ANNOUNCEMENT

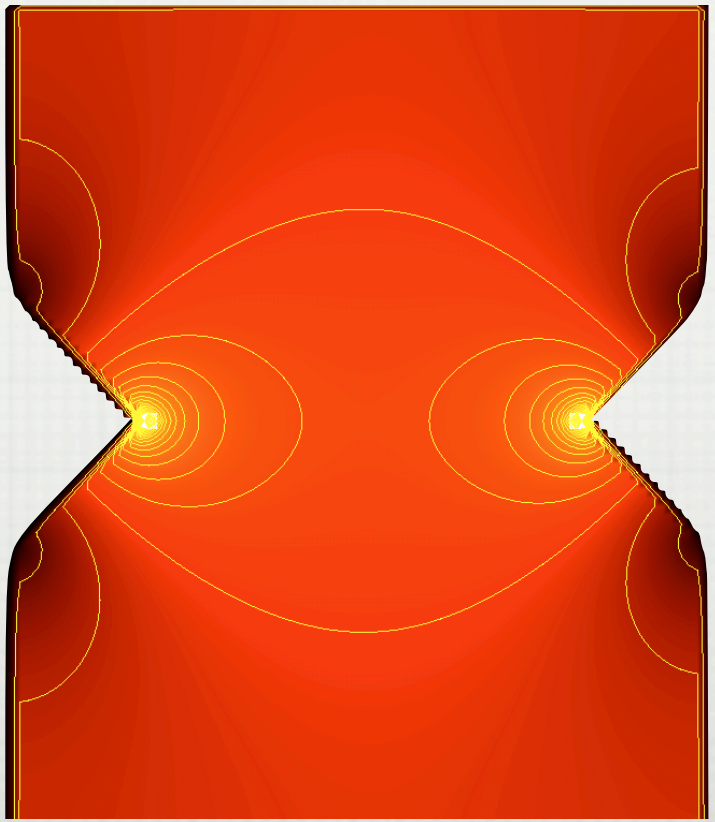
- **Creation of New Class**
  - **PHYS 6960 ADV COMPUTATIONAL PHYSICS**
  - **Will meet on Wednesday 5PM to 6:50 PM**
- **Prerequisite: 4810, QM**
-

POSSIBLE TOPICS

(1) finite difference methods;
(2) Molecular dynamics,
(3) wavelet transforms;
(4) Perturbation theory at low orders
(5) Random numbers and multidimensional integration (importance sampling)
(6) Dynamical Mean Field Theory for model Hamiltonians
(7) Local Density Approximation + Dynamical Mean Field Theory (LDA+DMFT) i action
(8) Parallel programming with MPI
(9) Recursion techniques
(10) Sparse ALgebra
(11) Solving Systems of Equations with Matrices
(12) Fractals & Statistical Growth
(13) More GPU
(14) PDEWaves: String, Quantum Packet, and E&M

PHY-4810
COMPUTATIONAL PHYSICS

LECTURE 10: PARTIAL DIFFERENTIAL EQUATIONS (PDE)



PDE: DEFINITION

Partial differential equations (PDEs) are a type of differential equations involving an unknown function (or functions) of several independent variables and their partial derivatives with respect to those variables.

$$F(x_1, \dots x_n, u, \frac{\partial}{\partial x_1}, \dots \frac{\partial}{\partial x_n} u, \frac{\partial^2}{\partial x_1 \partial x_1} u, \dots \frac{\partial^2}{\partial x_1 \partial x_2} u, \dots) = 0$$

EXAMPLES

- **2D Laplace equation**
- **Heat equation**
- **Wave equation**
- **Spherical waves**
- **Ginzburg Landau (superconductivity)**
- **Vibrating Membrane**

CLASSIFICATION

$$A\frac{\partial^2 U}{\partial x^2} + 2B\frac{\partial^2 U}{\partial x \partial y} + C\frac{\partial^2 U}{\partial y^2} + D\frac{\partial U}{\partial x} + E\frac{\partial U}{\partial y} = F$$

CLASSIFICATION

- **General Form**

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- **Types**

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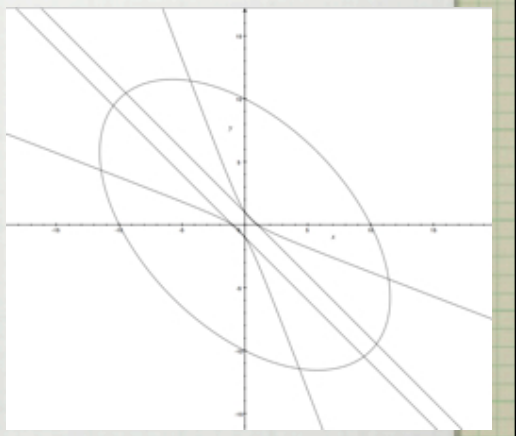
- **Types**

Elliptic	*Parabolic*	*Hyperbolic*
$d = AC - B^2 > 0$	$d = AC - B^2 = 0$	$d = AC - B^2 < 0$
$\nabla^2 U(x) = -4\pi\rho(x)$	$\nabla^2 U(\mathbf{x}, t) = a\partial U/\partial t$	$\nabla^2 U(\mathbf{x}, t) = c^{-2}\partial^2 U/\partial t^2$
Poisson's	Heat	Wave



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- If the boundary condition is the value of the **normal derivative** on the surrounding surface, we have a **Neumann boundary condition.**

- If both the **value** of solution and **its derivative** are specified on a closed boundary, we have a **Cauchy boundary condition** (***these are more initial conditions than boundary conditions!***)

BOUNDARY CONDITIONS

Boundary condition	Elliptic (Poisson equation)	Hyperbolic (Wave equation)	Parabolic (Heat equation)
Dirichlet open surface	Underspecified	Underspecified	*Unique and stable (1D)*
Dirichlet closed surface	*Unique and stable*	Overspecified	Overspecified
Neumann open surface	Underspecified	Underspecified	*Unique and stable (1D)*
Neumann closed surface	*Unique and stable*	Overspecified	Overspecified
Cauchy open surface	Unphysical	*Unique and stable*	Overspecified
Cauchy closed surface	Overspecified	Overspecified	Overspecified

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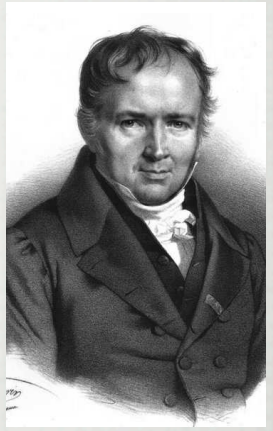
LAPLACE AND POISSON EQUATIONS

$$\frac{\partial^2 U(x,y)}{\partial x^2} + \frac{\partial^2 U(x,y)}{\partial y^2} = \begin{cases} 0 & \text{Laplace's equation} \\ -4\pi\rho(\mathbf{x}) & \text{Poisson's equation} \end{cases}$$



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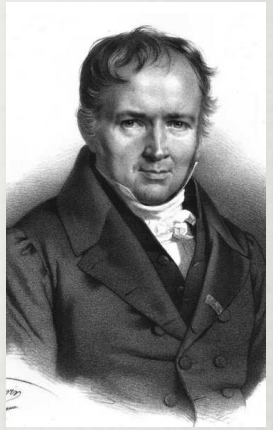

- **Dirichlet: impose potential U at the boundaries**
- **Neuman: impose electric field at the boundaries**

ANALYTICAL SOLUTIONS

$$U(x,y) = X(x)Y(y) \qquad \Rightarrow \qquad \frac{d^2X(x)/dx^2}{X(x)} + \frac{d^2Y(y)/dy^2}{Y(y)} = 0$$

ANALYTICAL SOLUTIONS

- **Electrodynamics: use of polynomial expansions (for instance, Fourier) using separation of variables.**

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- **Cons:**
  - **Solutions in infinite series end up being numerical!**
  - **Often hard to change specific boundary conditions in complicated geometries**

NUMERICAL SOLUTION

- **Remember Taylor or McLaurin (and homework #1):**

$$U(x+\Delta x,y) = U(x,y) + \frac{\partial U}{\partial x}\Delta x + \frac{1}{2}\frac{\partial^2 U}{\partial x^2}(\Delta x)^2 + \cdots$$

$$U(x-\Delta x,y) = U(x,y) - \frac{\partial U}{\partial x}\Delta x + \frac{1}{2}\frac{\partial^2 U}{\partial x^2}(\Delta x)^2 - \cdots$$

- **Adding equation yields the central difference approximation:**

$$\frac{\partial^2 U(x,y)}{\partial x^2} \simeq \frac{U(x+\Delta x,y)+U(x-\Delta x,y)-2U(x,y)}{(\Delta x)^2} + \mathcal{O}(\Delta x^4)$$

$$\frac{\partial^2 U(x,y)}{\partial y^2} \simeq \frac{U(x,y+\Delta y)+U(x,y-\Delta y)-2U(x,y)}{(\Delta y)^2} + \mathcal{O}(\Delta y^4)$$

LAPLACIAN OF U(X,Y)

$$\frac{U(x+\Delta x,y)+U(x-\Delta x,y)-2U(x,y)}{(\Delta x)^2} + \frac{U(x,y+\Delta y)+U(x,y-\Delta y)-2U(x,y)}{(\Delta y)^2} = -4\pi\rho$$

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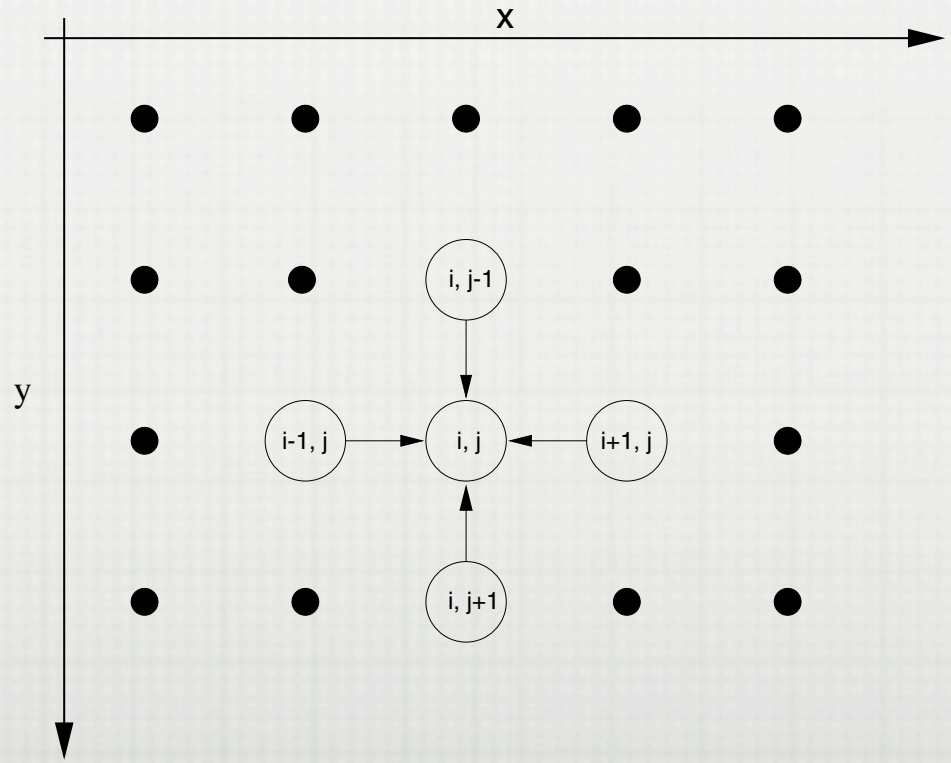
For equal spacing in x and y :

$$U(x+\Delta x,y)+U(x-\Delta x,y)+U(x,y+\Delta y)+U(x,y-\Delta y)-4U(x,y) = -4\pi\rho$$

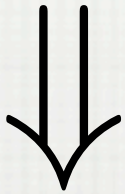
LET'S MEDITATE

$$U(x+\Delta x,y)+U(x-\Delta x,y)+U(x,y+\Delta y)+U(x,y-\Delta y)-4U(x,y)\ =-4\pi\rho$$



DISCRETIZED VERSION

$$U(x+\Delta x,y)+U(x-\Delta x,y)+U(x,y+\Delta y)+U(x,y-\Delta y)-4U(x,y) = -4\pi\rho$$



$$U_{i,j} = \tfrac{1}{4}\left[U_{i+1,j}+U_{i-1,j}+U_{i,j+1}+U_{i,j-1}\right]+\pi\rho(i\Delta,j\Delta)\Delta^2$$

$$x = x_0 + i\Delta, \qquad y = y_0 + j\Delta \qquad i,j = 0,\ldots,N_{\text{max-1}}$$

$$\Delta x = \Delta y = \Delta = L/(N_{\text{max}}-1)$$

RELAXATION: JACOBI METHOD (I)

$$\underbrace{U_{i,j}}_{\text{NEW}} = \frac{1}{4}\underbrace{\left[U_{i+1,j} + U_{i-1,j} + U_{i,j+1} + U_{i,j-1}\right]}_{\text{OLD}} + \pi\rho(i\Delta, j\Delta)\Delta^2$$

- **IMPOSE BOUNDARY CONDITIONS**
- **START WITH "REASONABLE GUESS" TO ACCELERATE CONVERGENCE**

RELAXATION: GAUSS-SEIDEL METHOD

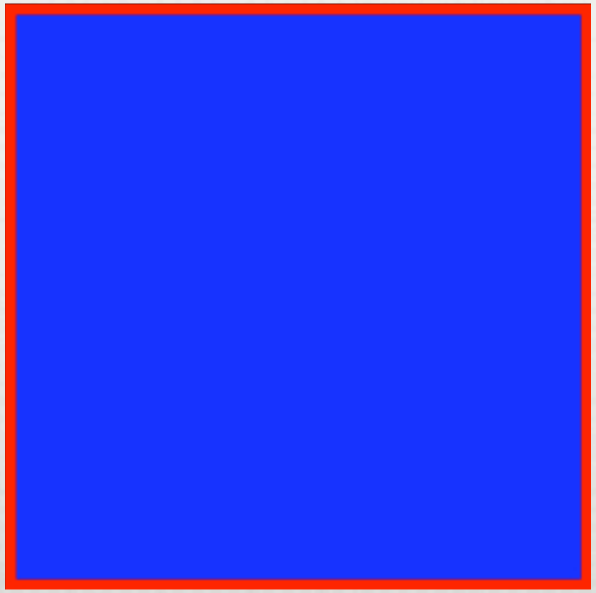
OLD OLD

$$U_{i,j} = \frac{1}{4}\left[U_{i+1,j} + U_{i-1,j} + U_{i,j+1} + U_{i,j-1}\right] + \pi\rho(i\Delta, j\Delta)\Delta^2$$

NEW NEW NEW

FIRST TEST: BOUNDARY CONDITIONS

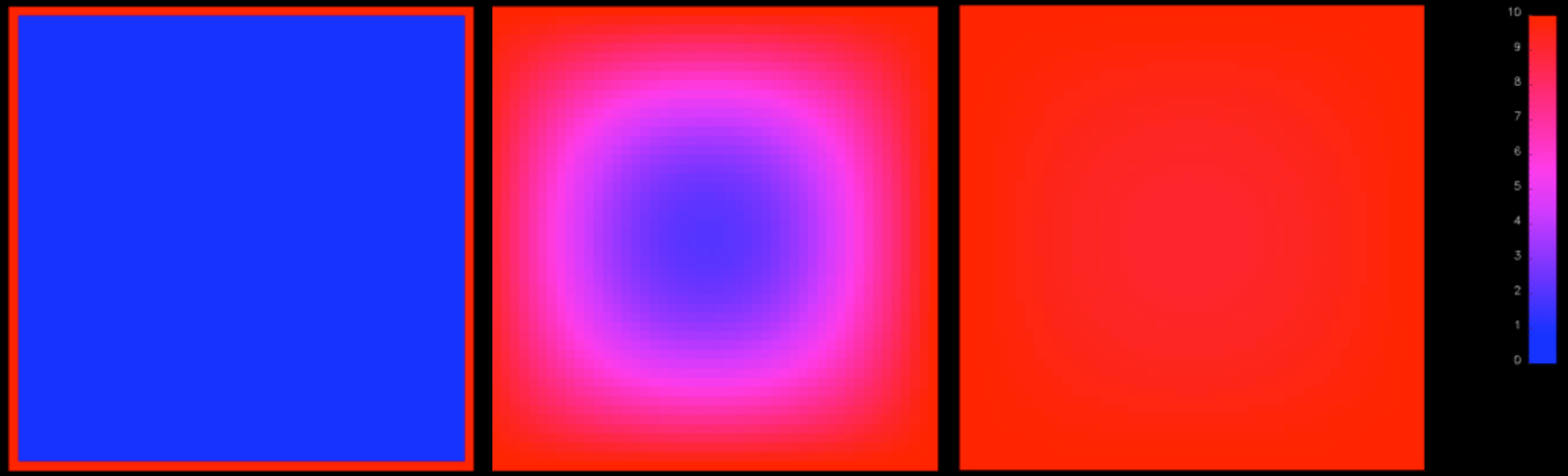
- **We should know the potential at the boundary (Dirichlet)**
- **We could know the derivative of the potential at the boundary (Neumann)**



V=10 VOLT

V=0 VOLT

INITIAL AFTER FEW ITERATIONS CONVERGED



V=10 V ON THE BOUNDARIES

HOW TO ACCELERATE CONVERGENCE: OVER- AND UNDER- RELAXATIONS

$$U_{i,j}^{(\text{new})} = U_{i,j}^{(\text{old})} + r_{i,j}$$

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$$u_{i,j}^{(\text{new})} = u_{i,j}^{(\text{old})} + r_{i,j}$$

$$r_{i,j} \equiv u_{i,j}^{(\text{new})} - u_{i,j}^{(\text{old})}$$

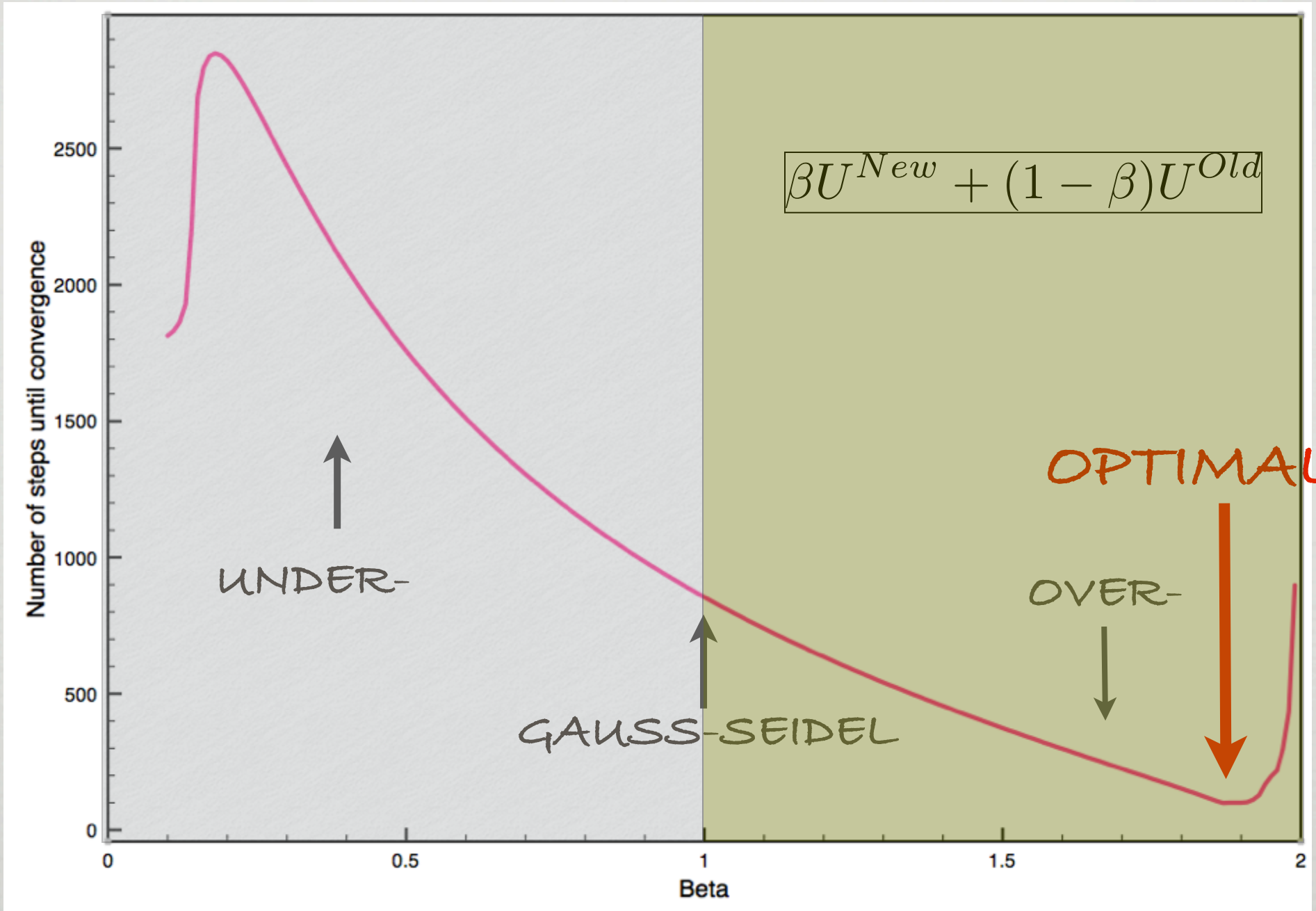
$$= \tfrac{1}{4}\left[u_{i+1,j}^{(\text{old})} + u_{i-1,j}^{(\text{new})} + u_{i,j+1}^{(\text{old})} + u_{i,j-1}^{(\text{new})} \right] - u_{i,j}^{(\text{old})}$$

