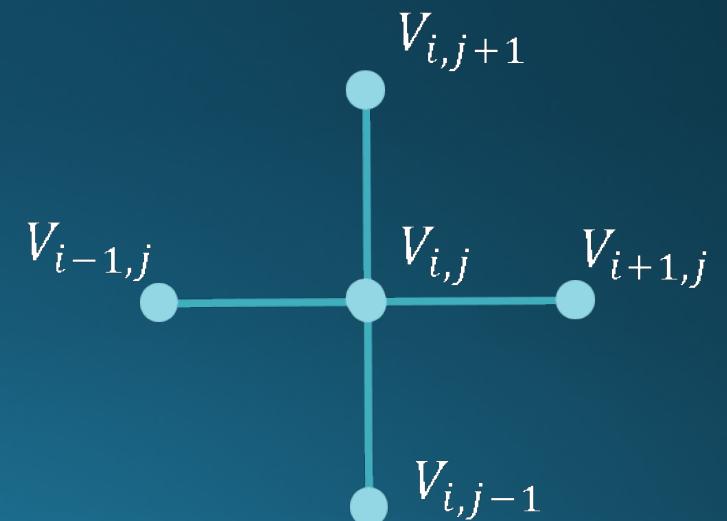
- These equations can be solved by forward, and back substitution respectively and thus no matrix inversion is necessary.

Iterative Method

- Every grid point estimated by the diffusion equation:

$$0 = \nabla^2 V \Rightarrow \frac{\partial V}{\partial t} = \nabla^2 V$$

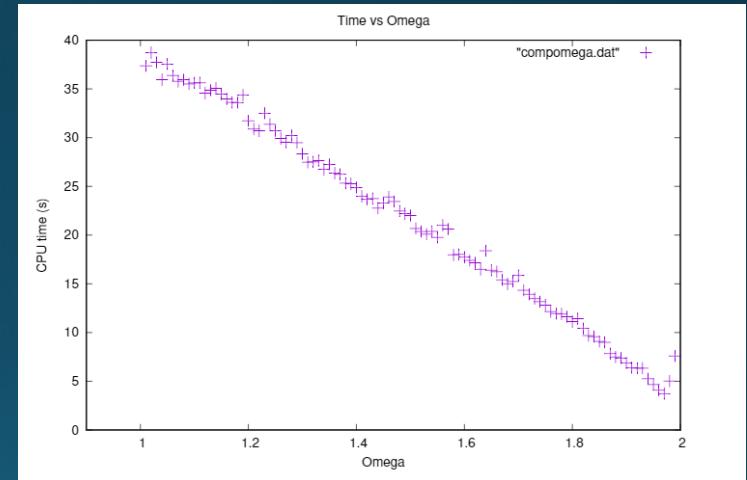
- t is a dummy index of estimations.
- First guess is poor.
- Eventual Convergence to Laplace
- Can we do better?



Iterative Optimization

- We introduce Successive Over-relaxation (SOR)
- 'Steal' future information at rate ω .
- ω is called the relaxation factor.

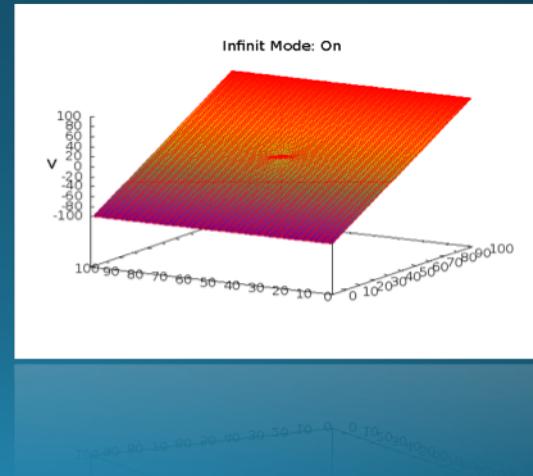
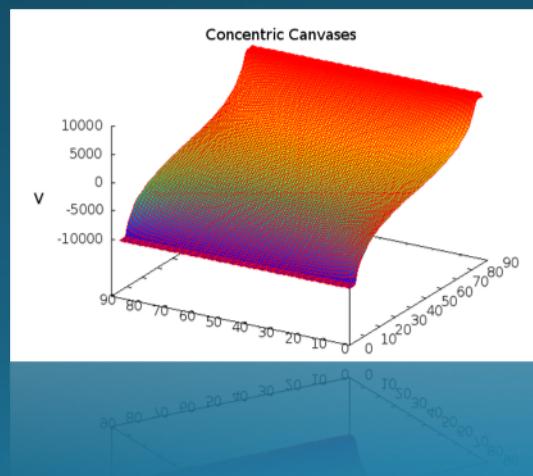
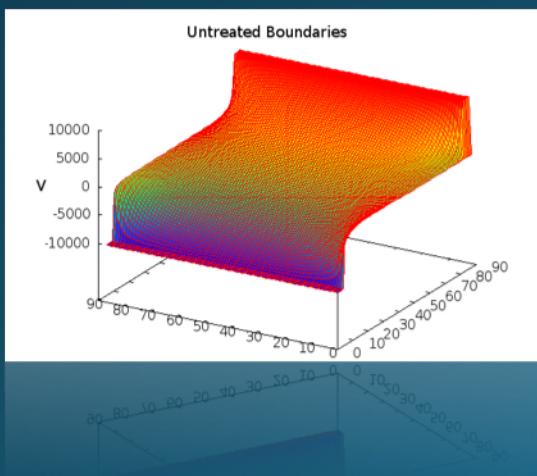
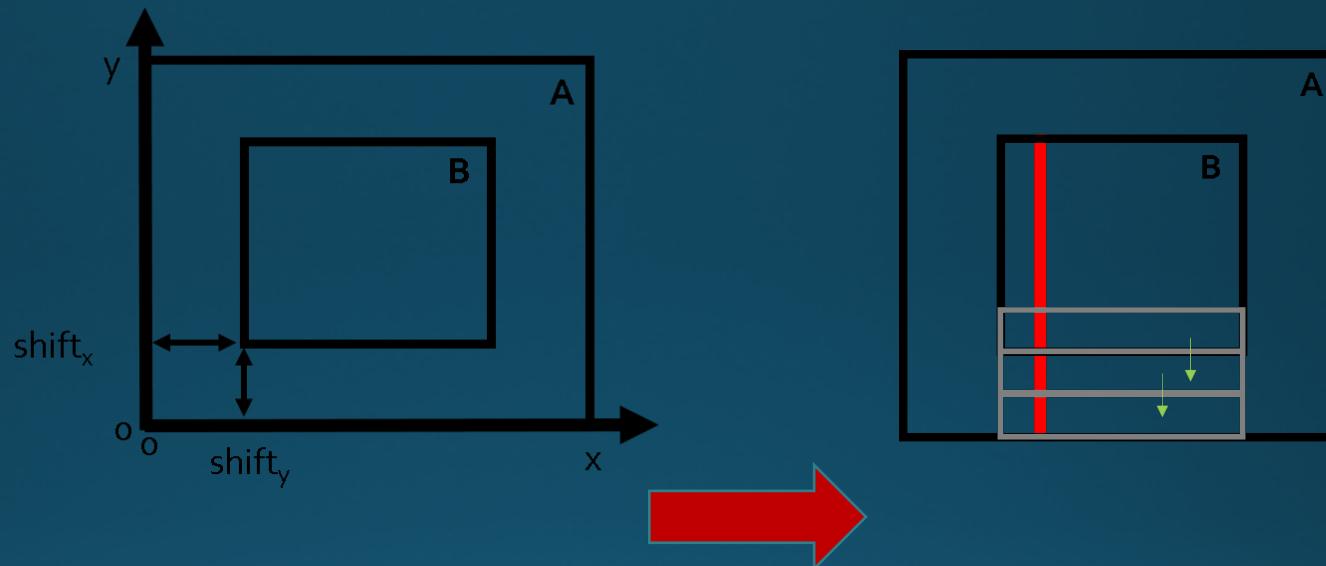
$$\omega_{optimum} \approx \frac{2}{1 + \sin(\frac{\pi}{N})}$$



$$V_{i,j}^{n+1} = V_{i,j}^n + \frac{\Delta t}{\Delta^2} \omega (V_{i+1,j}^n + V_{i-1,j}^{n+1} + V_{i,j+1}^n + V_{i,j-1}^{n+1} - 4V_{i,j}^n)$$