$$u_{i,j}^{(\text{new})} = u_{i,j}^{(\text{old})} + \omega\, r_{i,j}$$

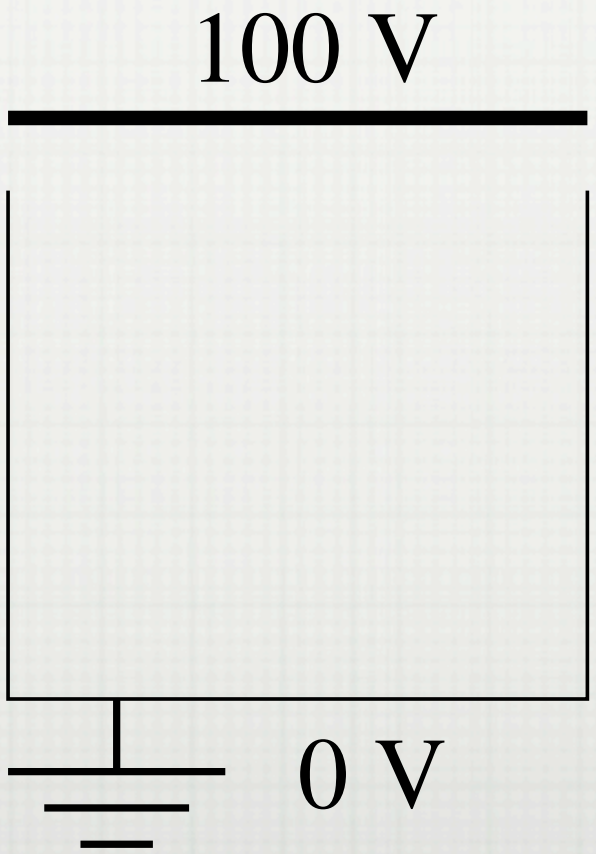
ω < 1: under-relaxation

ω = 1: Gauss-Seidel

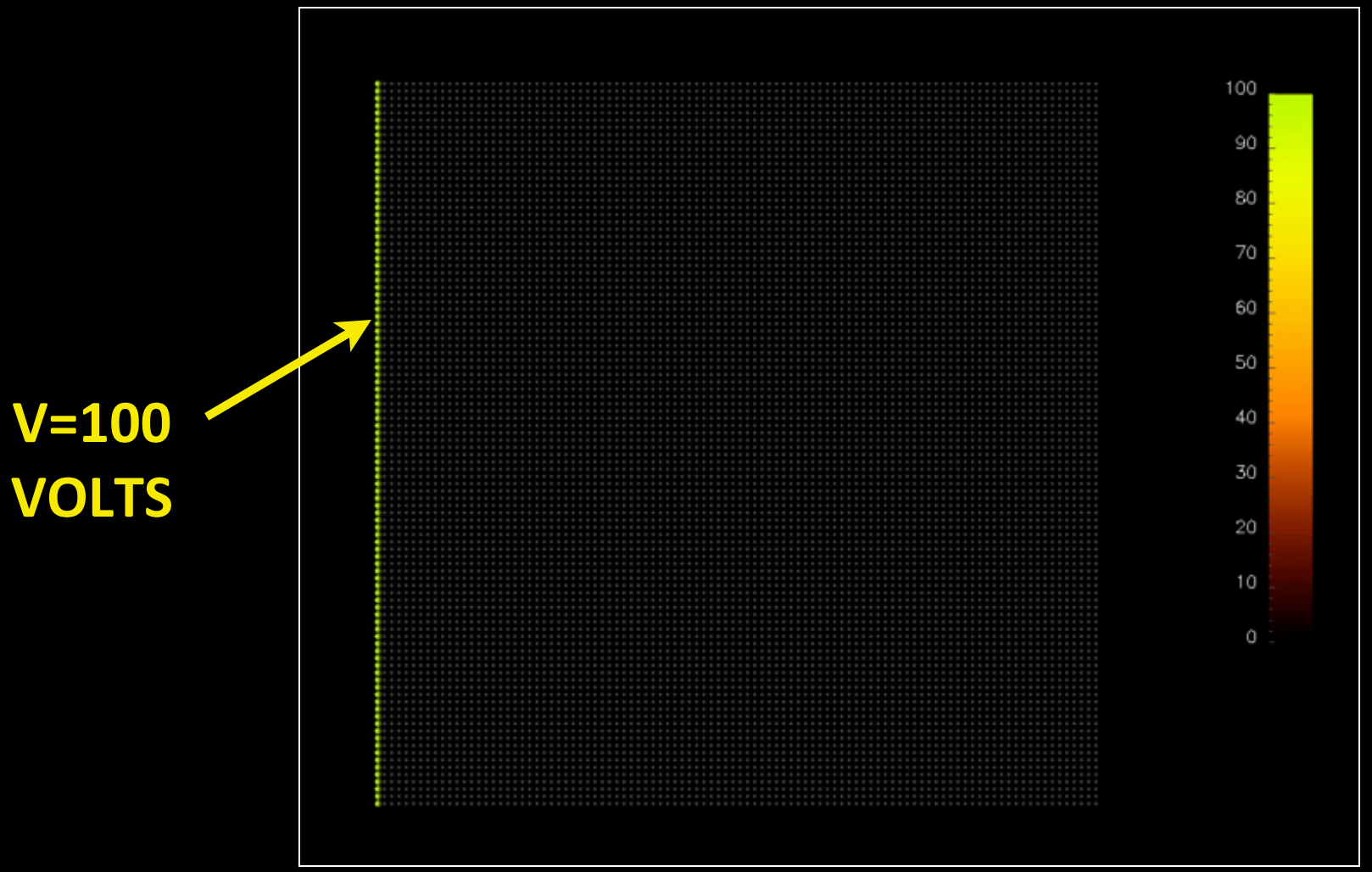
ω ≥ 1: over-relaxation


Number of steps until convergence
2500
2000
1500
1000
500
0
0
0.5
1
1.5
2
Beta
$\beta U^{New} + (1-\beta)U^{Old}$
UNDER-
GAUSS-SEIDEL
OVER-
OPTIMAL

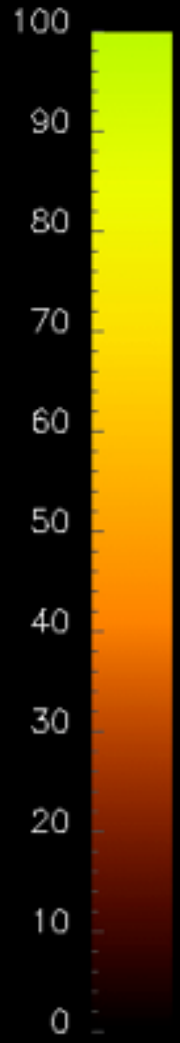
OTHER EXAMPLE: SINGLE METALLIC PLATE CAPACITOR