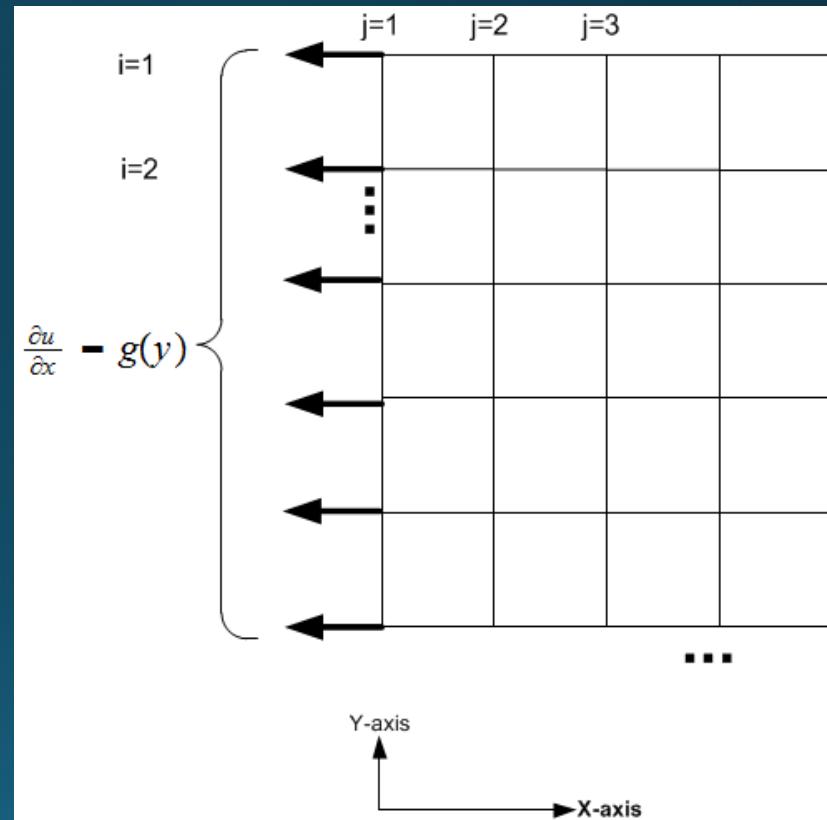
Treating boundaries: Concentric Canvases

No treatment



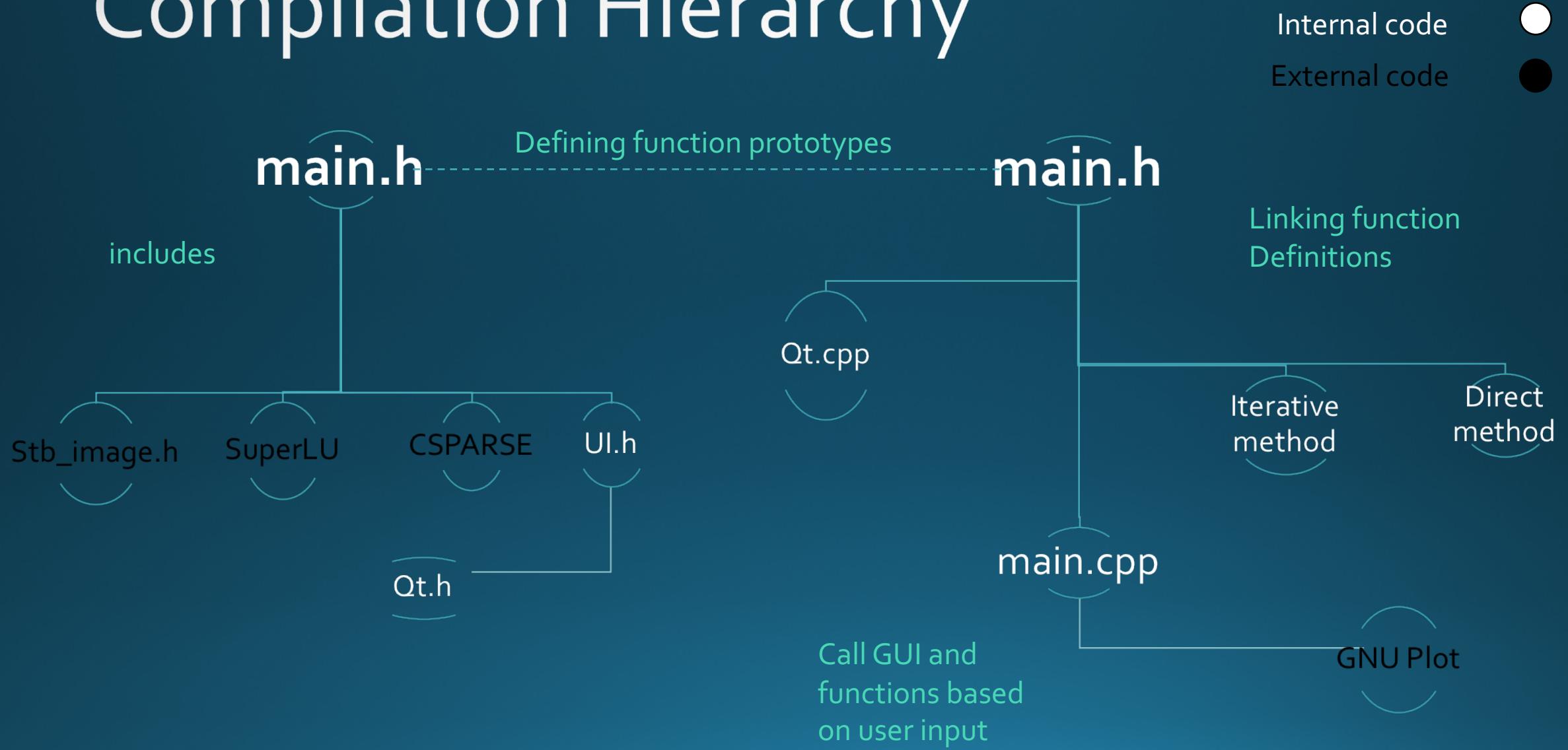
Von Neumann Boundary condition

- Assume slopes are, with good approximation, equal to each other
- $\frac{V_{2,i} - V_{0,i}}{2h} = g(y) = \frac{V_{3,i} - V_{1,i}}{2h}$
- $V_{0,i} = V_{2,i} - 2hg(y)$



https://www.12000.org/my_courses/UC_davis/fall_2010/math_228a/HWs/HW3/Neuman_BC/Neuman_BC.htm