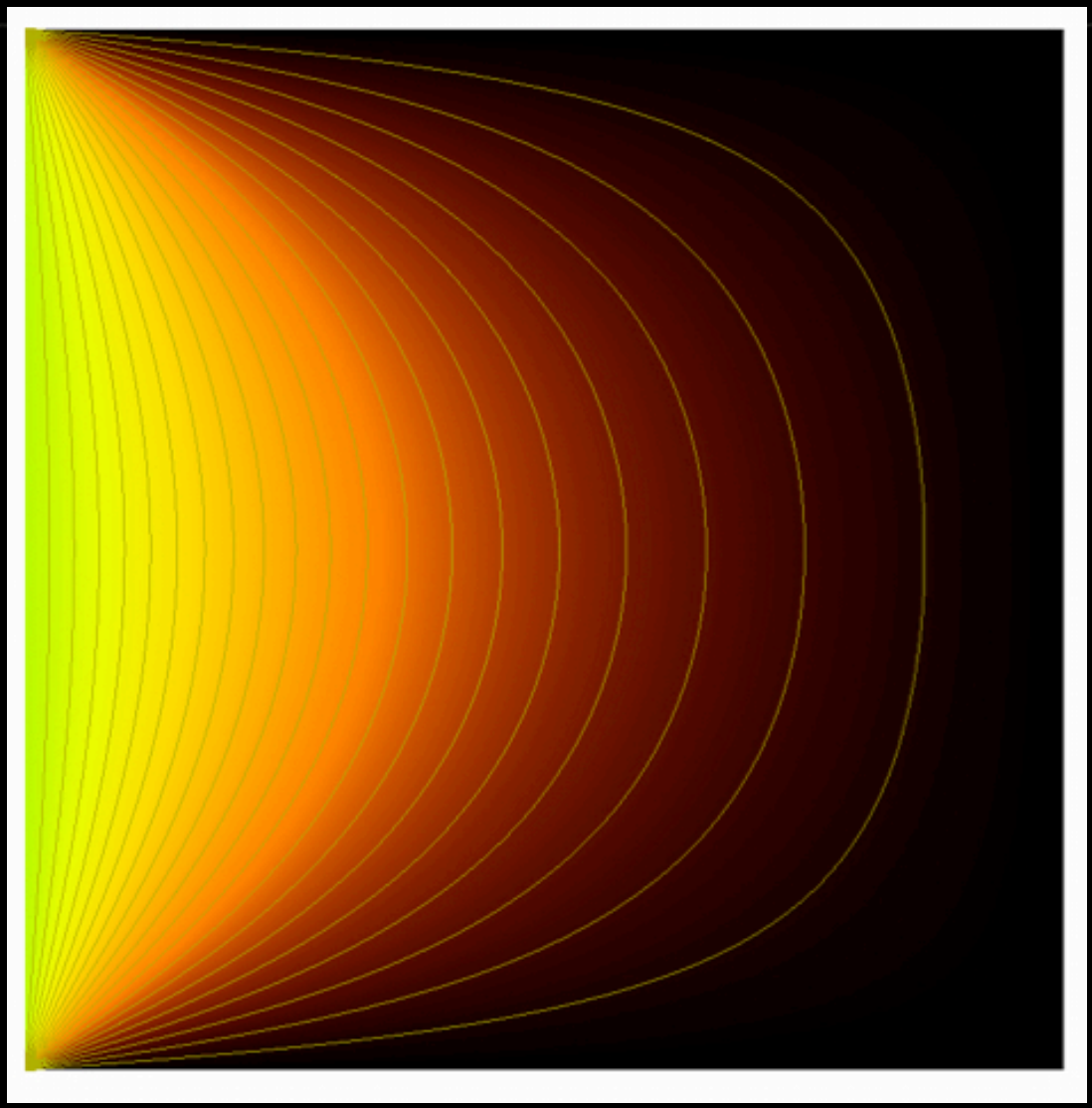


INITIAL CONDITIONS

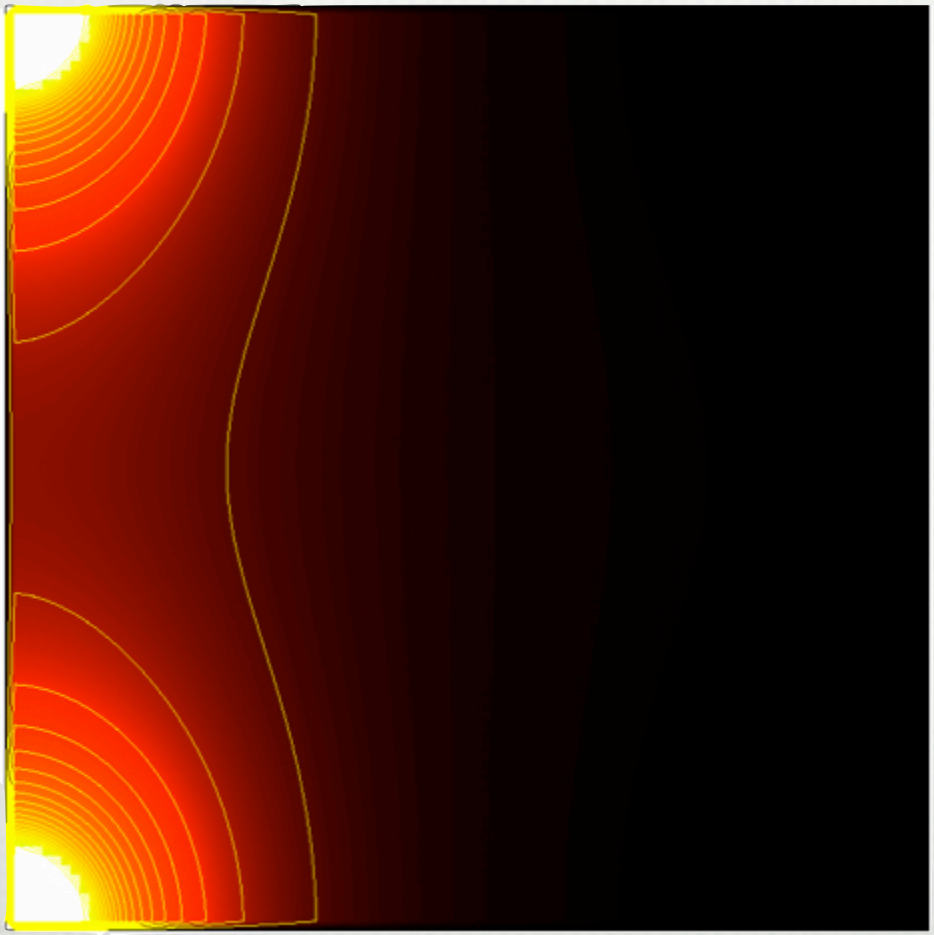


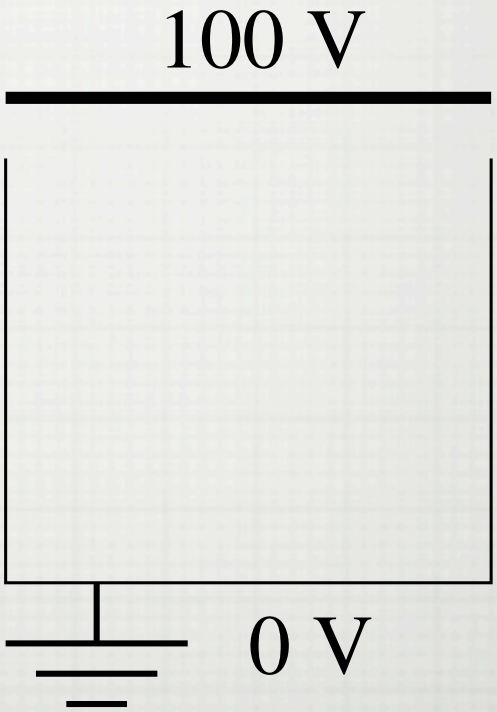
AFTER CONVERGENCE



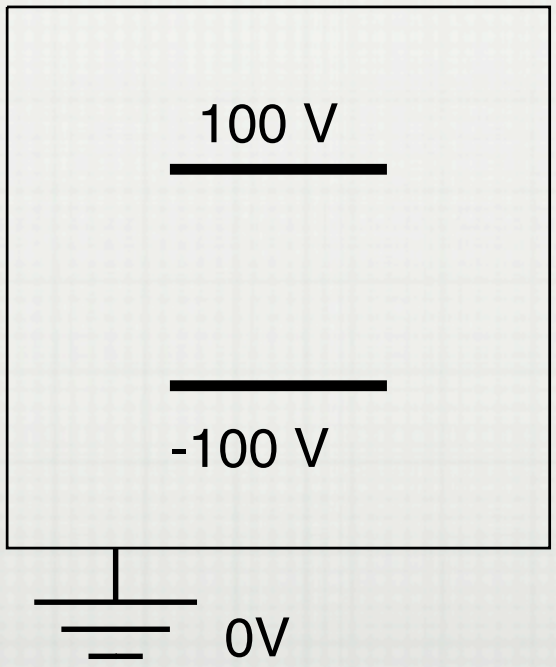


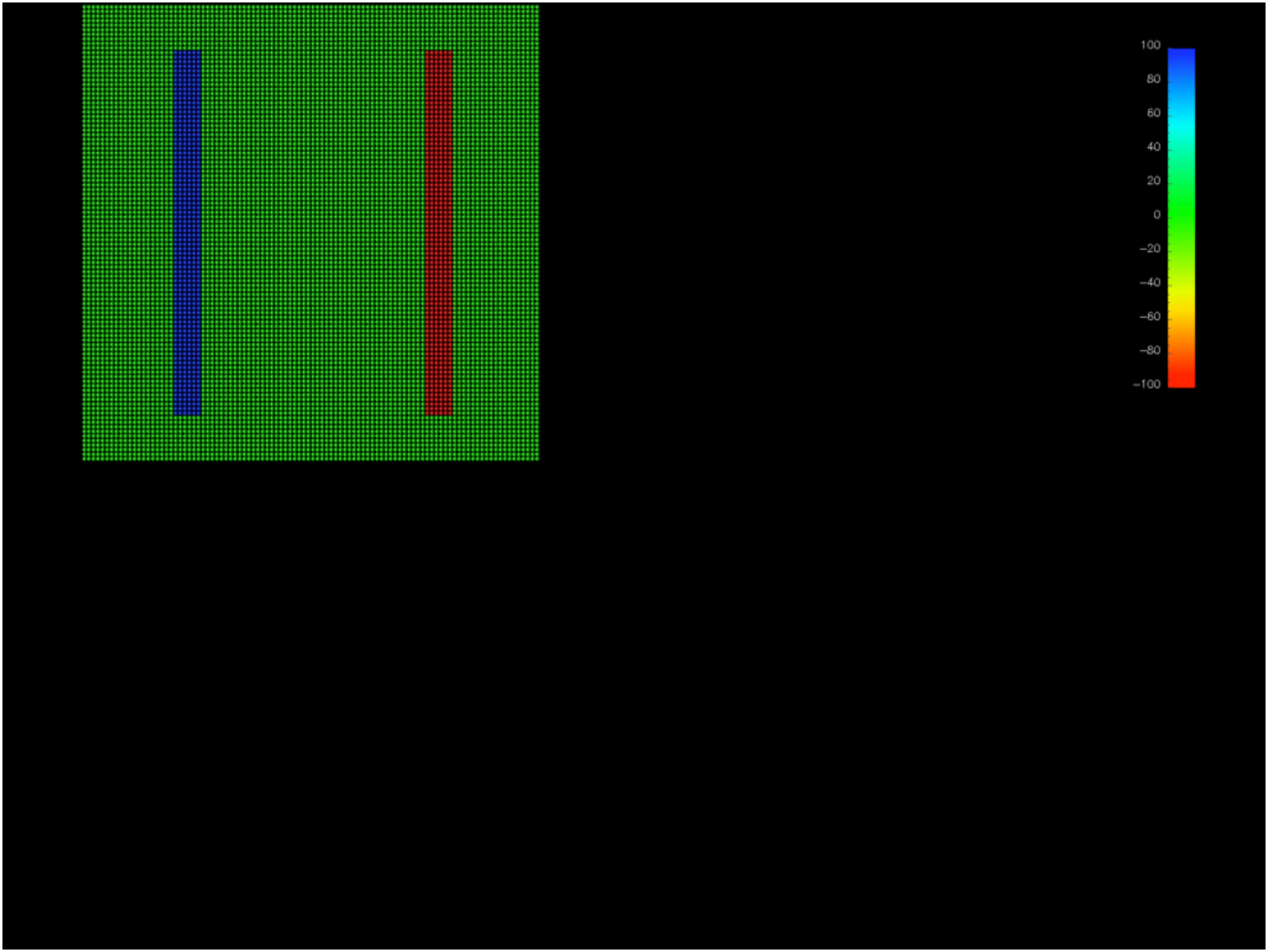
ELECTRIC FIELD





PARALLEL PLATE CAPACITOR

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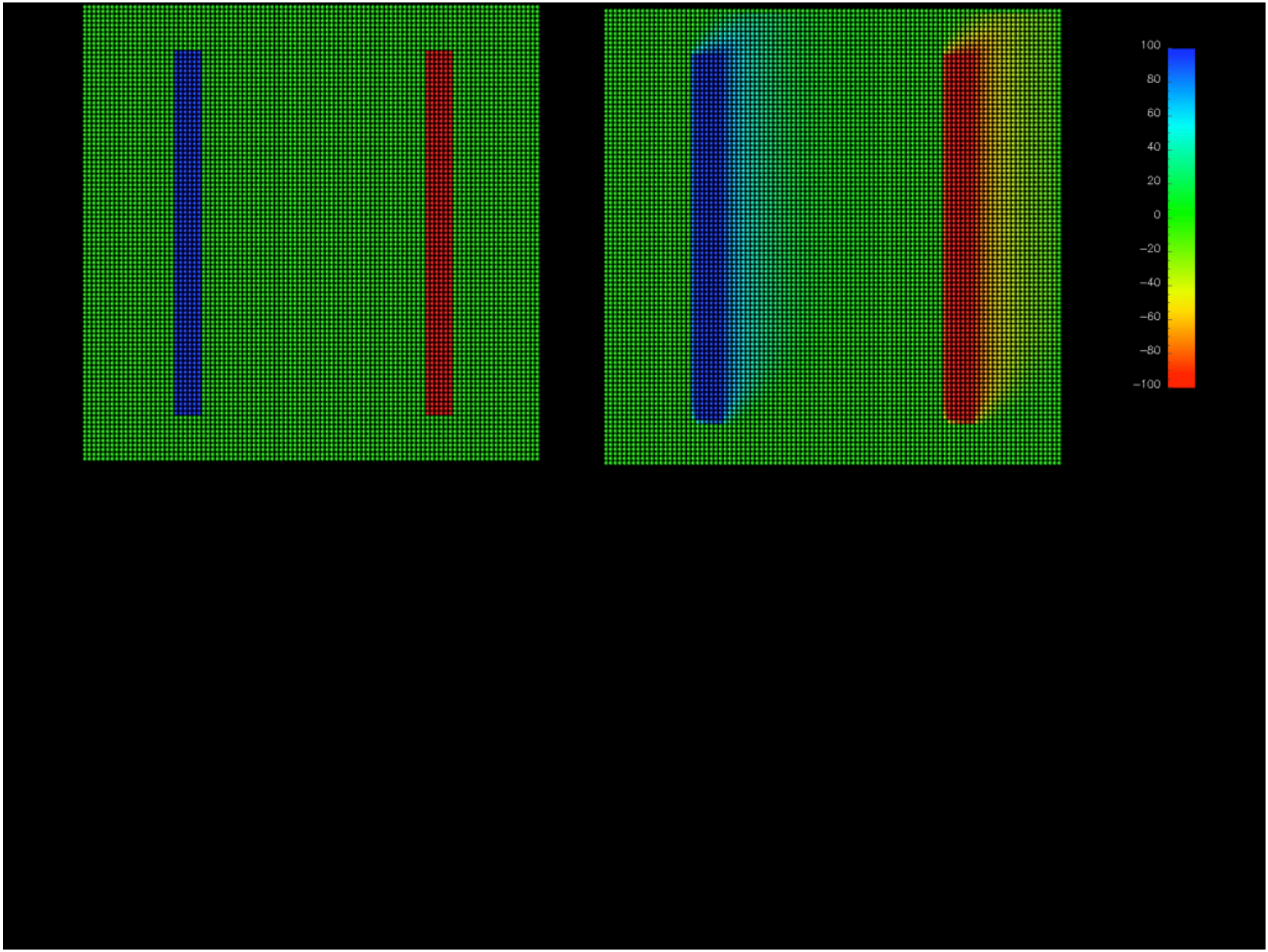
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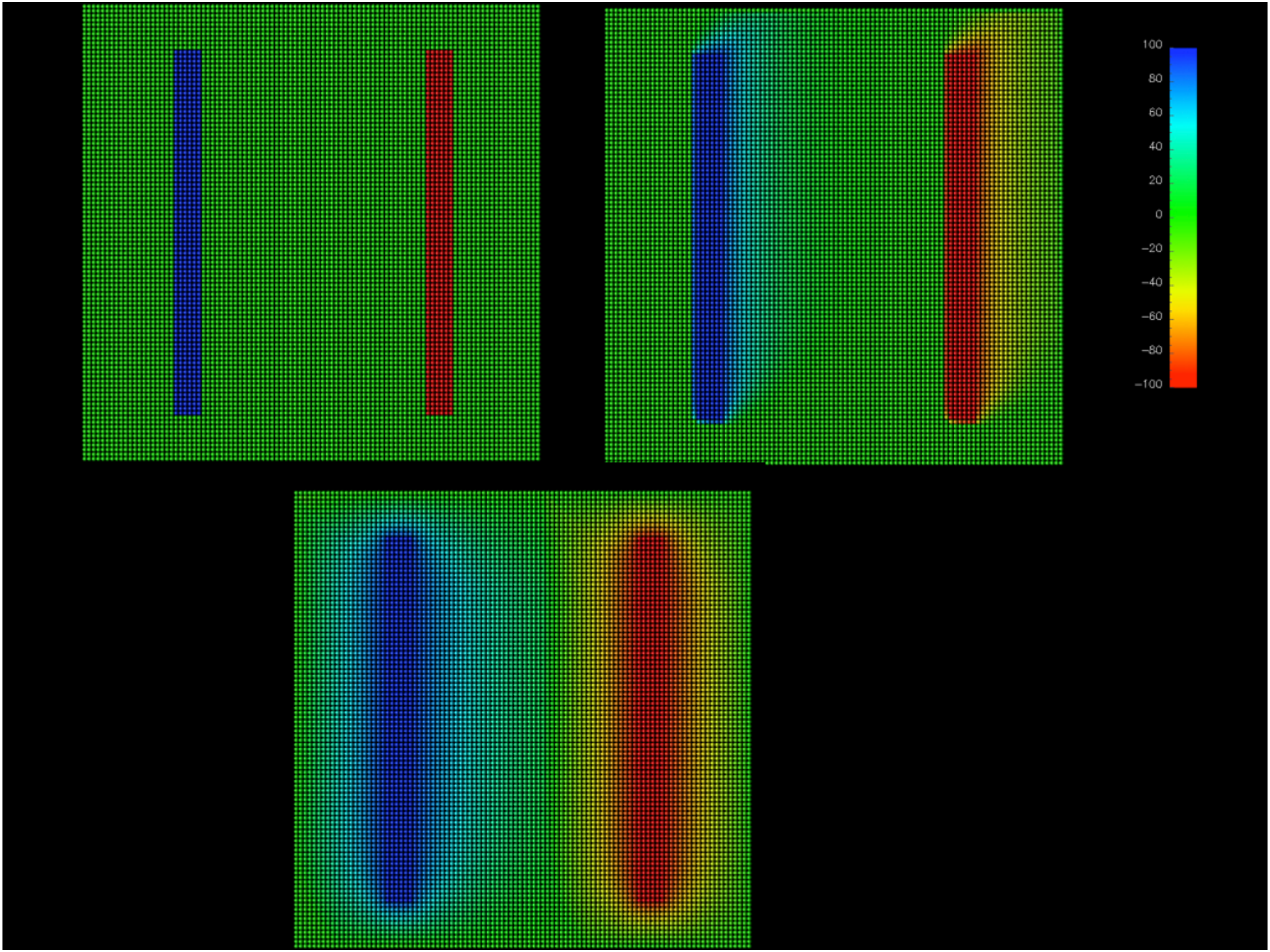
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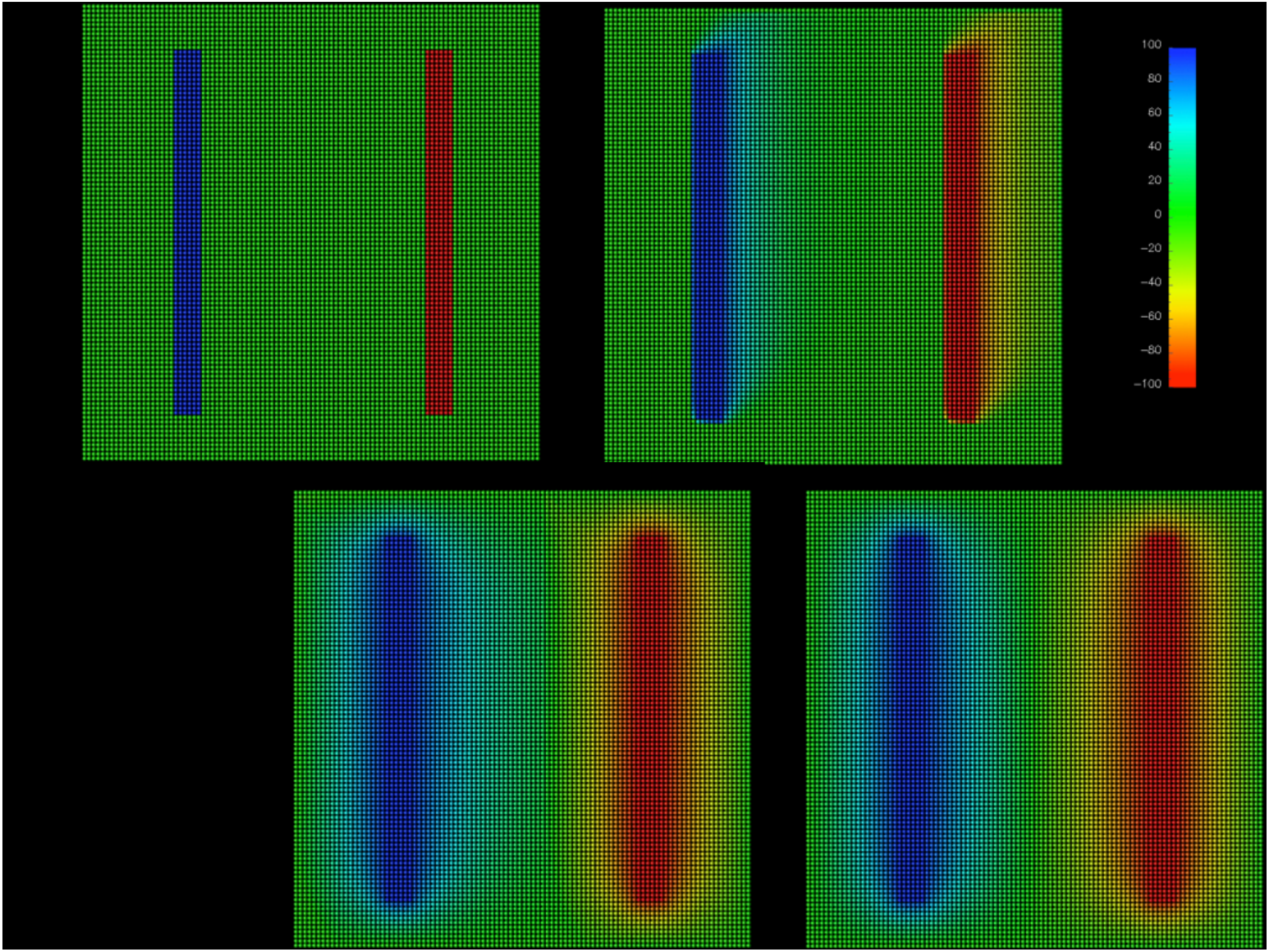
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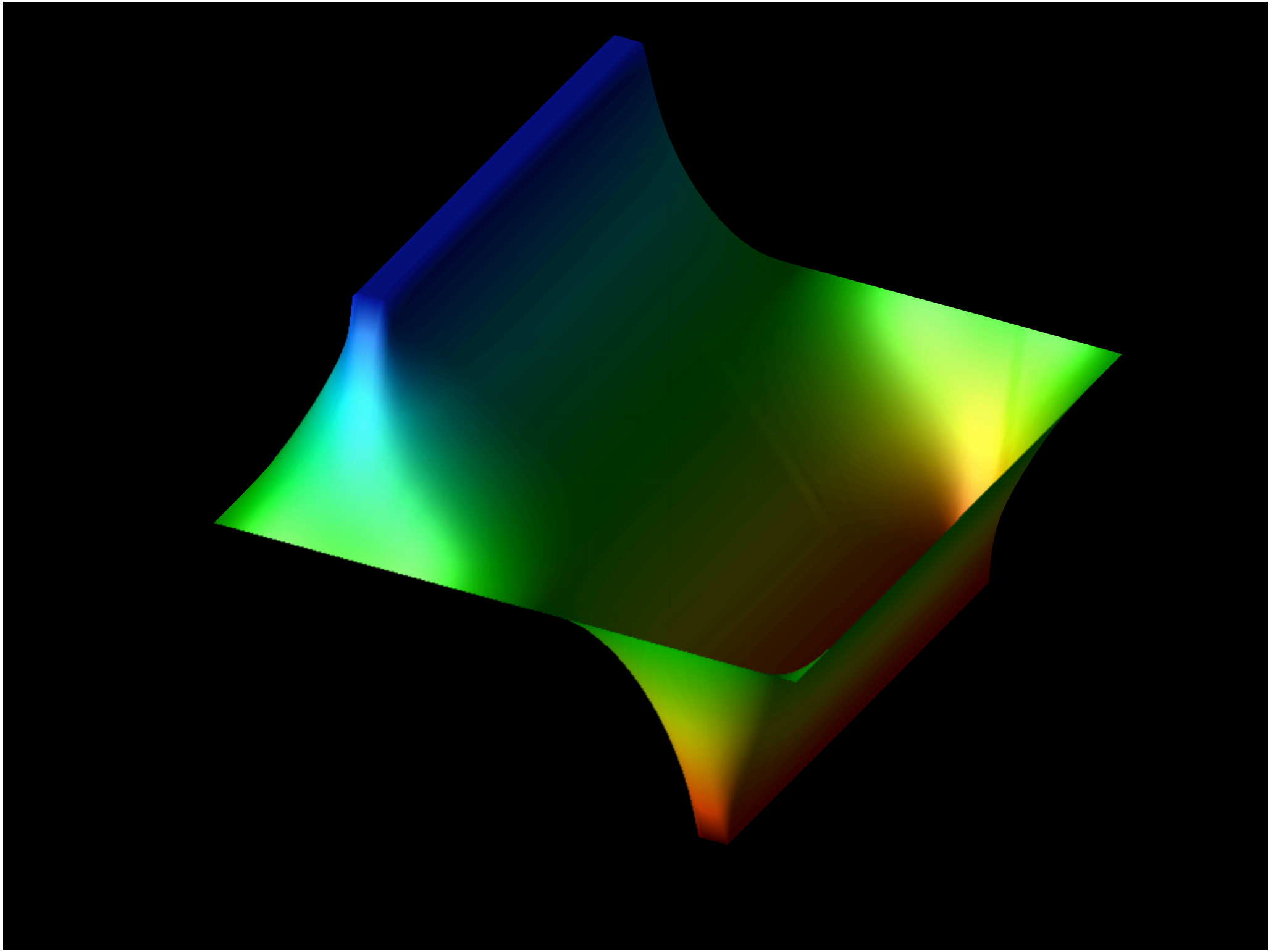
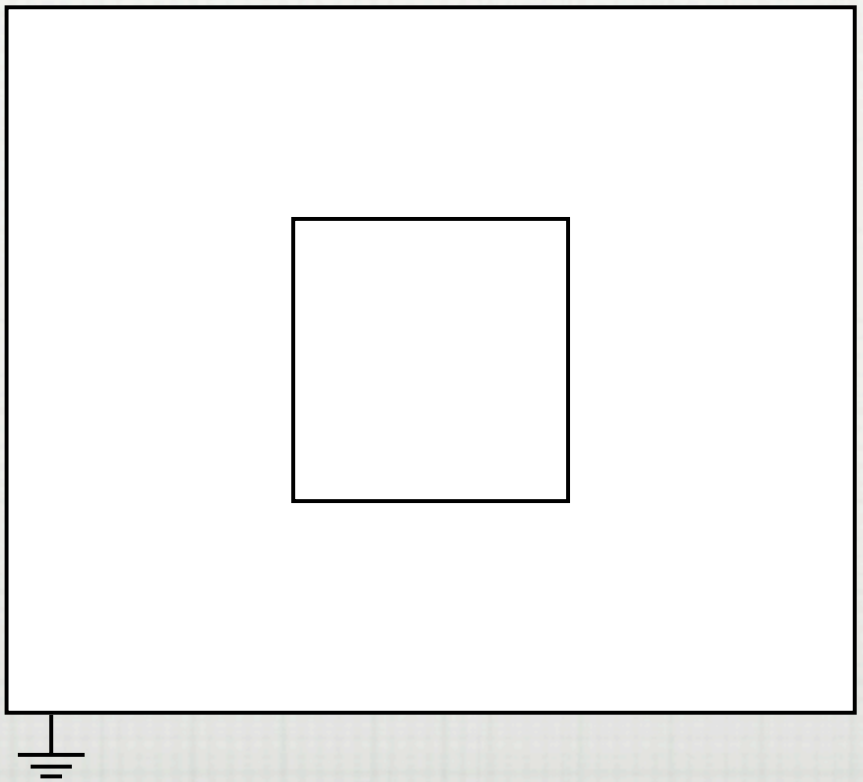
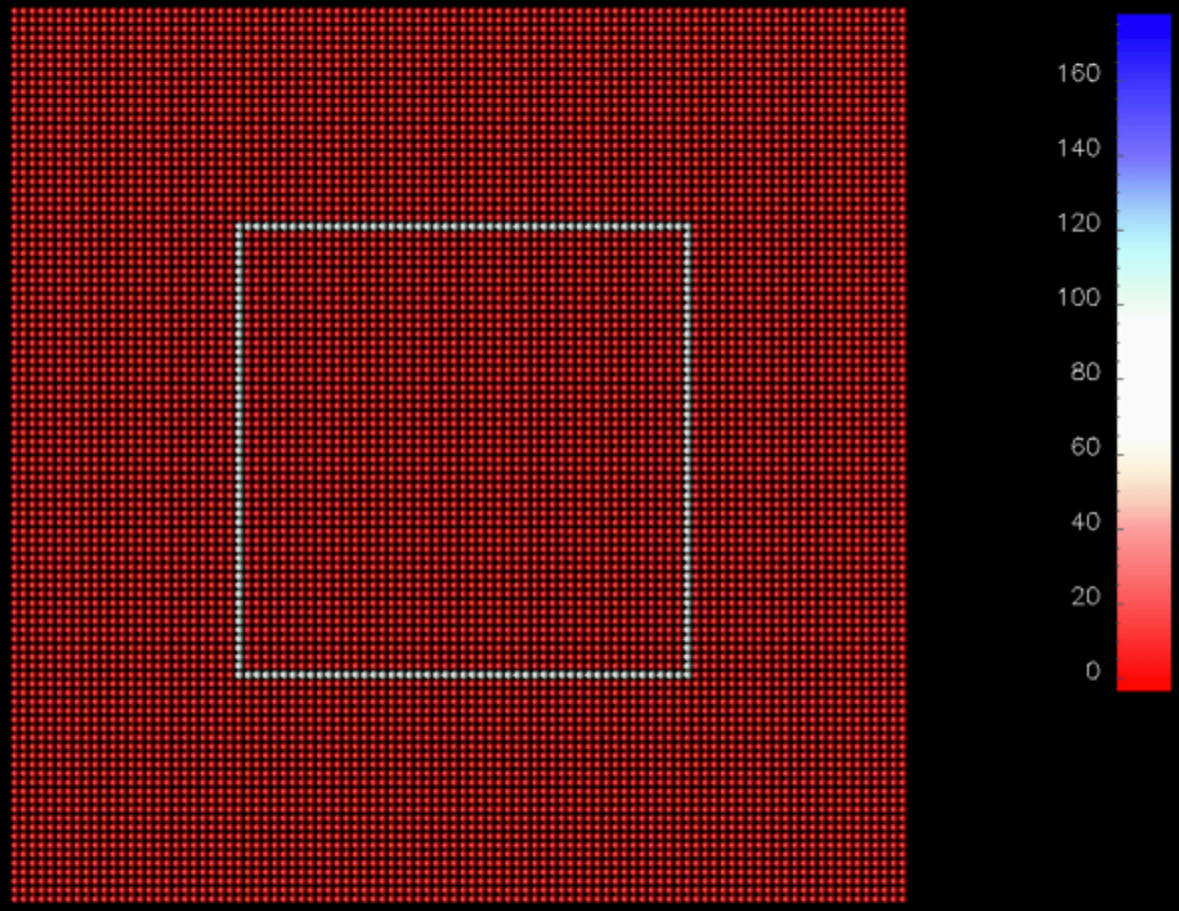


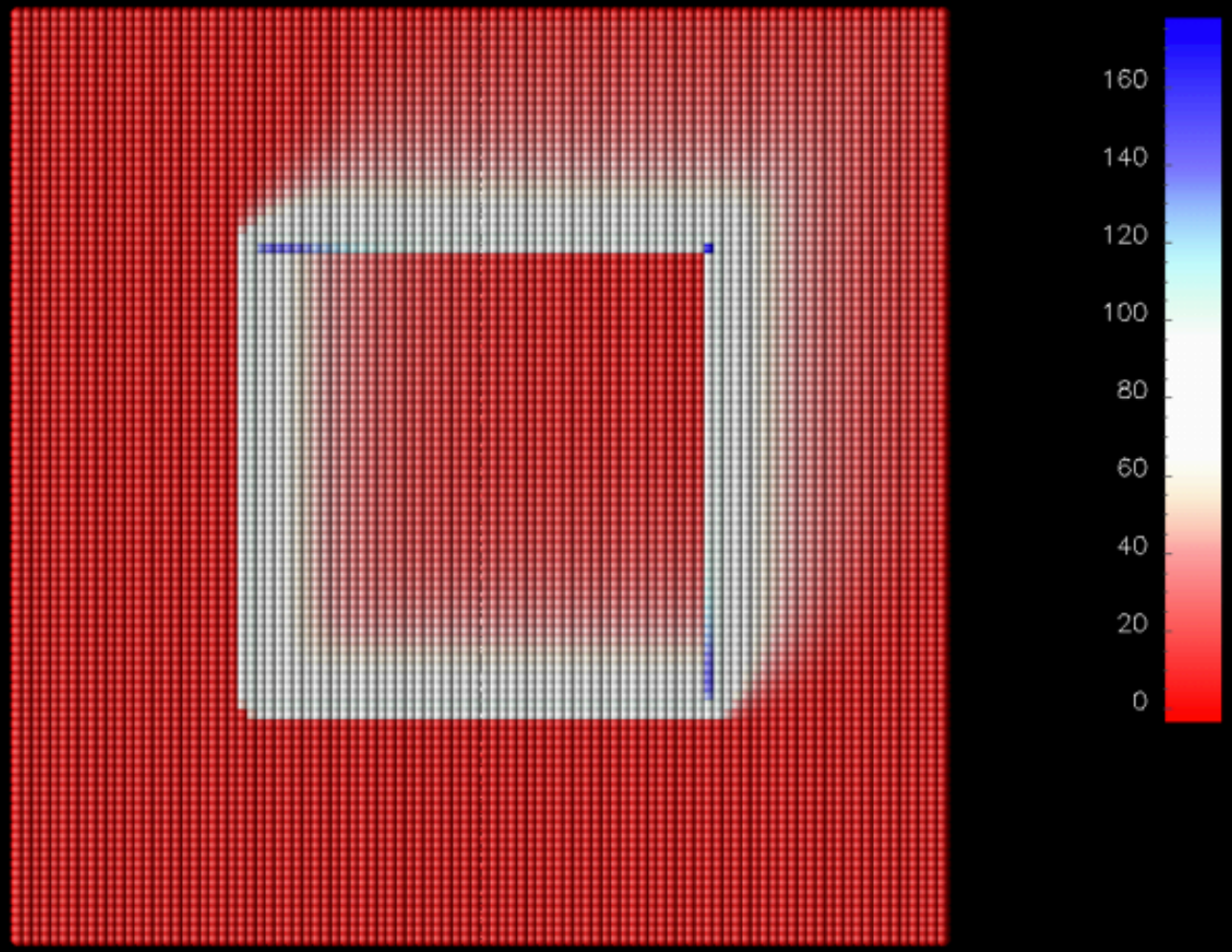
SQUARE IN A SQUARE



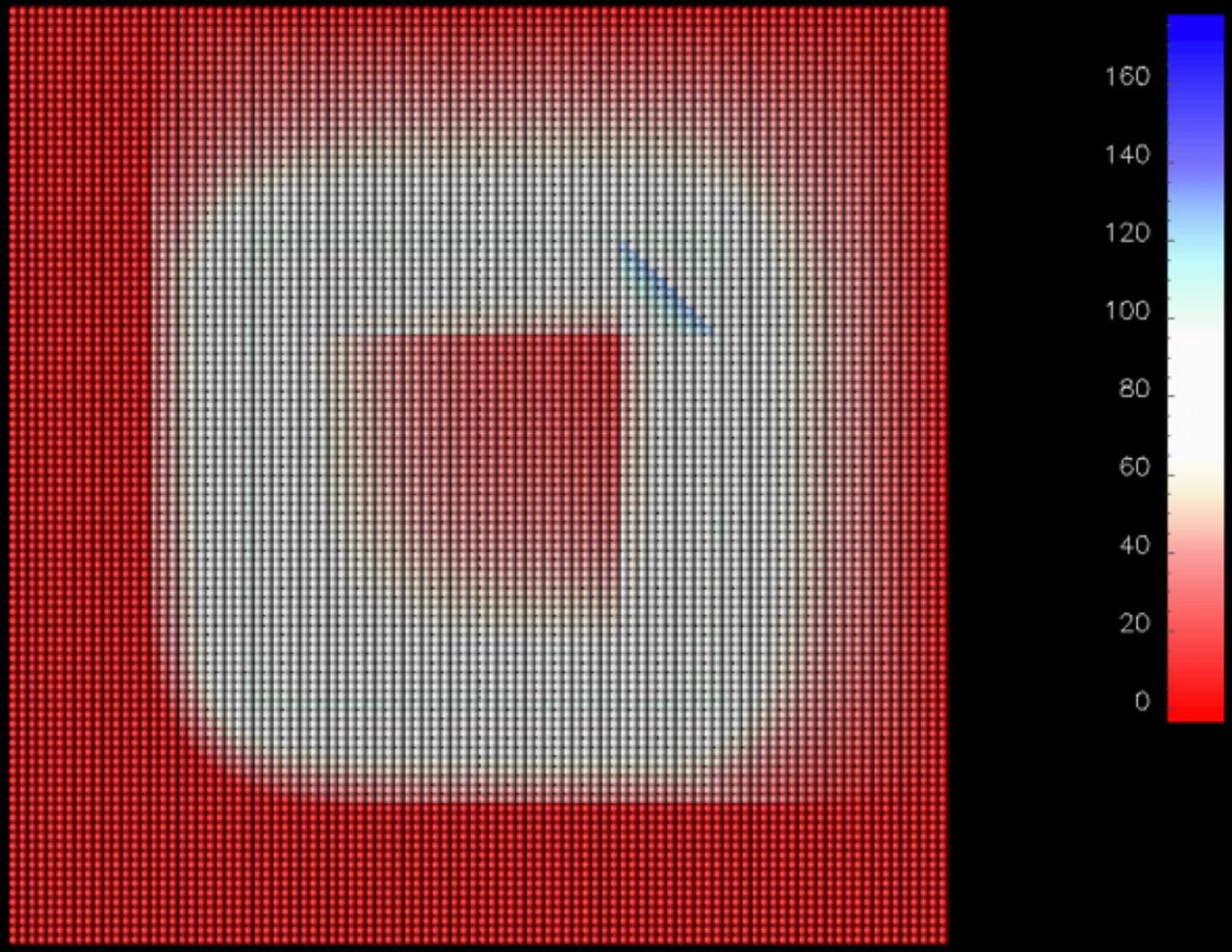
INITIAL CONDITIONS



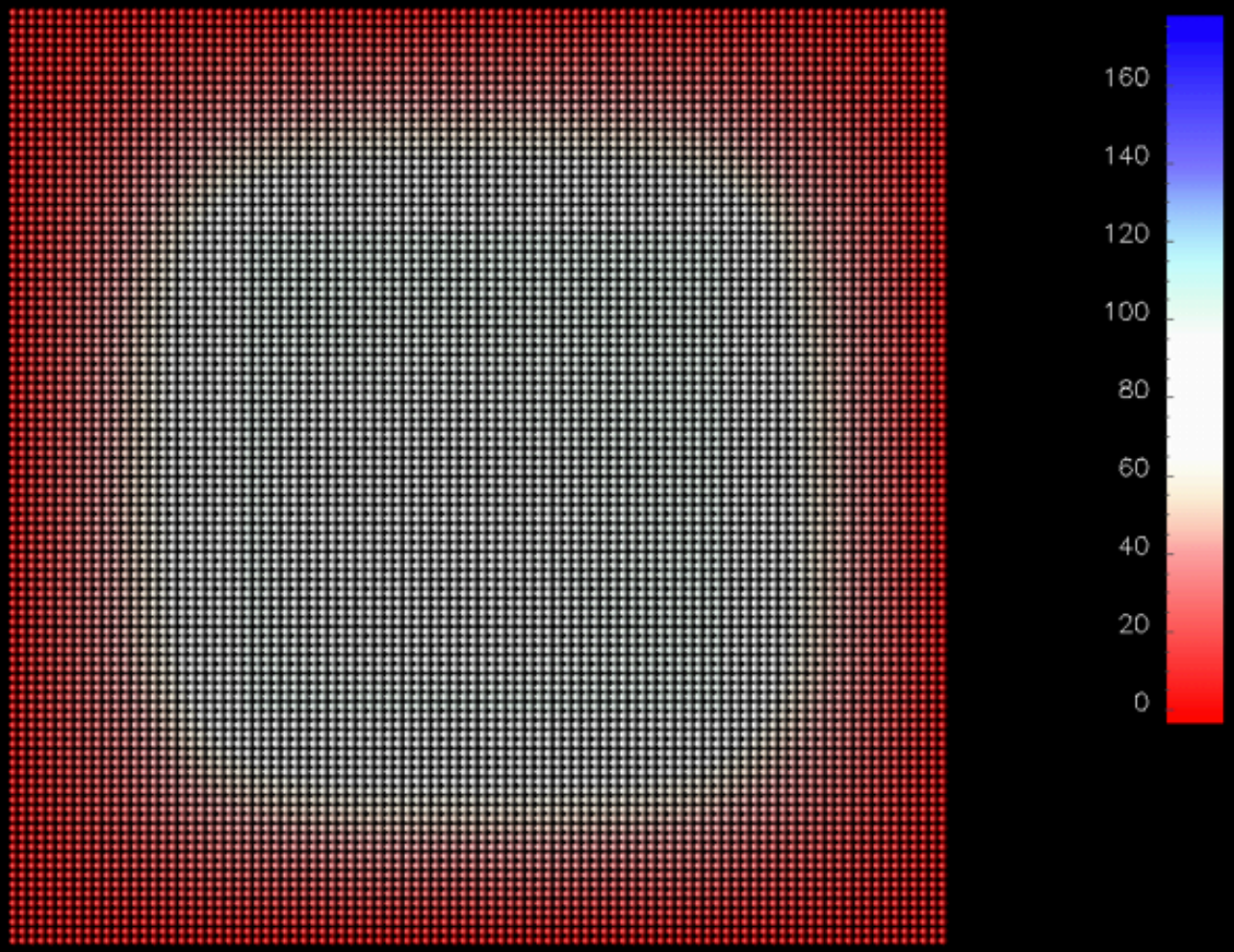
STEP 1



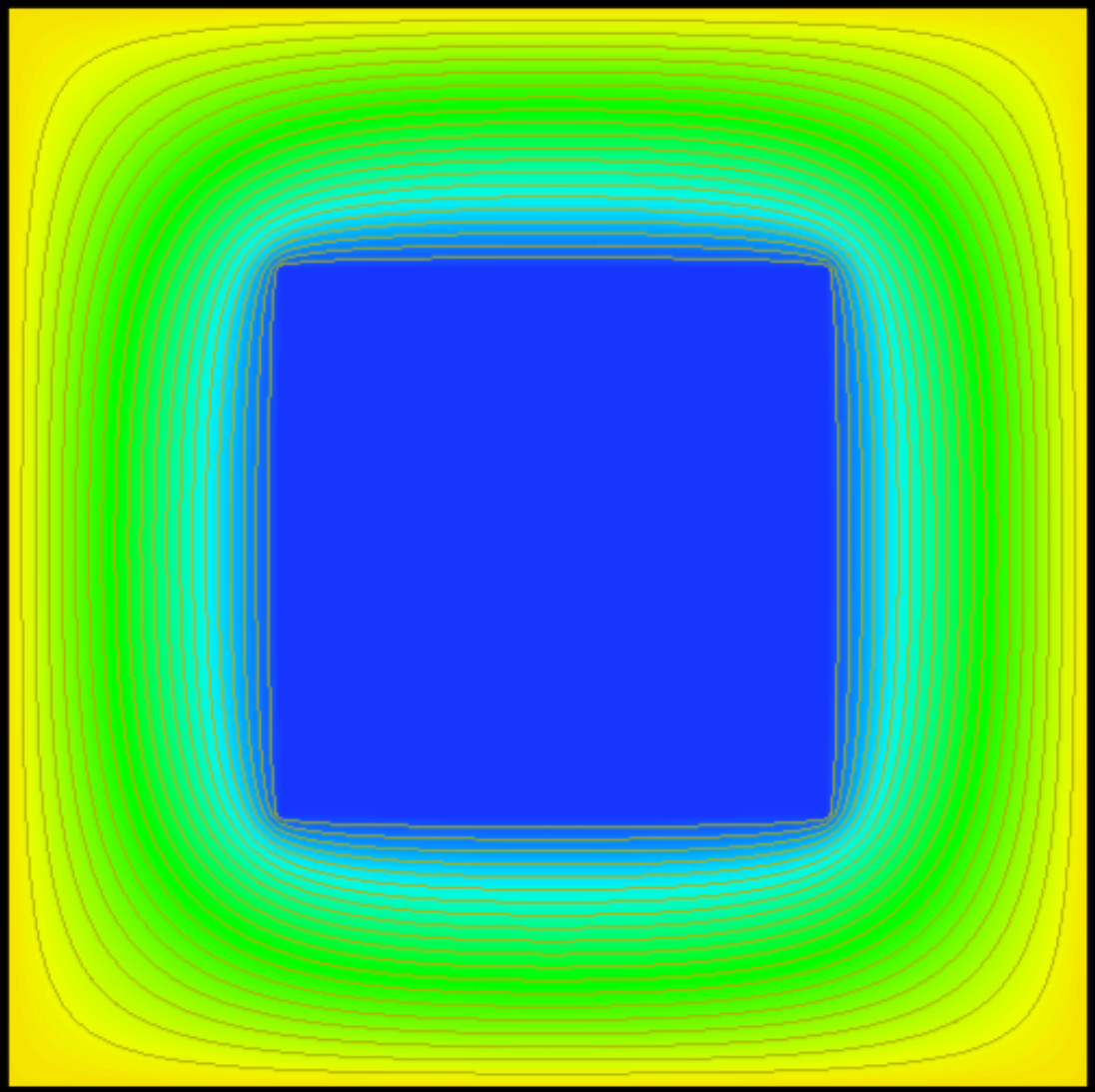
STEP 50



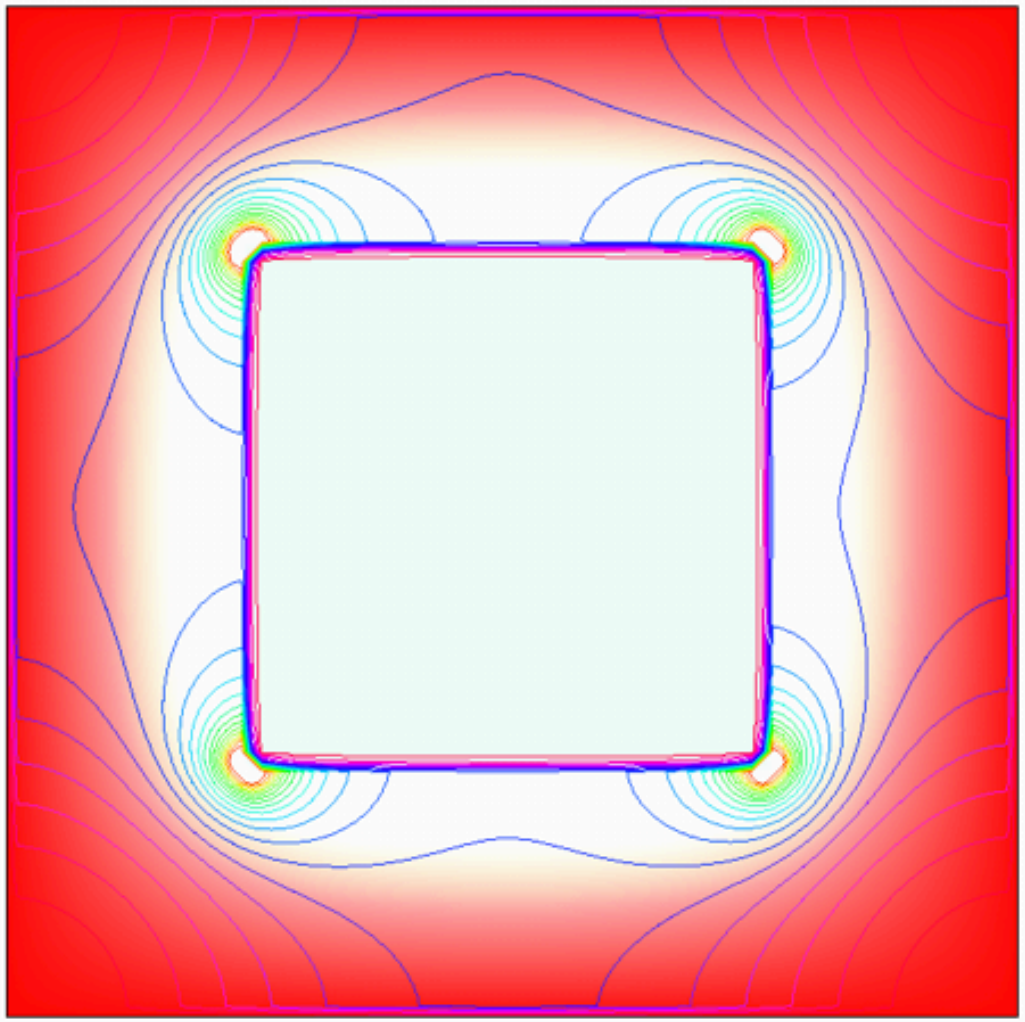
CONVERGED

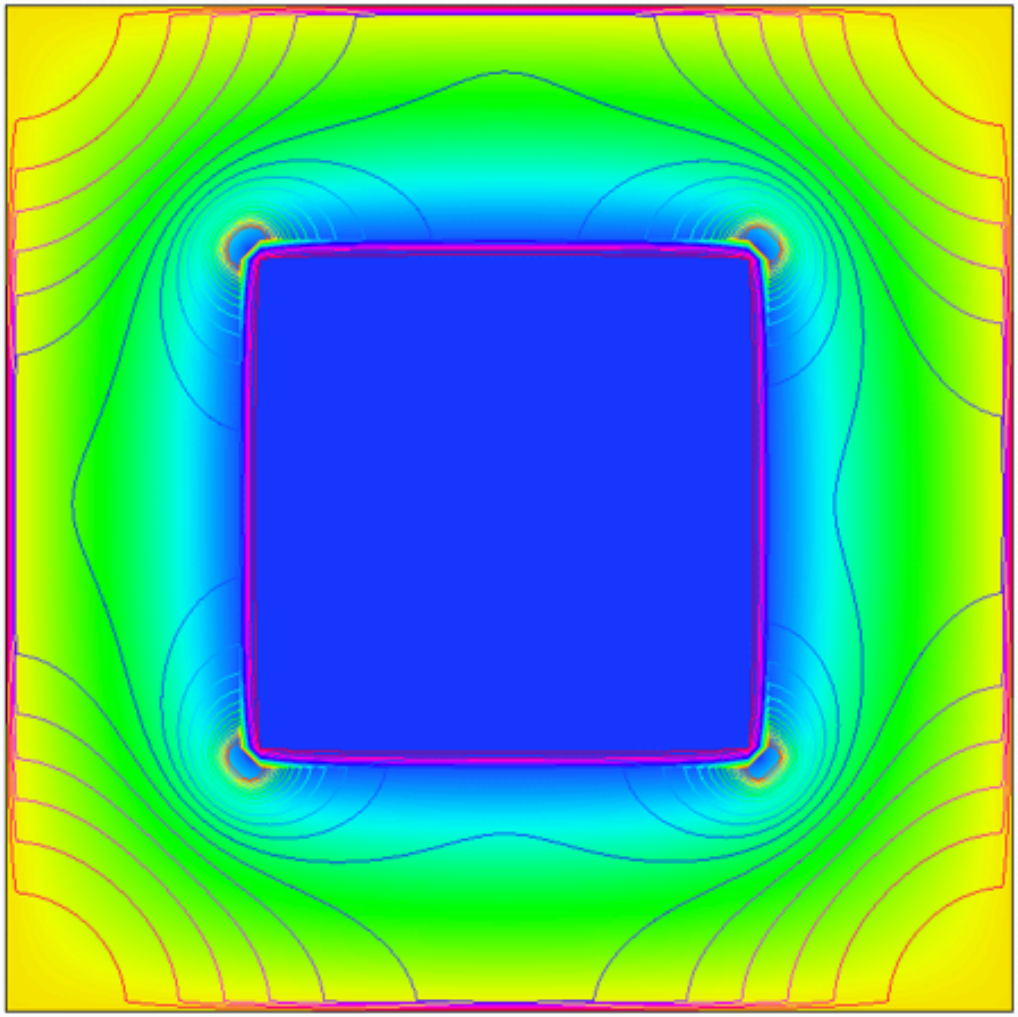


POTENTIAL



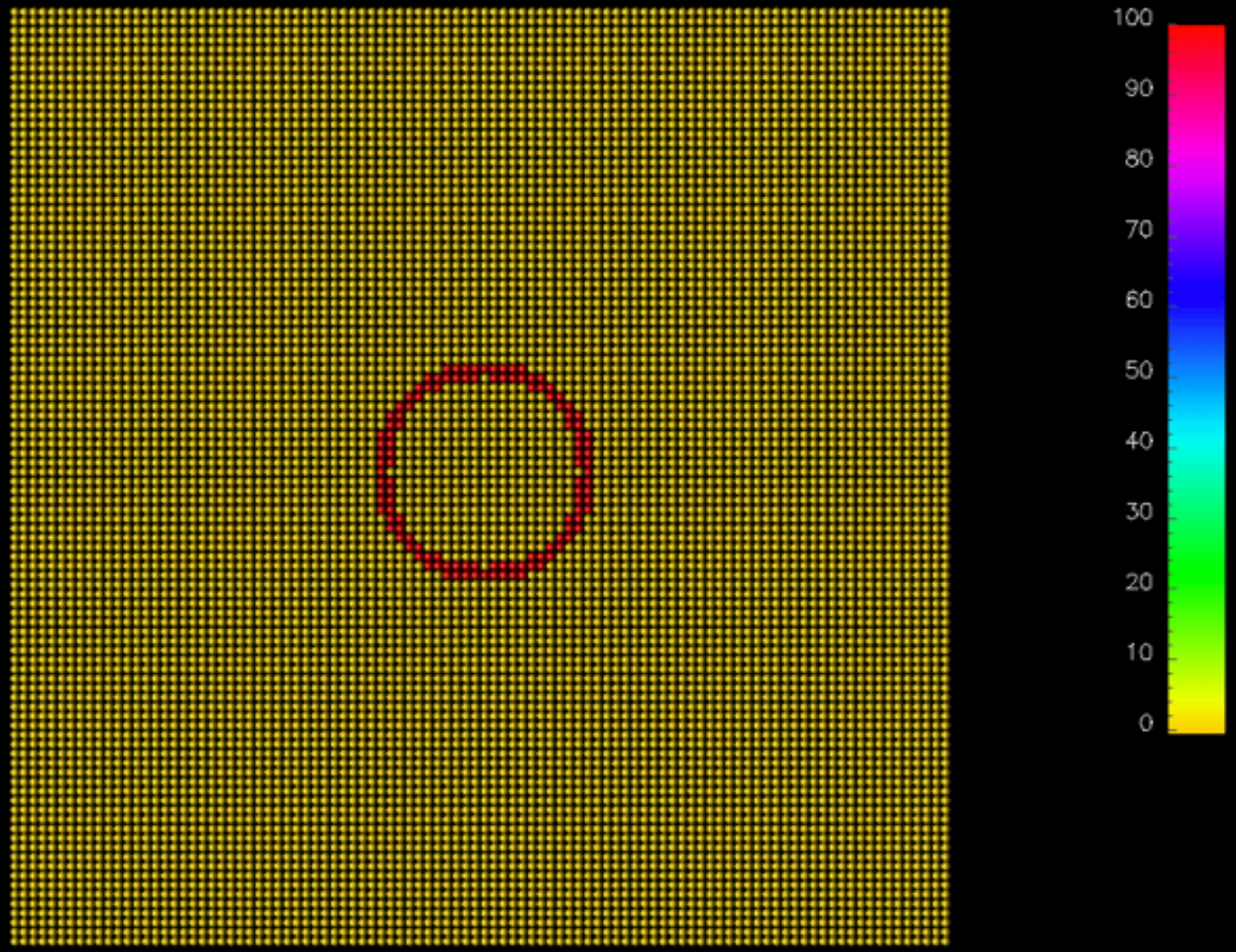