Compilation Hierarchy

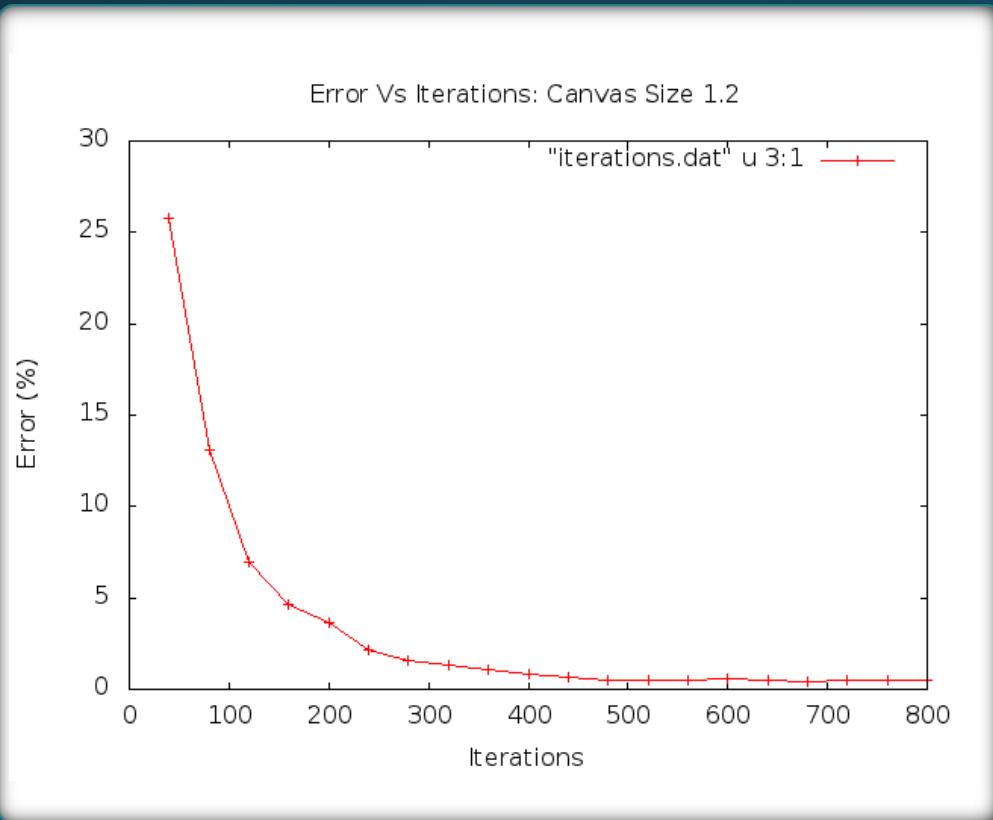


Performance of the Direct Method

Measurement	Problem 0	Problem 1	Nobel Problem
Time	8.684 s	15.130 s	4.857 s
Memory	705.830 MB	1059.962 MB	502.983 MB
Error	0.312%	0.869%	-N/A-

Tests conducted with a 350 x 350 grid.

Controlling Iterative Errors



- The error of the iterative method can be reduced by adjusting the tolerance.
- The direct and iterative methods agree at larger iterations.
- We were able to achieve relative errors as low as 0.487% for Problem 0 and 0.740% for Problem 1

Comparison of the Solvers

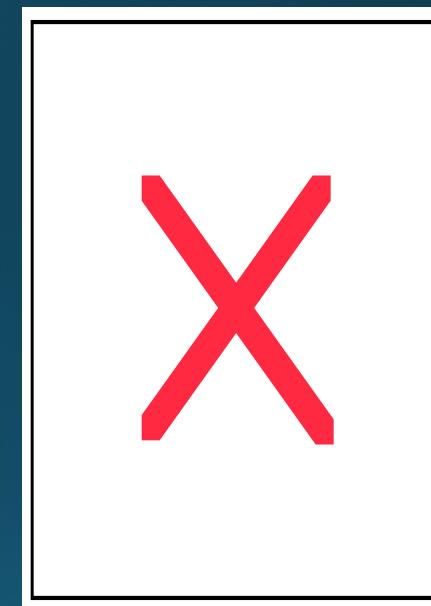
- The direct method was taken as the reference point since no analytical solution was available.
- The iterative method converged to a relative error of 0.075% after 460 iterations (4.48s).