ELECTRIC FIELD



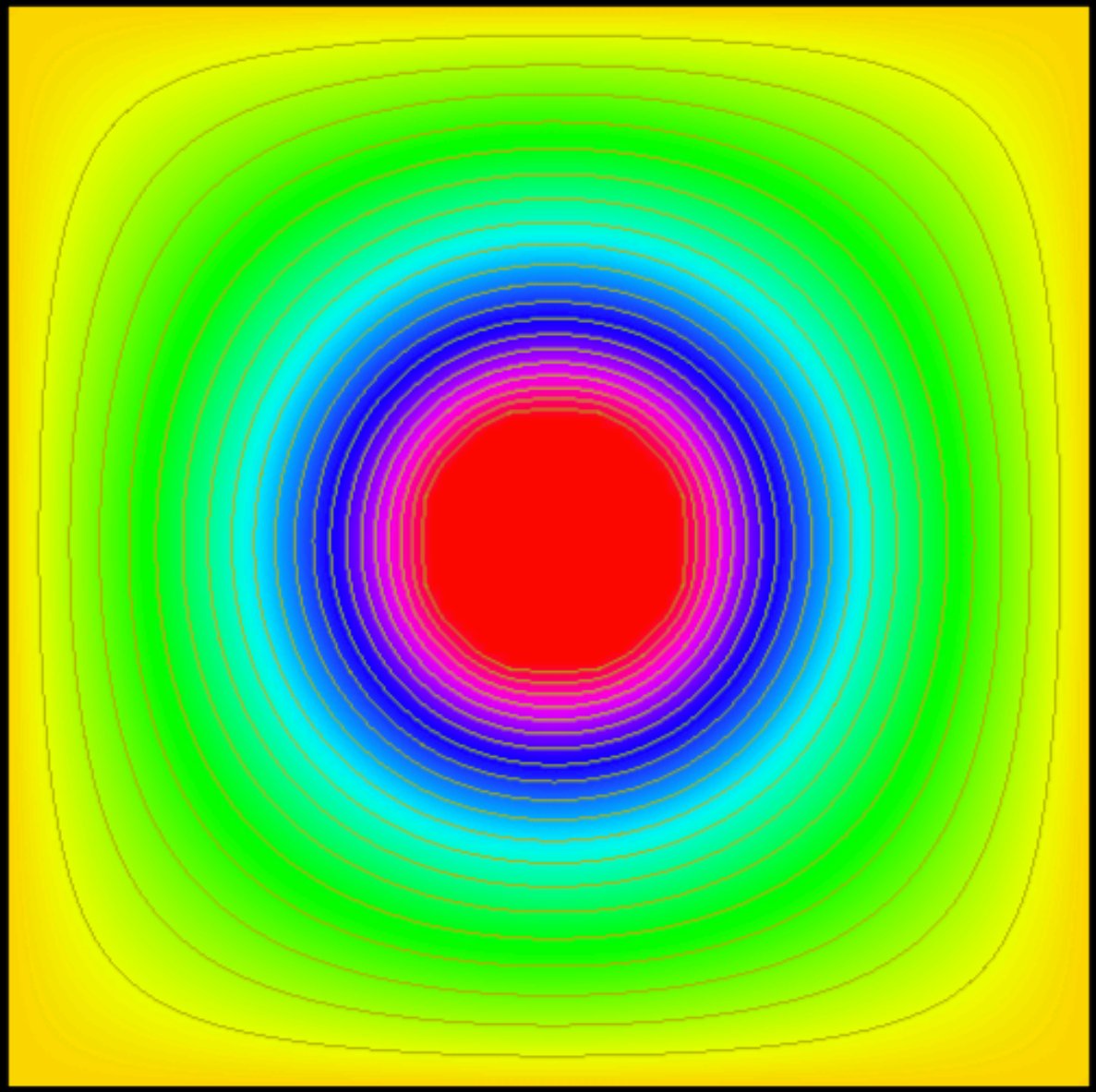


HOW CAN WE REDUCE THE ELECTRIC FIELD?

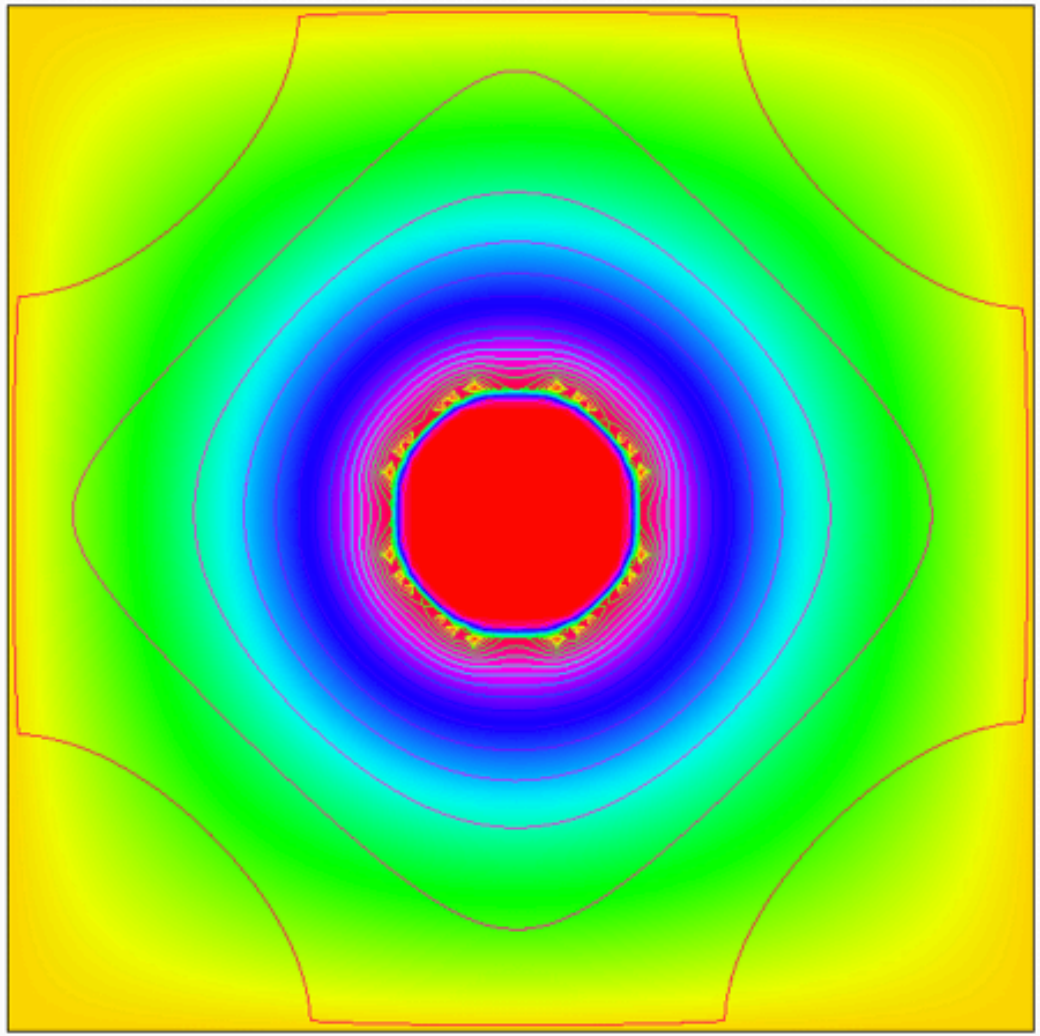
INITIAL CONDITIONS



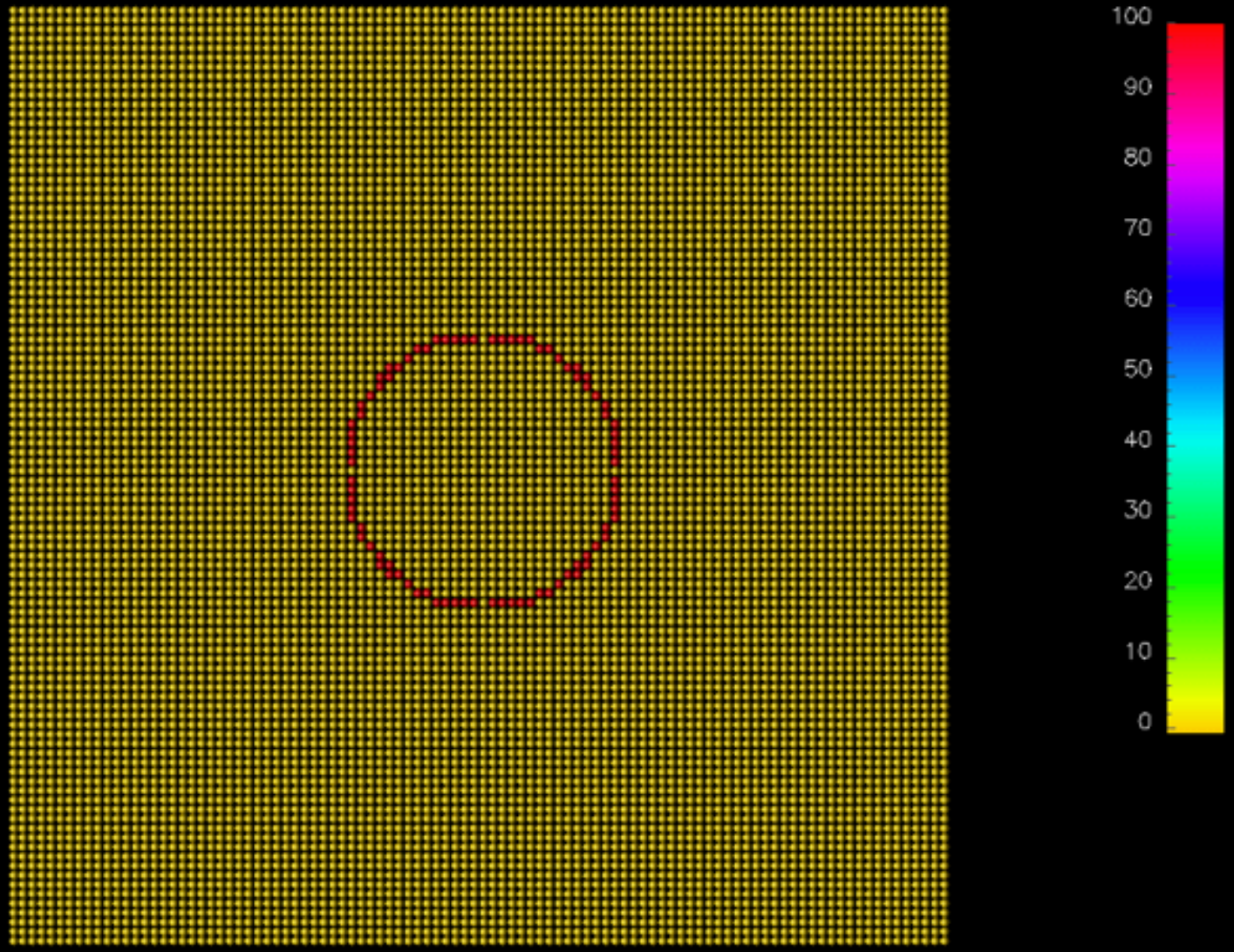
CONVERGED POTENTIAL

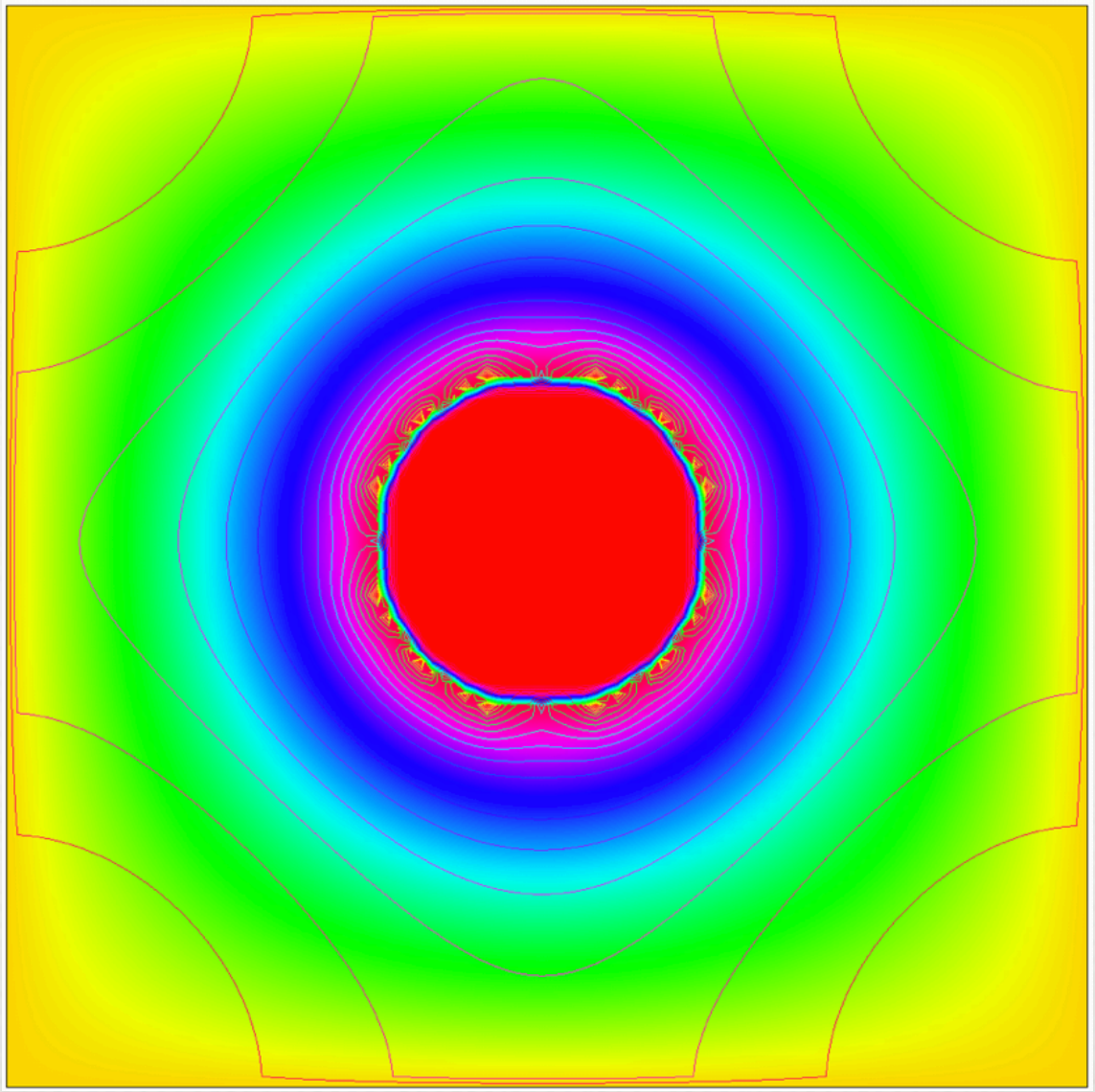


FIELD

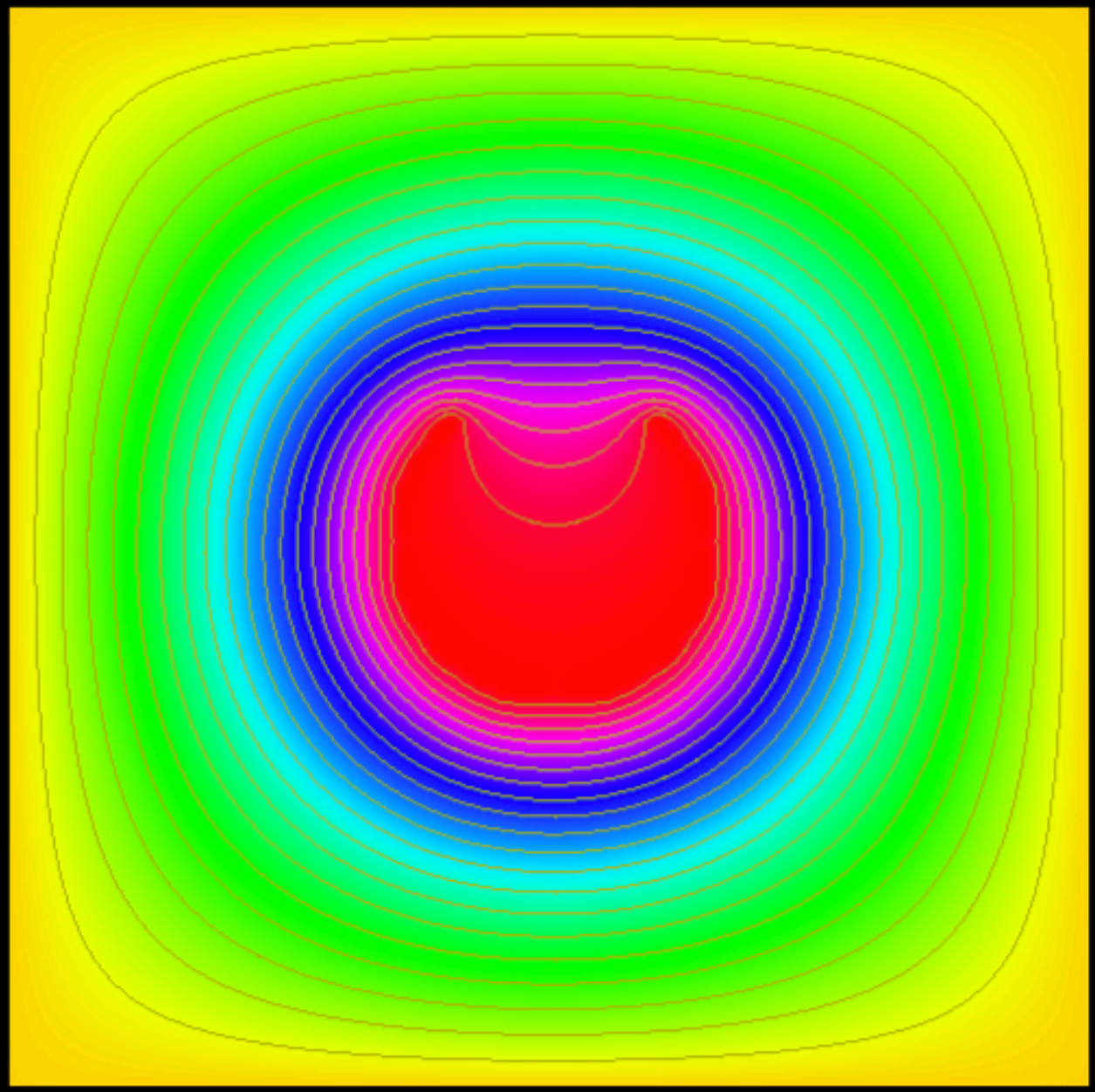


INITIAL CONDITIONS (MODIFIED)

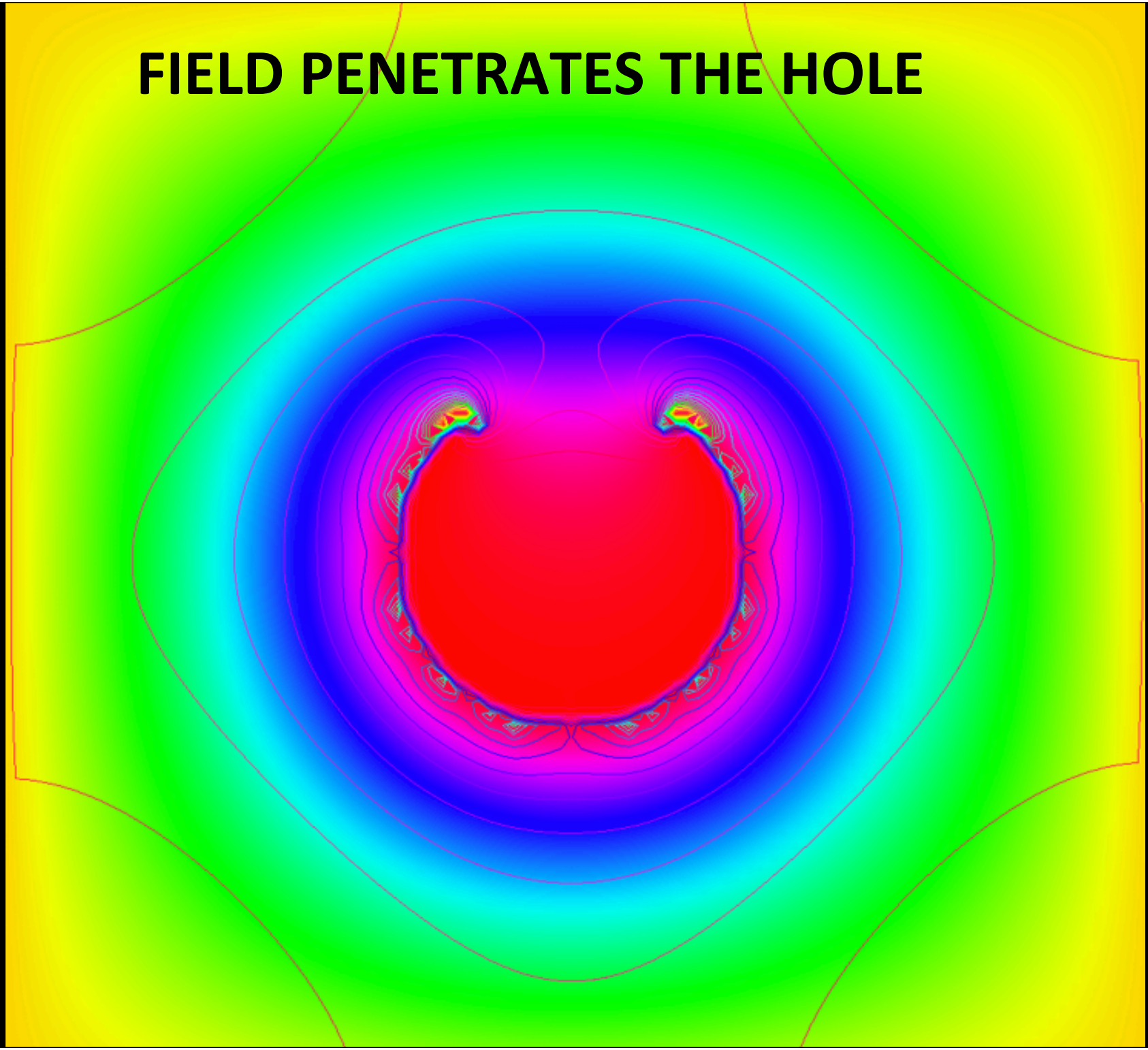


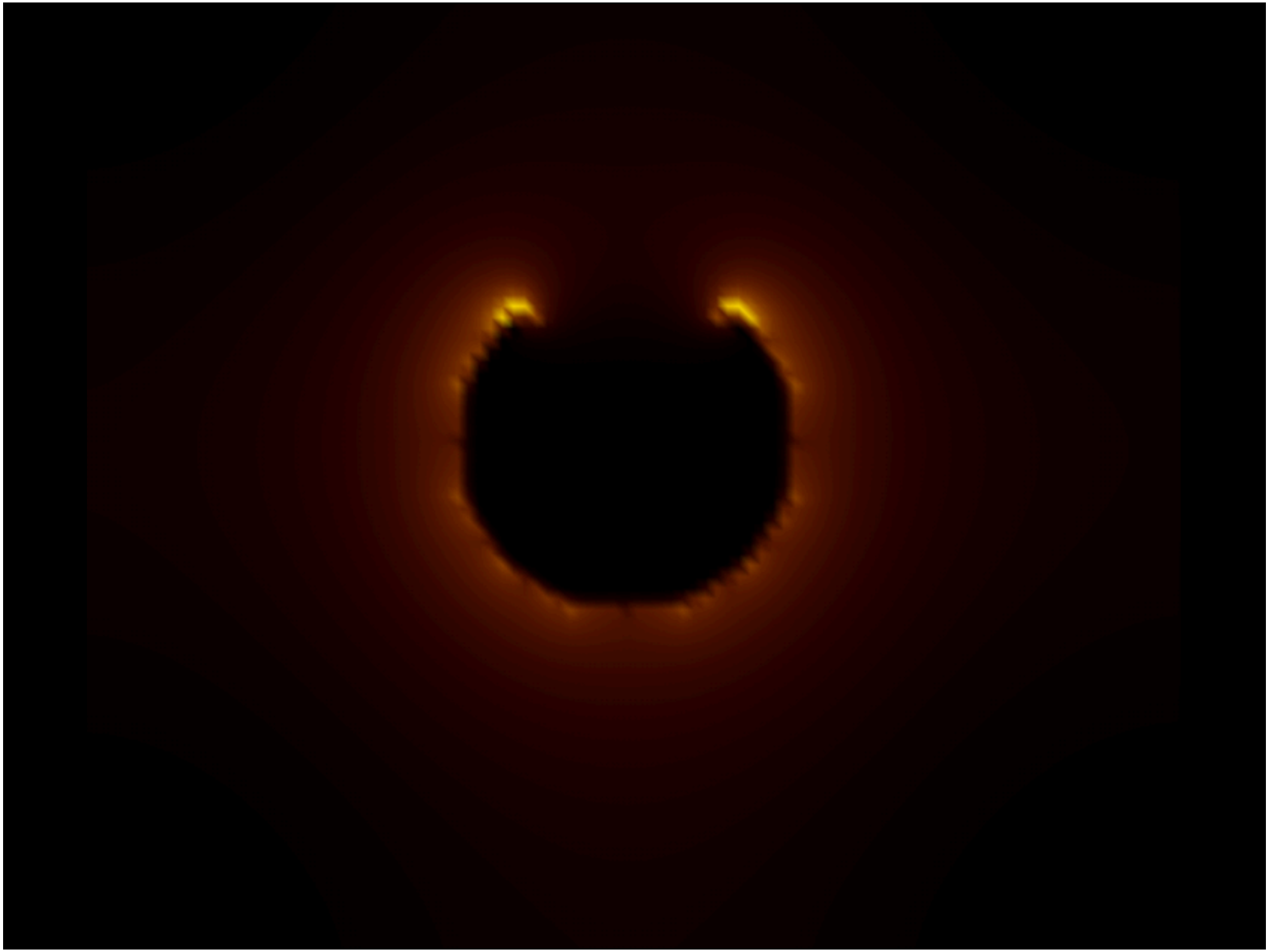


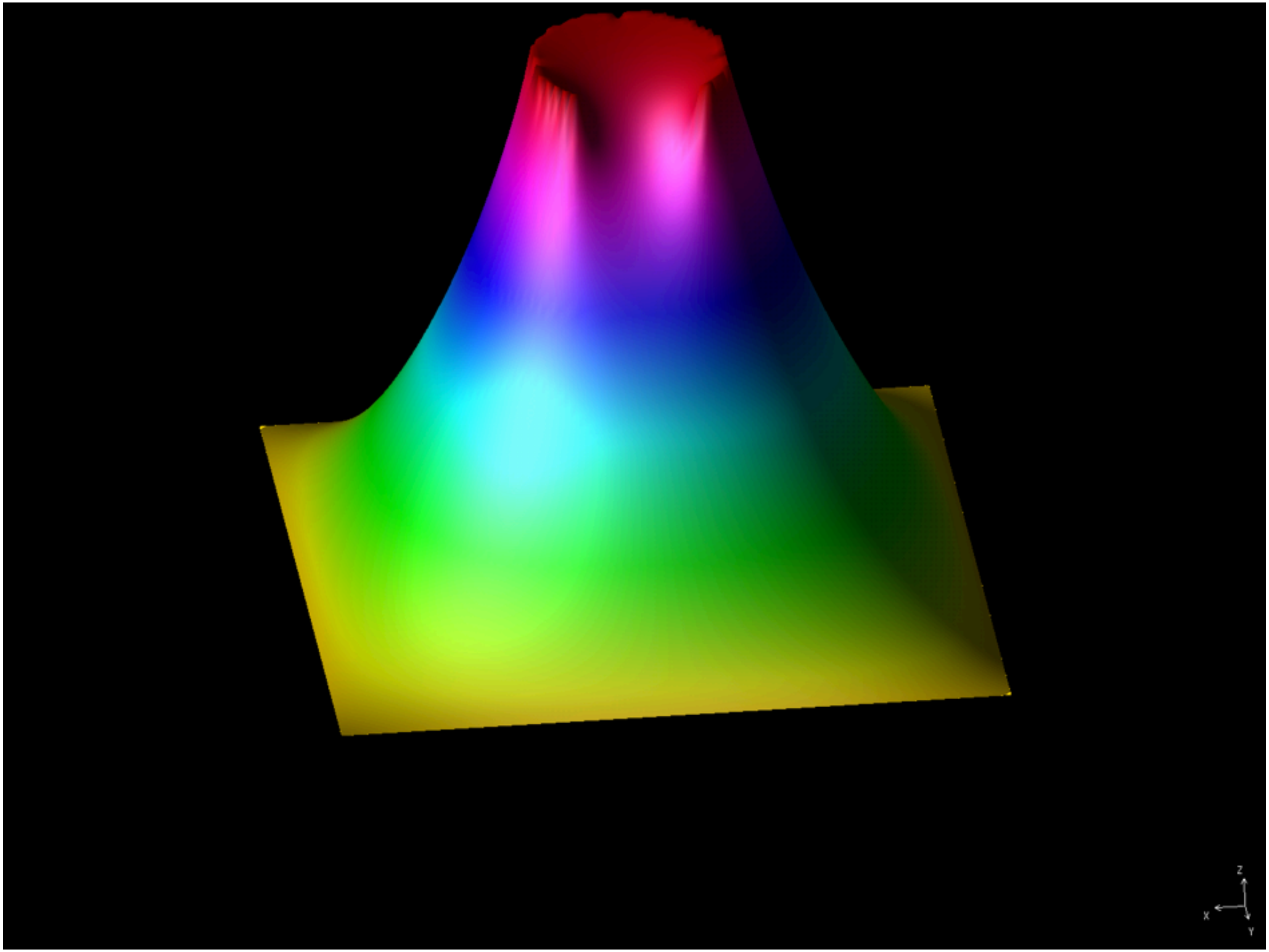
WITH A HOLE

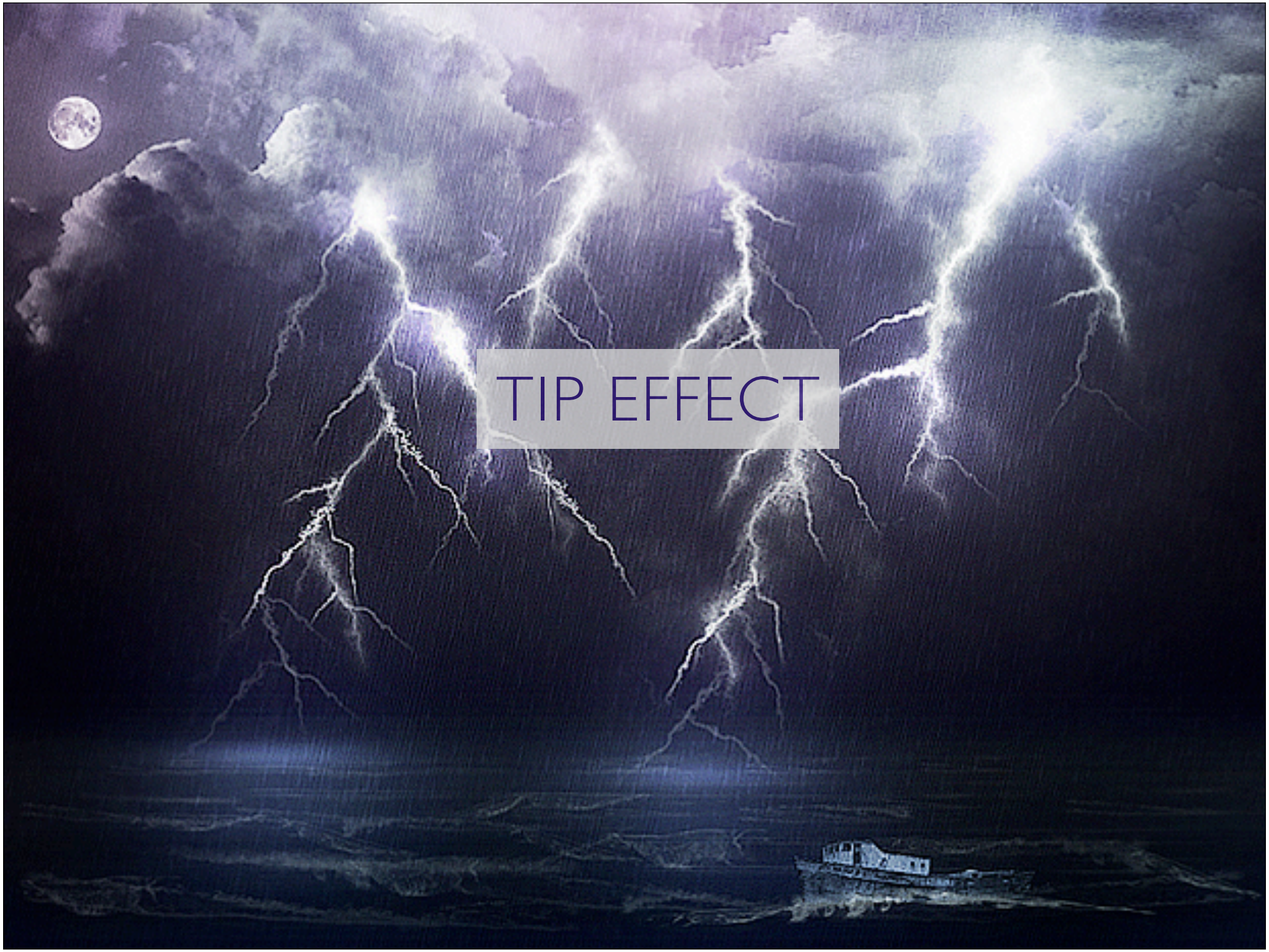


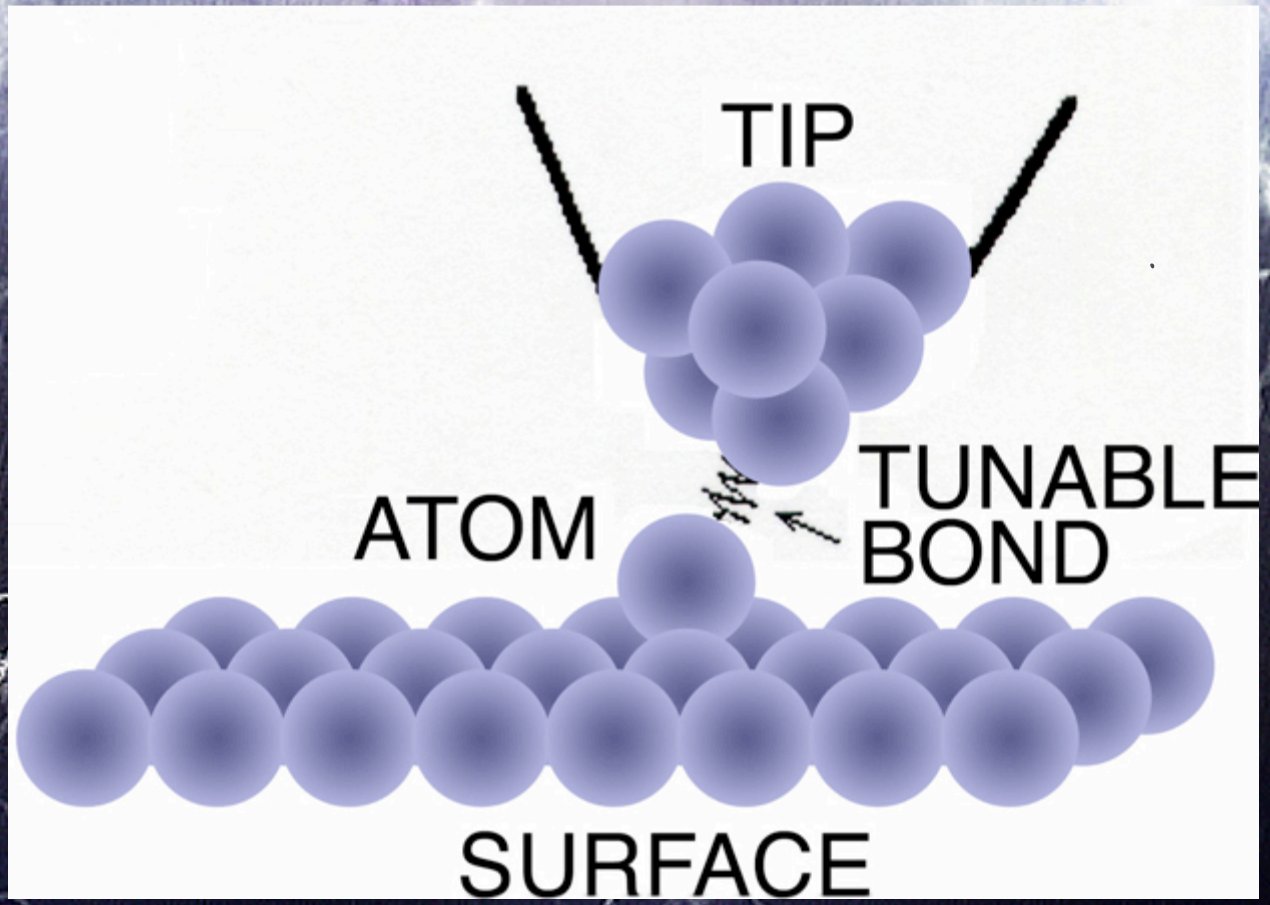
FIELD PENETRATES THE HOLE



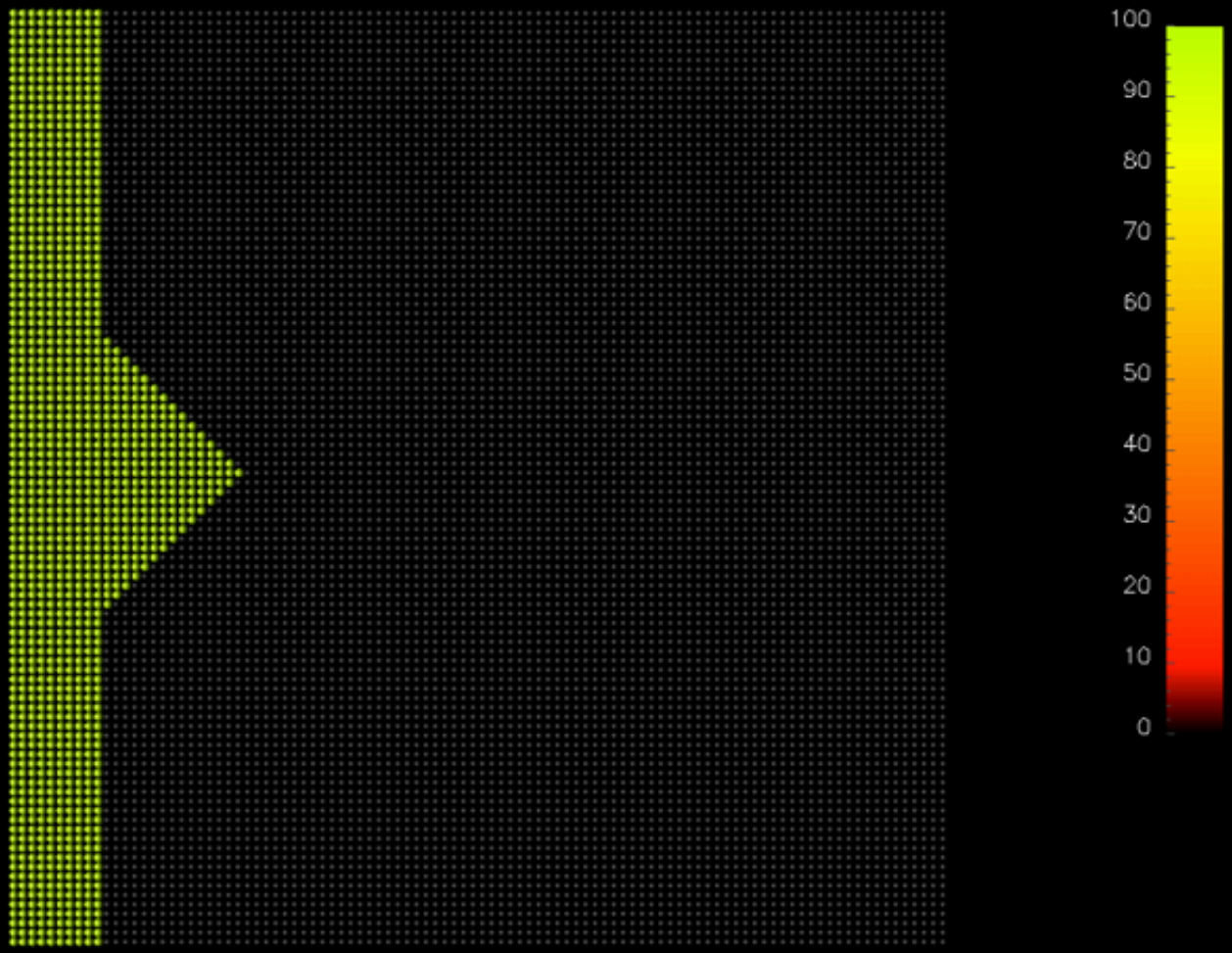


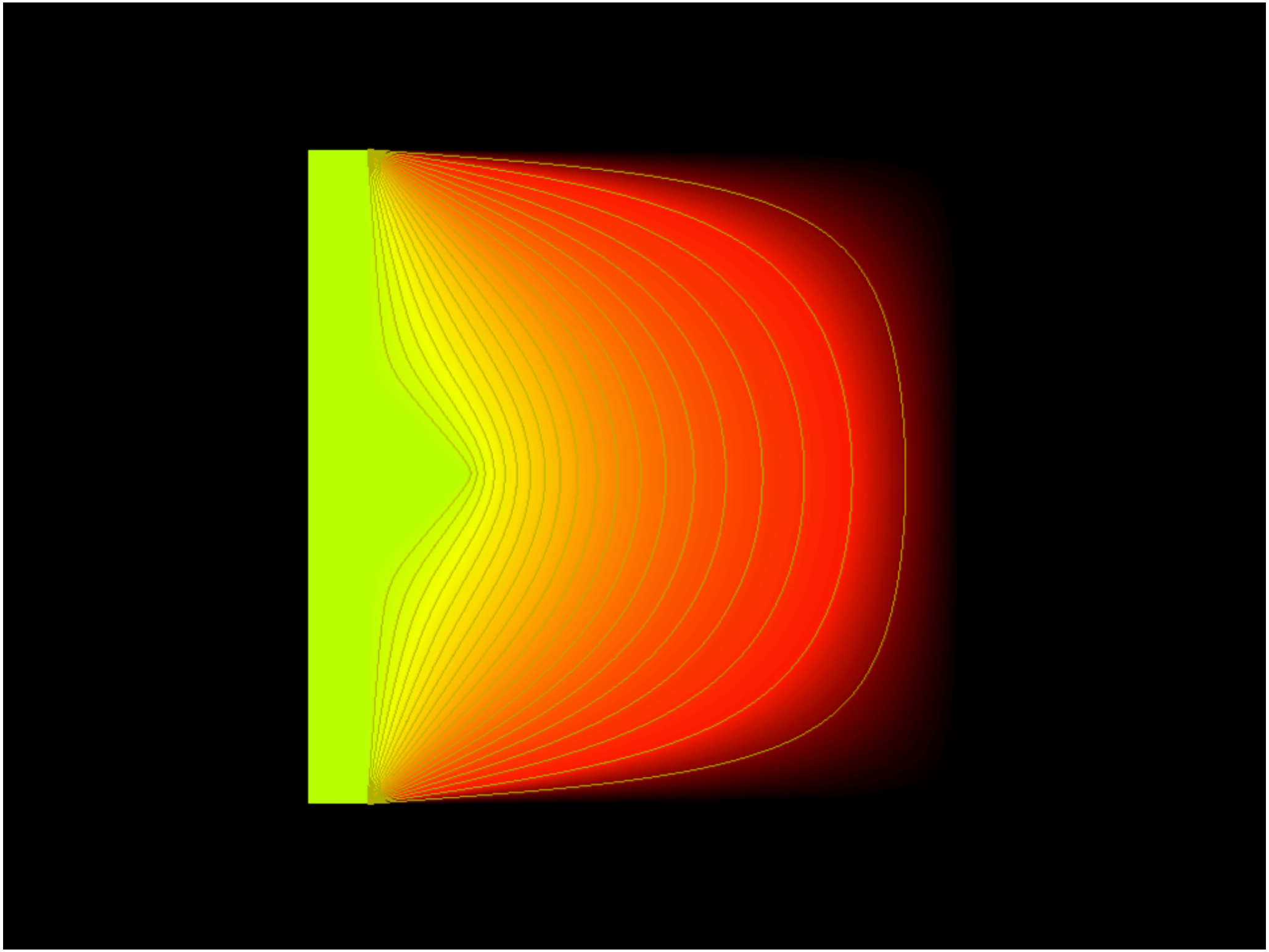

Z
X
Y


TIP EFFECT

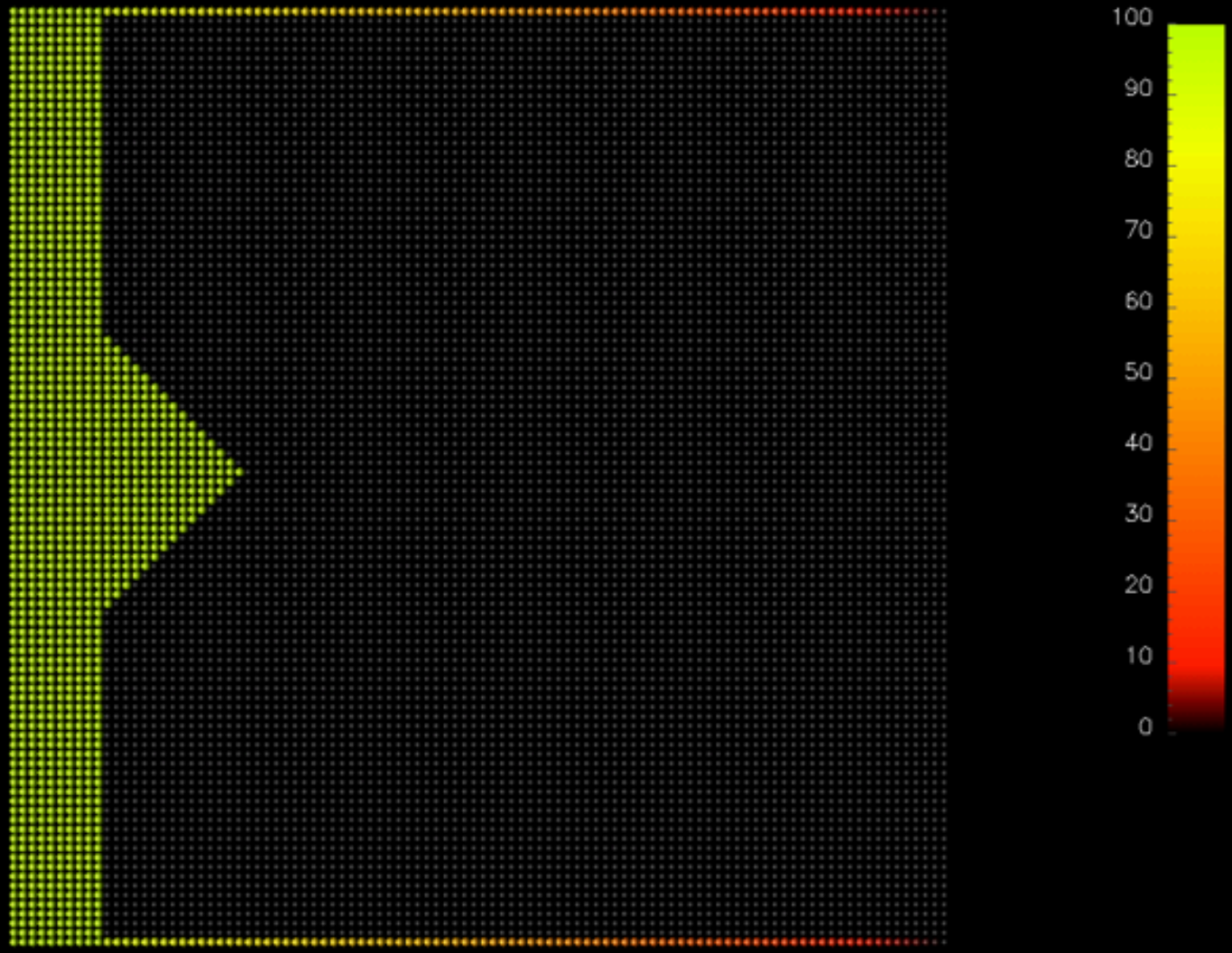

TIP
TUNABLE
BOND
ATOM
SURFACE

INITIAL CONDITIONS

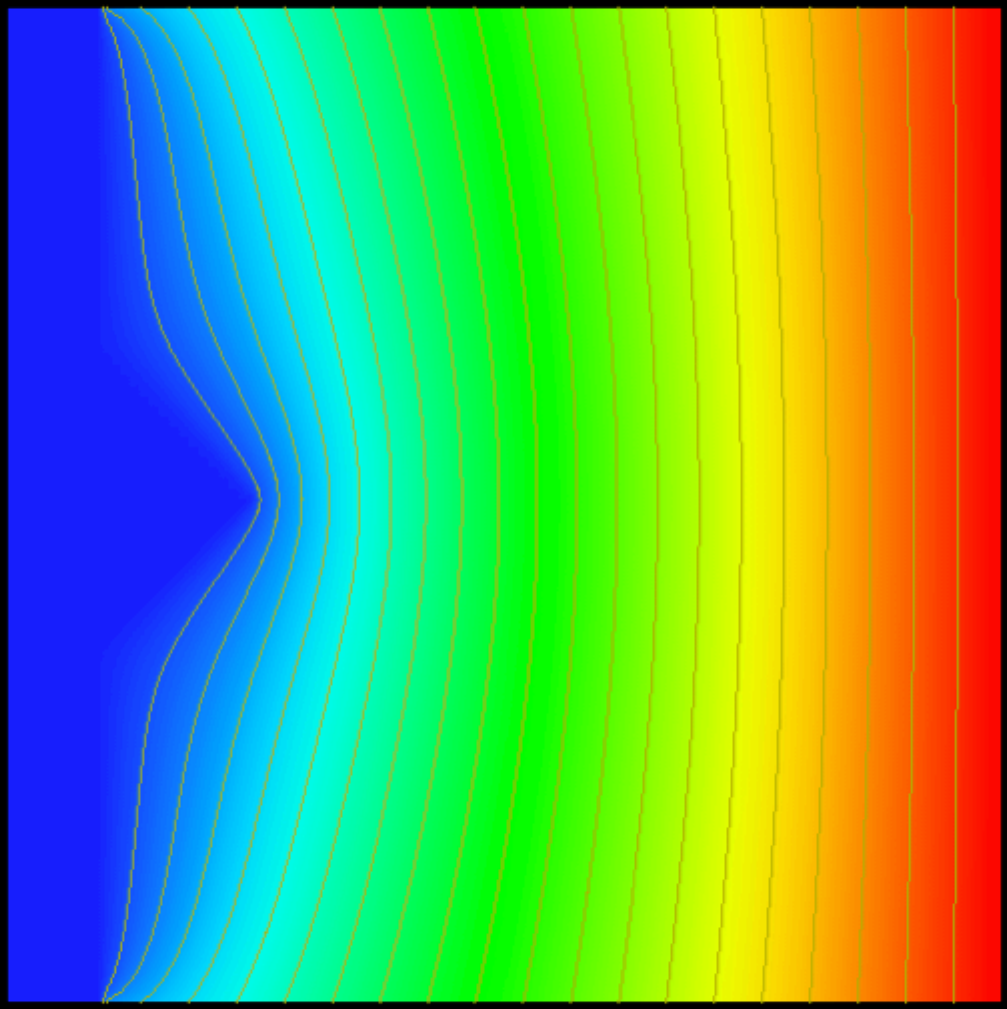




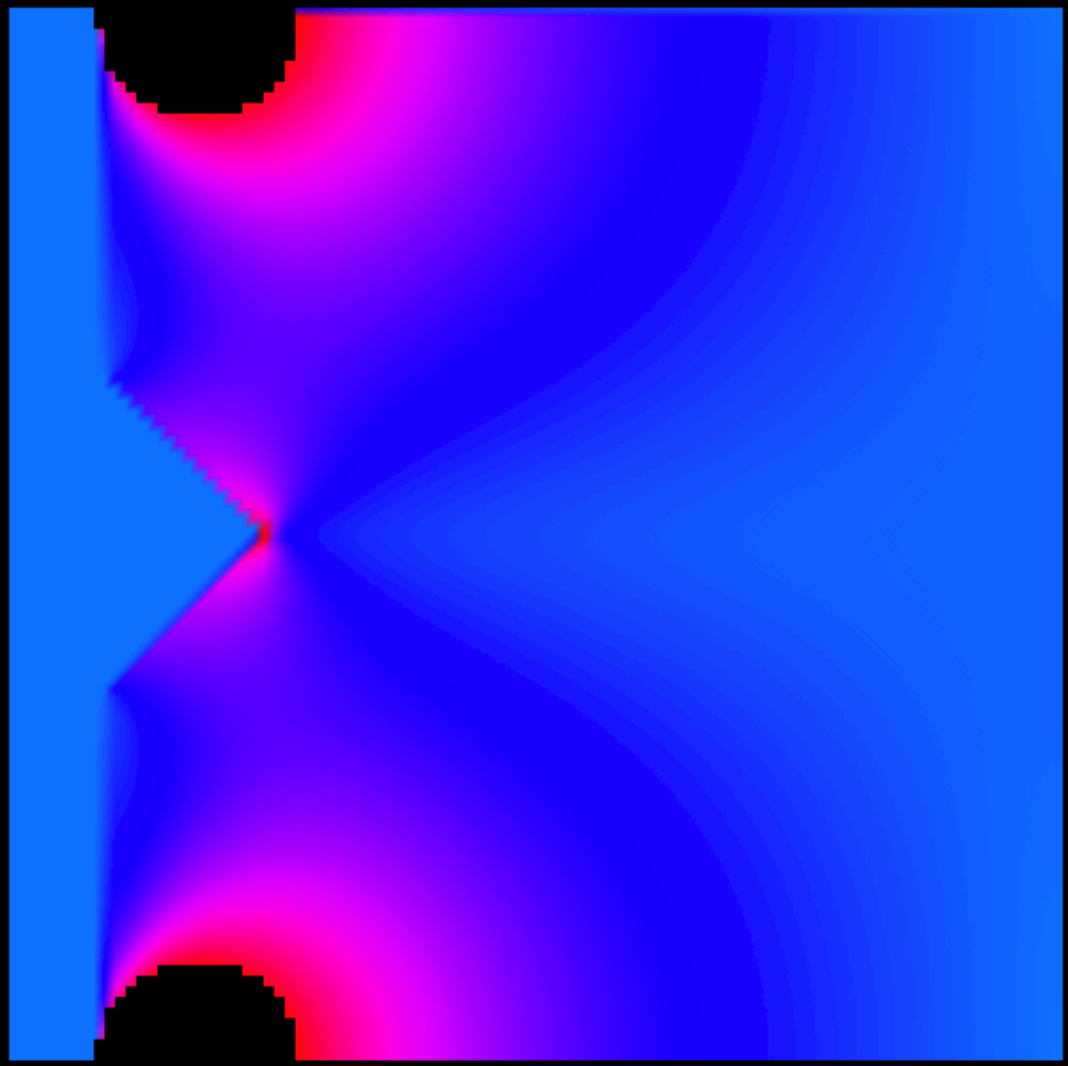
MODIFIED INITIAL CONDITIONS



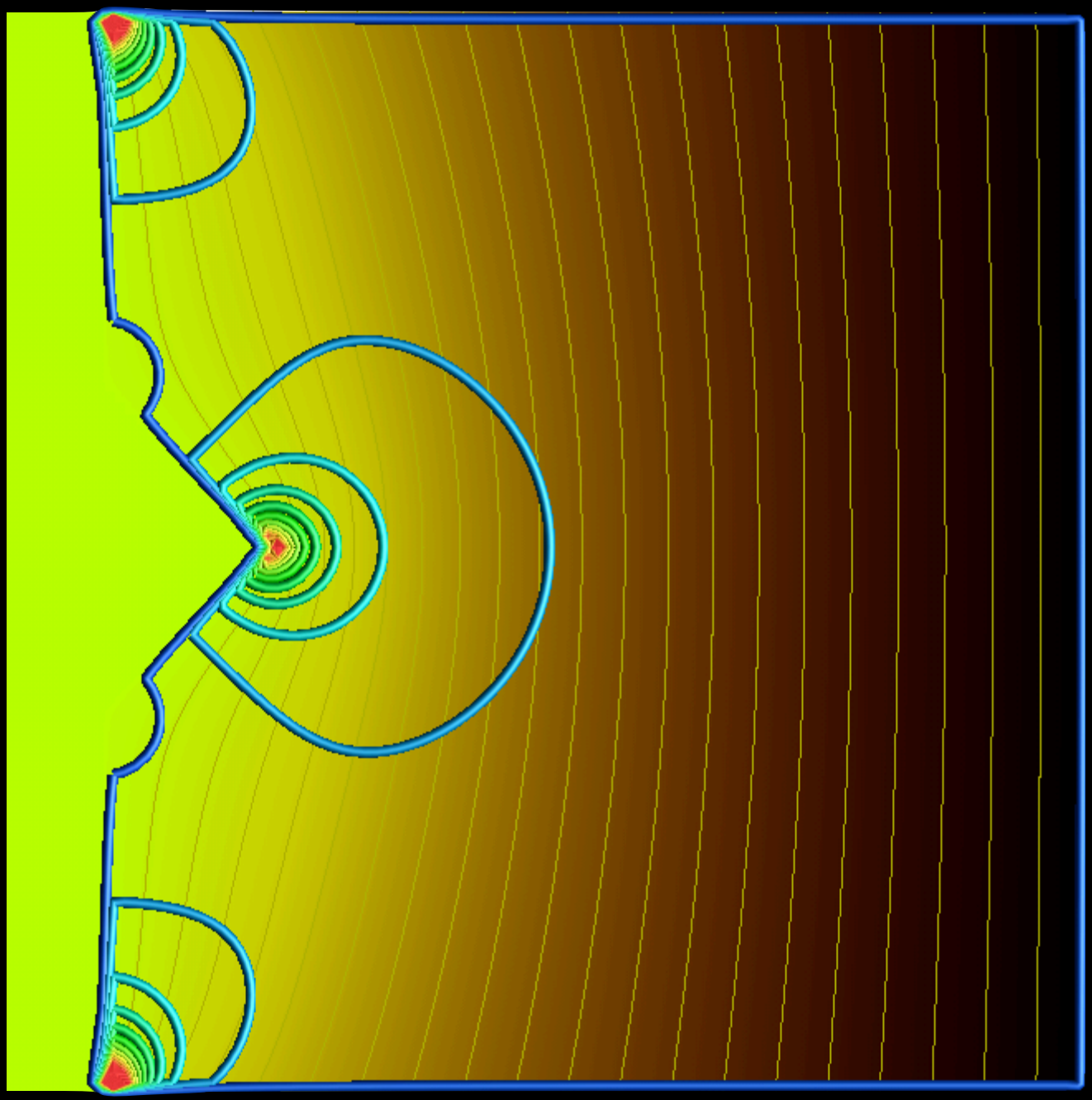
CONVERGED POTENTIAL



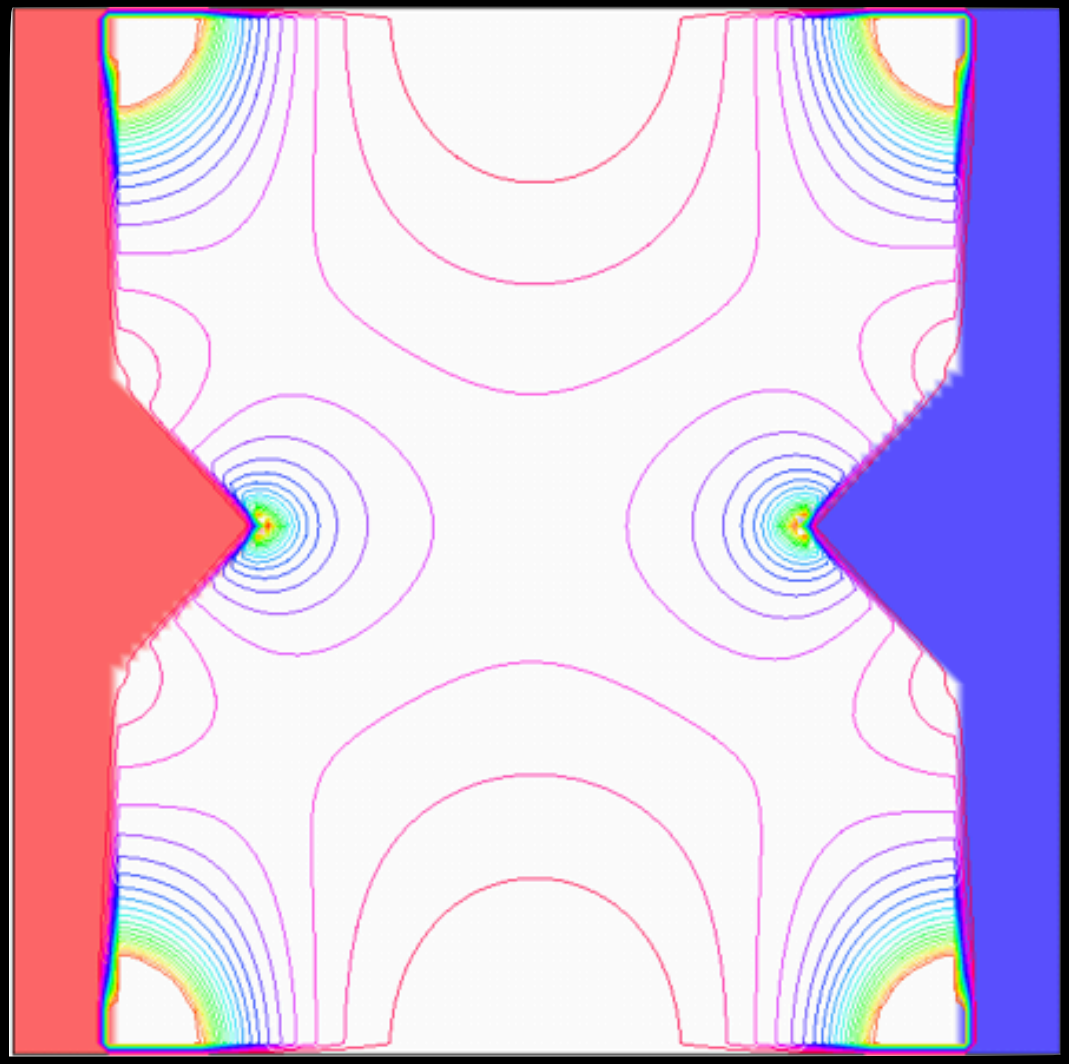
ELECTRIC FIELD



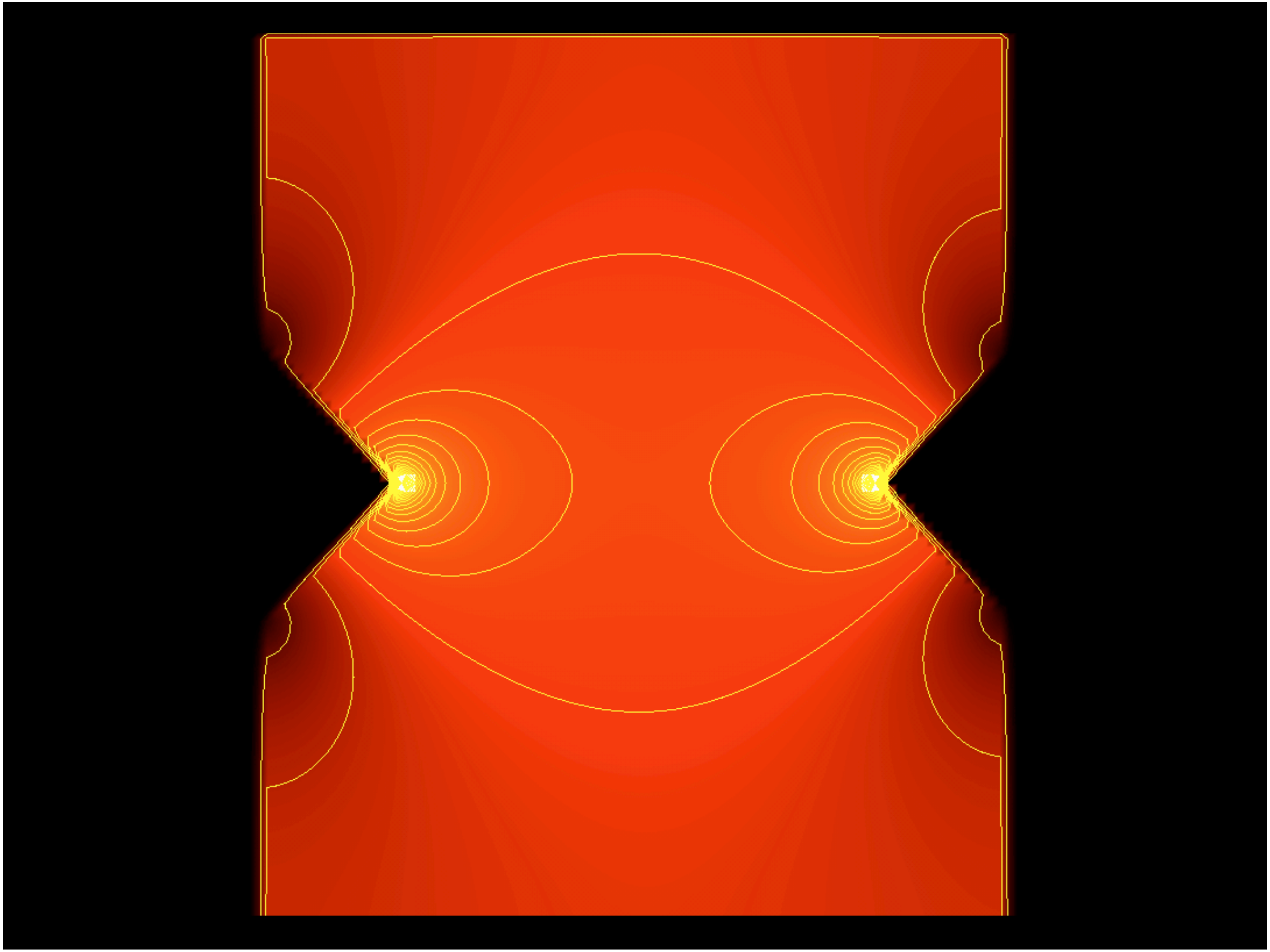
ELECTRIC FIELD AND POTENTIAL

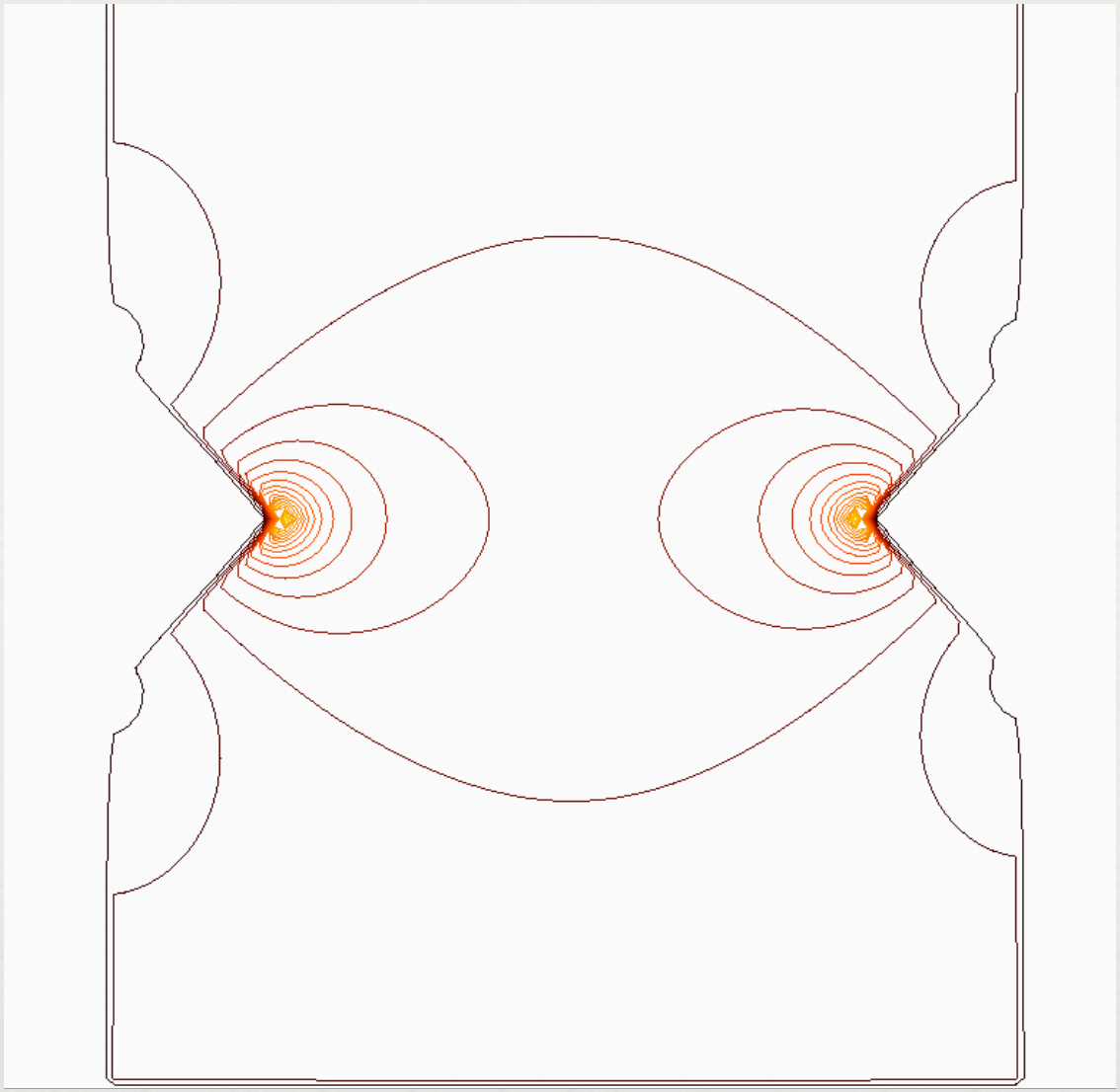


TWO-TIPS AT OPPOSITE POTENTIALS



HOW CAN WE GET RID OF SIDE FIELD?

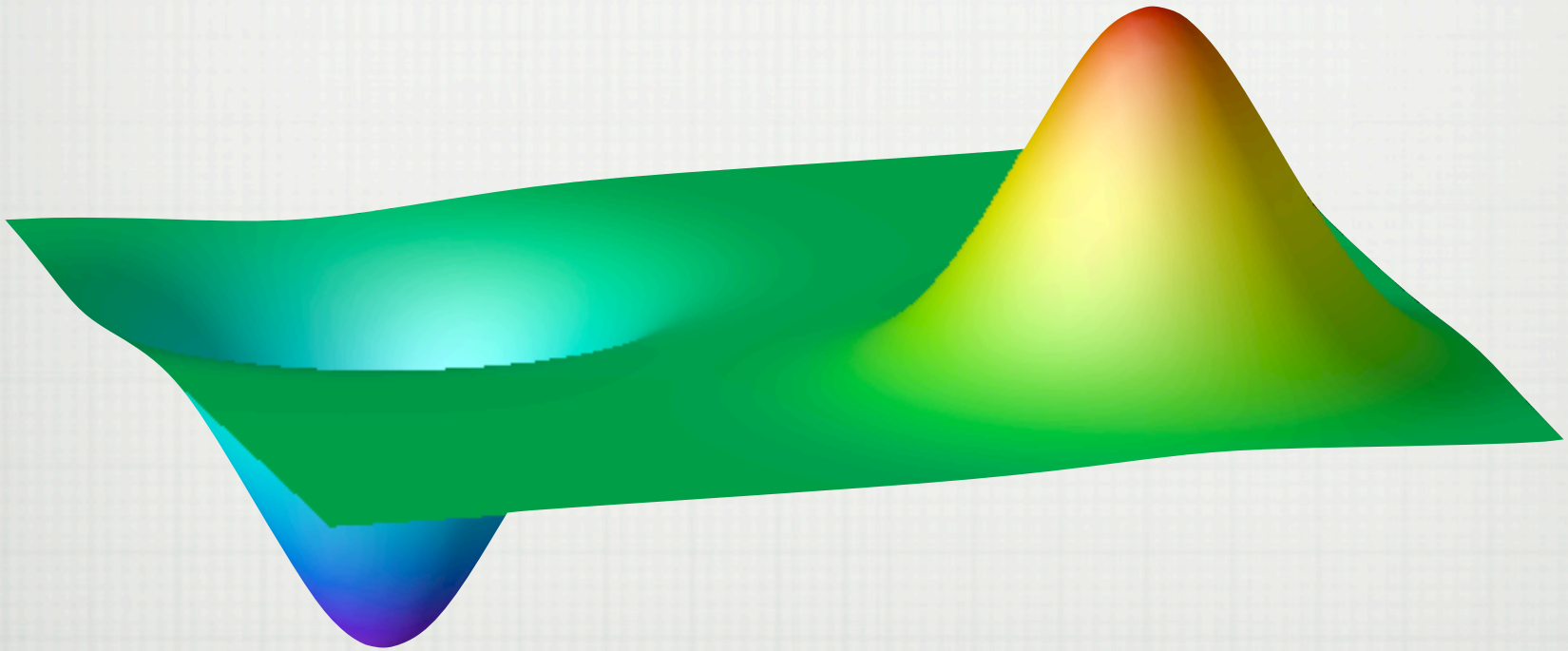




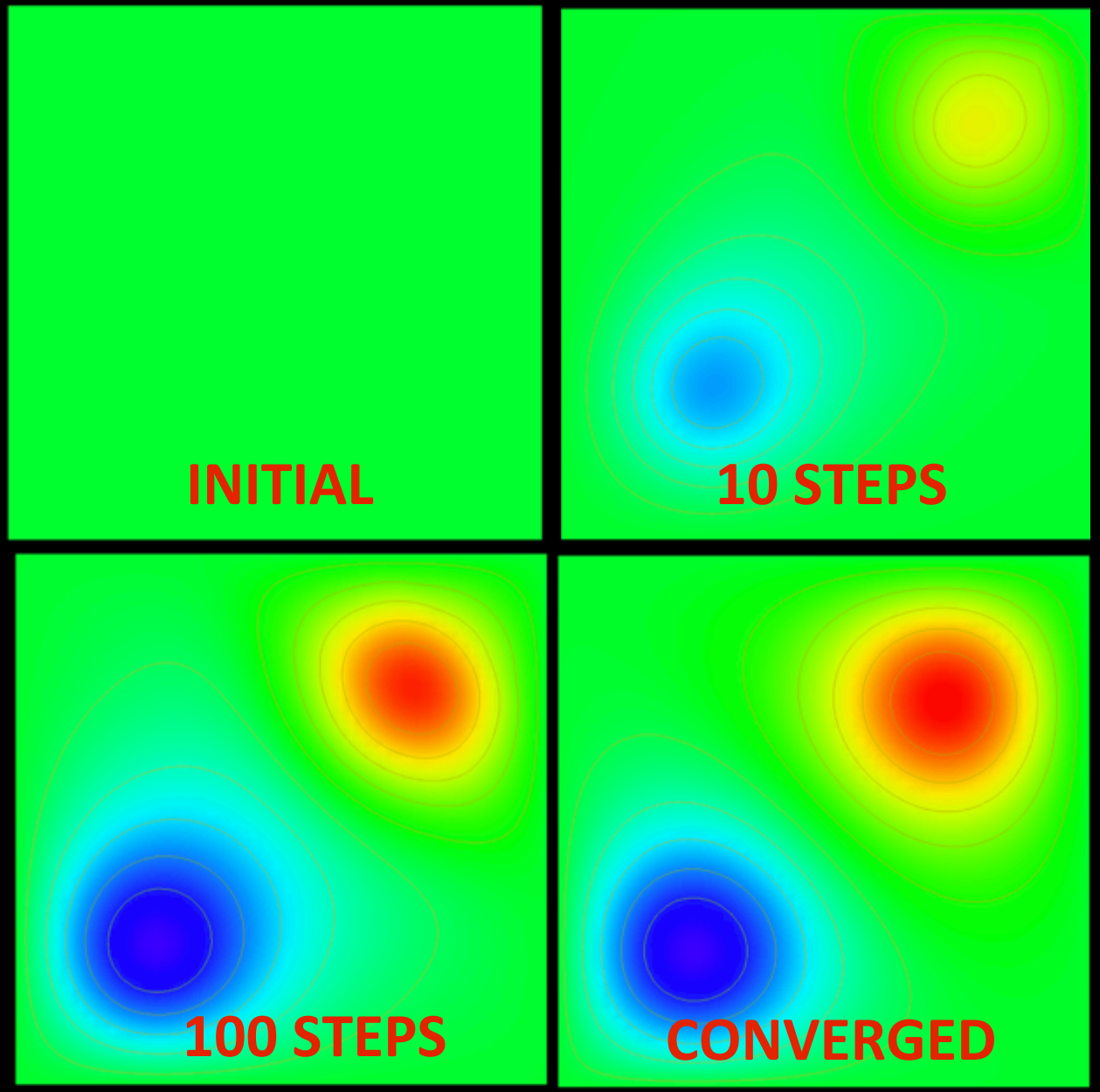
POISSON EQUATION

$$\frac{\partial^2 U(x,y)}{\partial x^2} + \frac{\partial^2 U(x,y)}{\partial y^2} = \begin{cases} 0 & \text{Laplace's equation} \\ -4\pi\rho(\mathbf{x}) & \text{Poisson's equation} \end{cases}$$