Multiwire Proportional Chamber

Nobel Prize, Georges Charpak (1992)

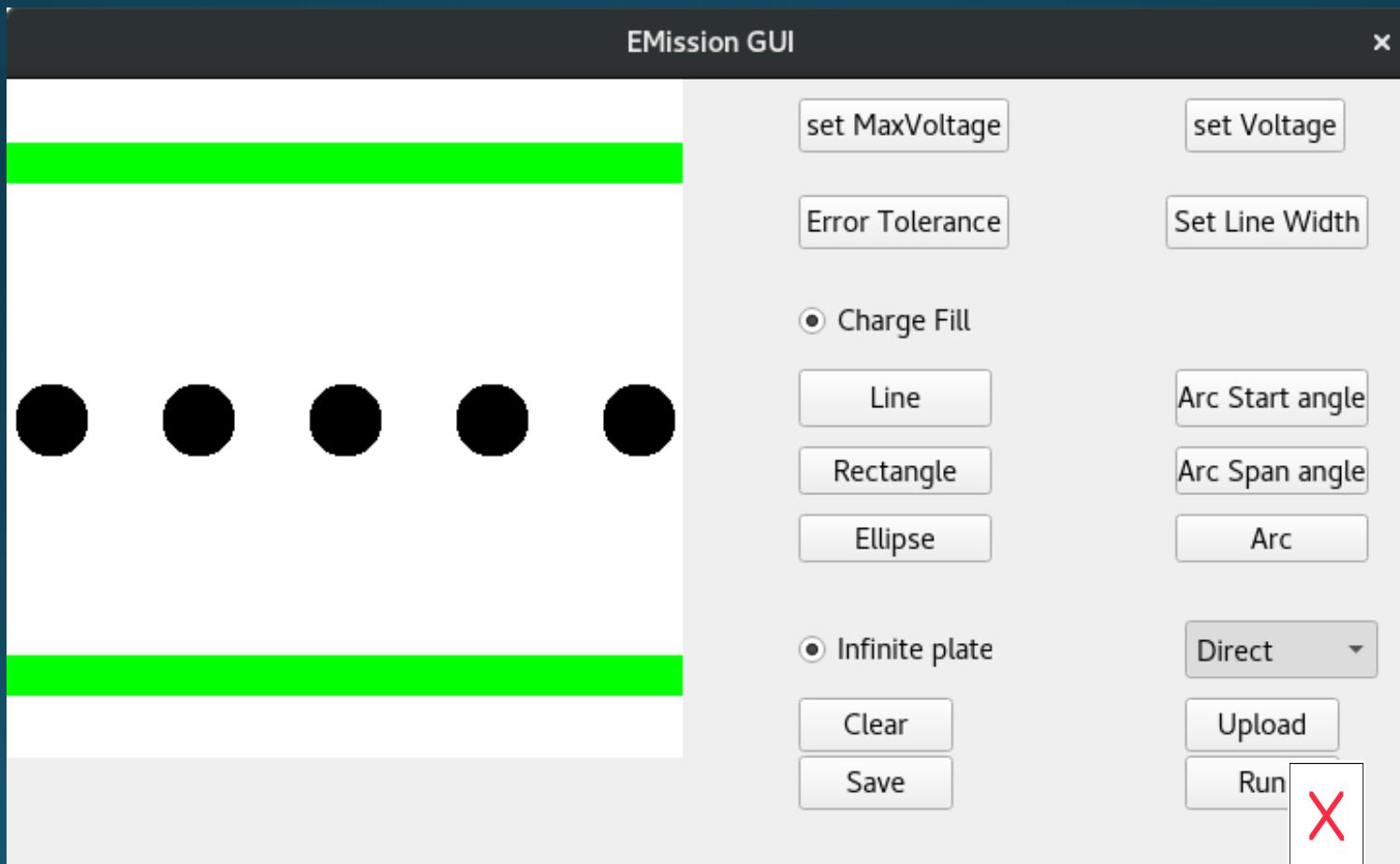


Multi wire proportional chamber

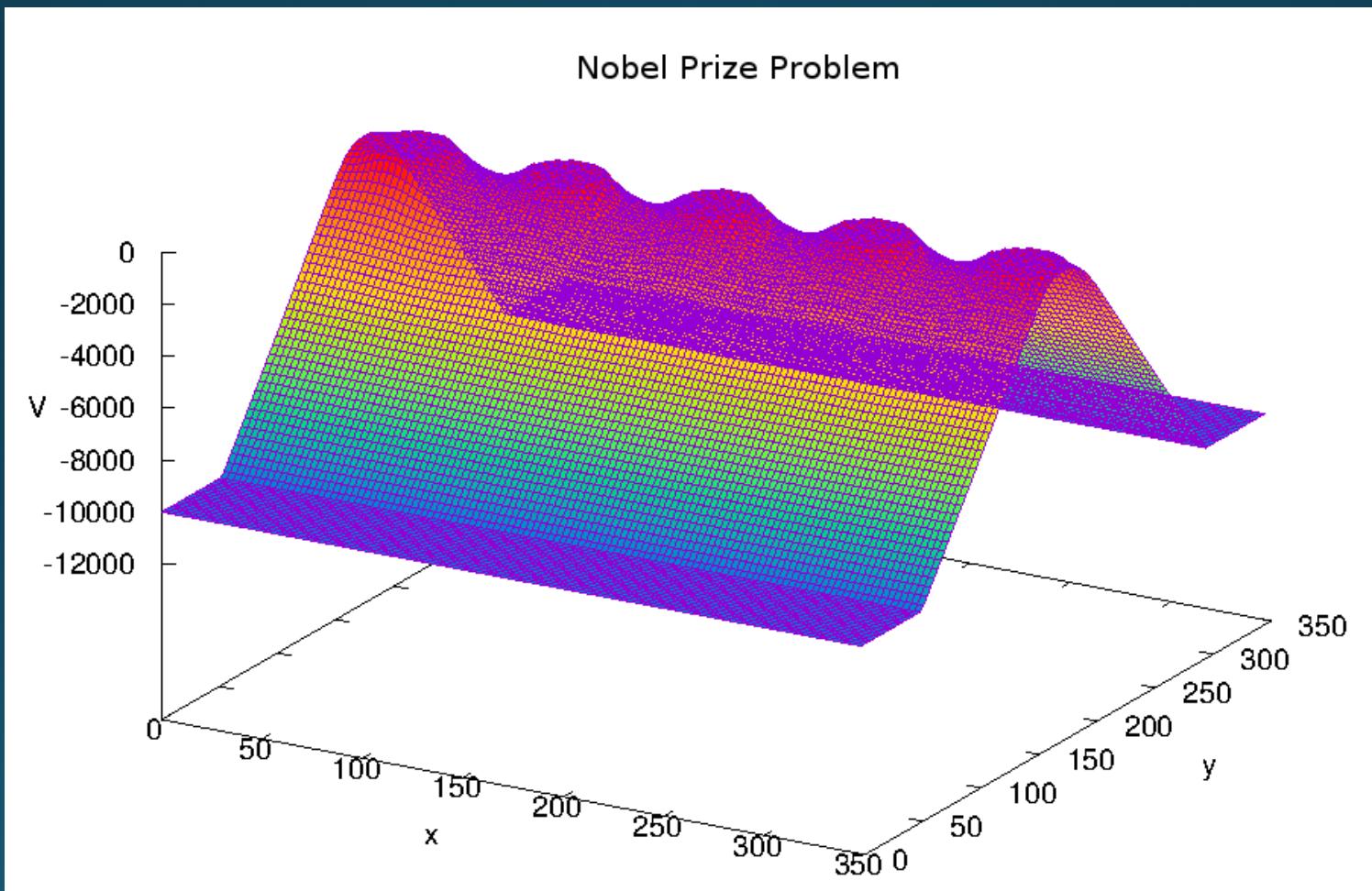


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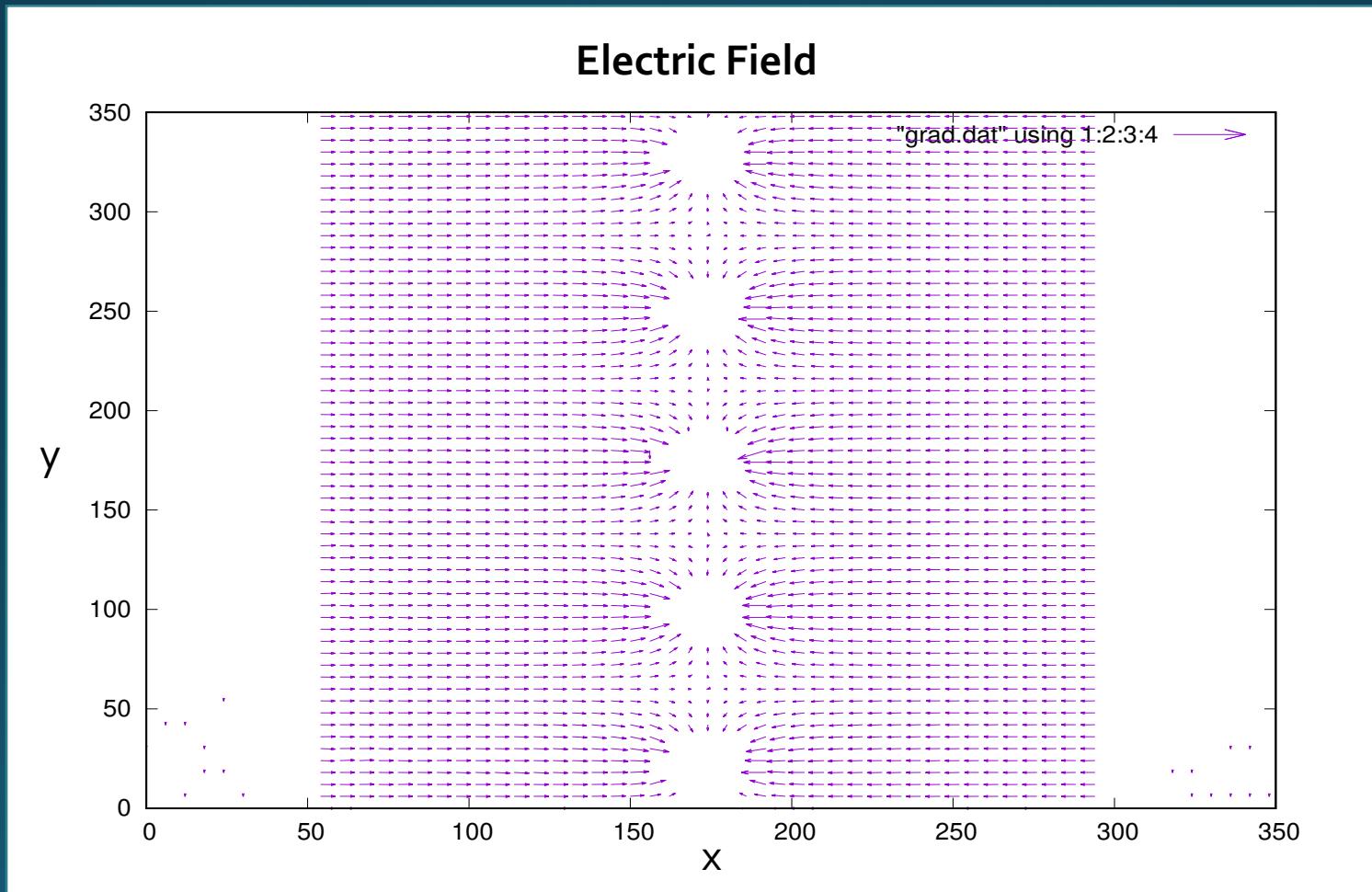
Example Run



Results:



Results:



Summary

- Created a custom GUI to make problem specification general and easy.
- Developed two numerical solvers that accomplish the goals of the projects through the iterative and direct paradigm.
- Coordinated the entire project through a publicly accessible repository.

Possible Improvements

- Support for dielectrics.
- Create a statically linked version to allow for easy distribution of the code.
- Implementation of multigrid methods.

On behalf of the Emission group, thank you for your attention.