POISSON: POTENTIAL OF A DIPOLE?



POISSON EQUATION: DIPOLE



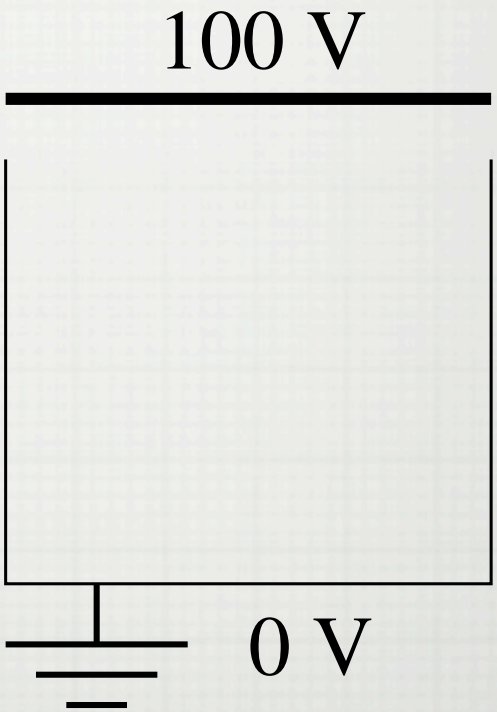
ACTUAL IMPLEMENTATION: C++ CODES

BOUNDARY CONDITIONS

```
for (ix=0;ix<n;ix++){
    for (iy=0;iy<n;iy++){
       donotcompute[ix][iy]=false;
       func[ix][iy]=0.0;
    }
}
for (iy=0;iy<n;iy++){
    if(periodic==0){
       donotcompute[0][iy]=true;
       donotcompute[n-1][iy]=true;
    }
    func[0][iy]=0.0;
    func[n-1][iy]=0.0;

}
for (ix=0;ix<n;ix++){
    donotcompute[ix][0]=true;
    donotcompute[ix][n-1]=true;
    func[ix][0]=0.0;
    func[ix][n-1]=0.0;

}
```

SPECIAL CONDITIONS

```
for (ix=0;ix<n;ix++){
    for (iy=0;iy<n;iy++){
       donotcompute[ix][iy]=false;
       func[ix][iy]=0.0;
    }
}
for (iy=0;iy<n;iy++){
    if(periodic==0){
       donotcompute[0][iy]=true;
       donotcompute[n-1][iy]=true;
    }
    func[0][iy]=0.0;
    func[n-1][iy]=0.0;

}
for (ix=0;ix<n;ix++){
    donotcompute[ix][0]=true;
    donotcompute[ix][n-1]=true;
    func[ix][0]=100.0;
    func[ix][n-1]=0.0;

}
```

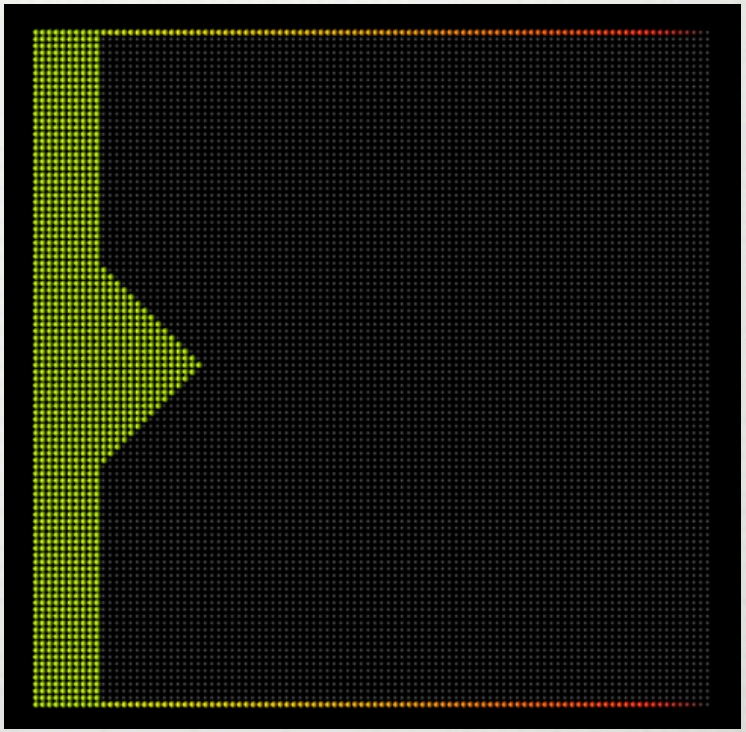


SPECIAL CONDITIONS: DOUBLE-PLATE

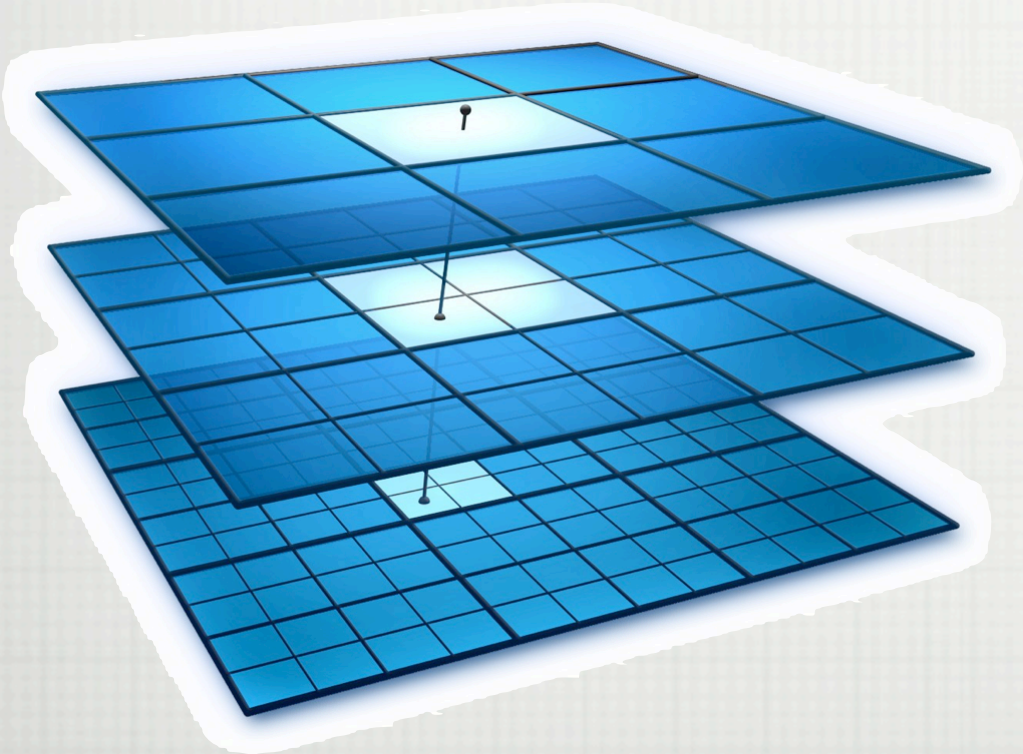
```
for (ix=10;ix<n-10;ix++){
      for(iy=20; iy<26;iy++){
         donotcompute[ix][iy]=true;
         donotcompute[ix][n-iy]=true;
         func[ix][iy]=result[ix][iy];
         func[ix][n-iy]=result[ix][n-iy];
      }
   }
}
```

SPECIAL CONDITIONS: TIP

```
for (ix=0;ix<n;ix++){
    for(iy=0; iy<n;iy++){
        if(iy<ix-25 && iy < -ix+75)
                {
            donotcompute[ix][iy]=true;
            func[ix][iy]=100;
        }
    }
}
for (ix=0;ix<n;ix++){
    for (iy=0;iy<10;iy++){
        donotcompute[ix][iy]=true;
        func[ix][iy]=100.0;
    }
}
```



HOW TO MAKE IT EVEN FASTER?



- **Solve on coarse grid and use the converged result on finer and finer grid.**

- **The preconditioning avoid spending too much time on the early stages of convergence**

SUMMARY

- **We covered relaxation methods for Laplace and Poisson's equation**
- **Over- and under- relaxation yield vast improvements to overall speed**
- **The "art" is to set up boundary conditions**