Electrostatics

C. J. F. Solano

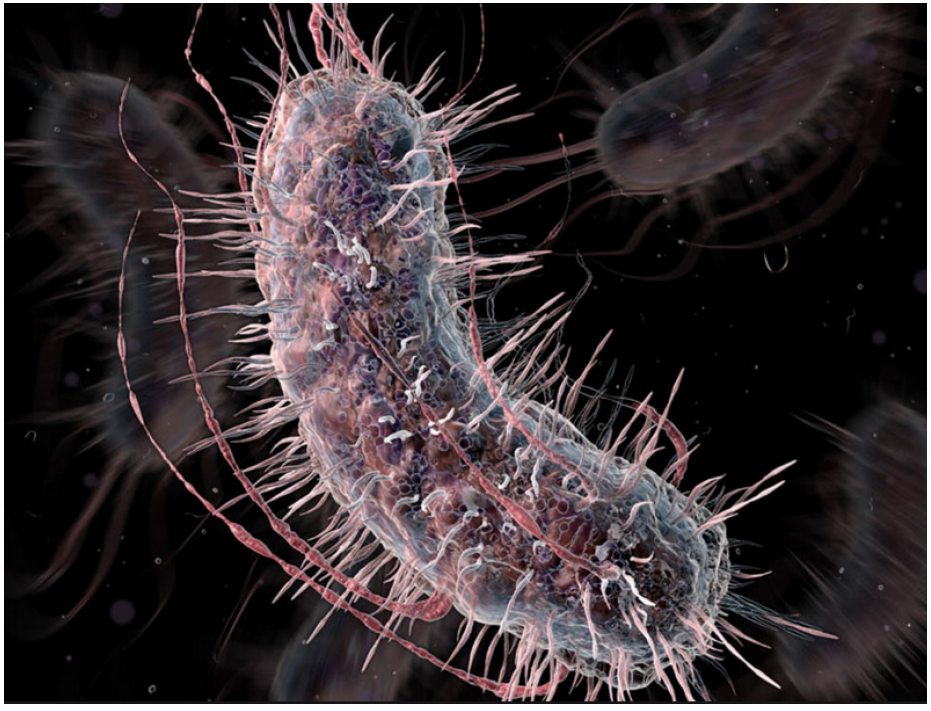
Jacobs University Bremen

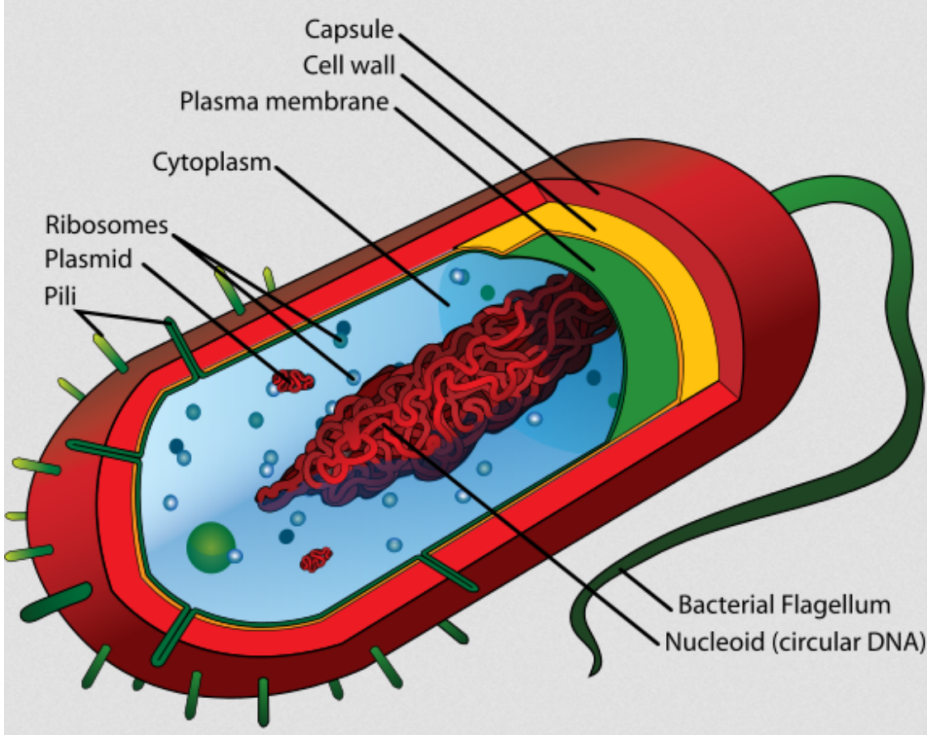
Outline

Motivation: E. Coli as an example

Escherichia coli:

- Gram-negative bacteria
- Two membranes protecting the interior

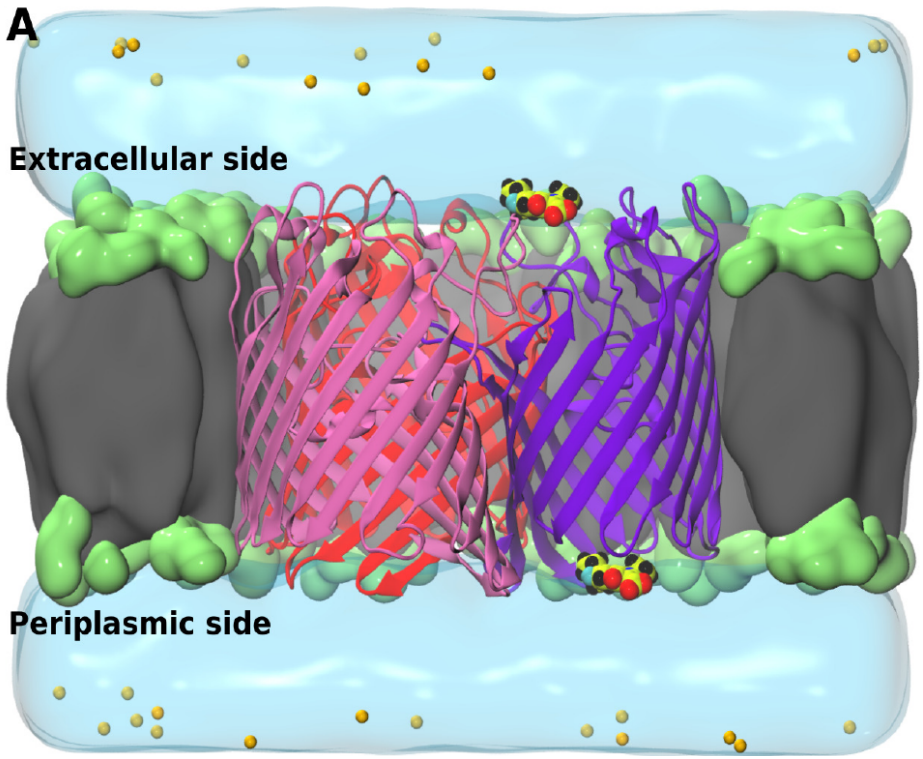




Motivation: E. Coli as an example

Outer membrane porins:

- Porins allow the permeation of ions and hydrophilic compounds
- The structure of some porins has been determined experimentally
- Electrostatic interactions play a key role in the permeation process



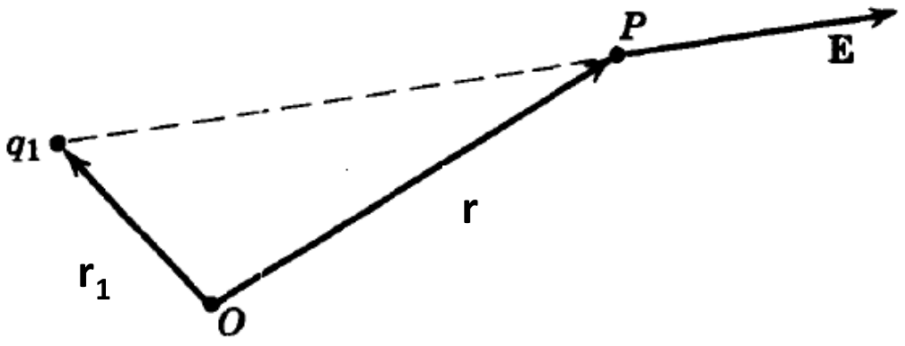
Outline

Electric field: definition

- An **electric field** is a **vector field** that associates to each point in space the Coulomb force that would be experienced by a test charge at that point
- The electric field at the point $\mathbf{r}$ due to a static charge q_1 at the point $\mathbf{r}_1$ is given by:

$$\mathbf{E}(\mathbf{r}) = kq_1 \frac{(\mathbf{r} - \mathbf{r}_1)}{|\mathbf{r} - \mathbf{r}_1|^3}$$

where k is a constant of proportionality



Electric field: units

The constant of proportionality k depends on the system of units used:

- **SI units** (mks units)

$$k = \frac{1}{4\pi\varepsilon_0}$$

  where $\varepsilon_0 = 8.854 \times 10^{-12}\, C^2 kg^{-1} m^{-3} s^2$ is permittivity of free space
  - Unit of charge is called *Coulomb*: $1\, C = 1\, As^{-1}$
  - $k \approx 9.0 \times 10^9 C^{-2} kgm^3 s^{-2}$
  - **This choice of units is not convenient for computer programs**
- **Gaussian units** (cgs units)

$$k = 1$$

  - Unit of charge is called *Stat-Coulomb*: $1\, statC = 1\, g^{1/2} cm^{3/2} s^{-1}$
  - The electric and magnetic field have the same dimension
  - **This choice of units is convenient for computer programs**

Electric field: superposition principle

The electric field at **r** due to a **system of static point charges** $\{q_1, \ldots, q_n\}$, located at $\mathbf{r}_i$ with $i = 1, \ldots, n$, can be written as the vector sum (parallelogram law)

$$\mathbf{E}(\mathbf{r}) = \sum_{i=1}^{n} \mathbf{E}_i(\mathbf{r}) = k \sum_{i=1}^{n} q_i \frac{(\mathbf{r} - \mathbf{r}_i)}{|\mathbf{r} - \mathbf{r}_i|^3}$$

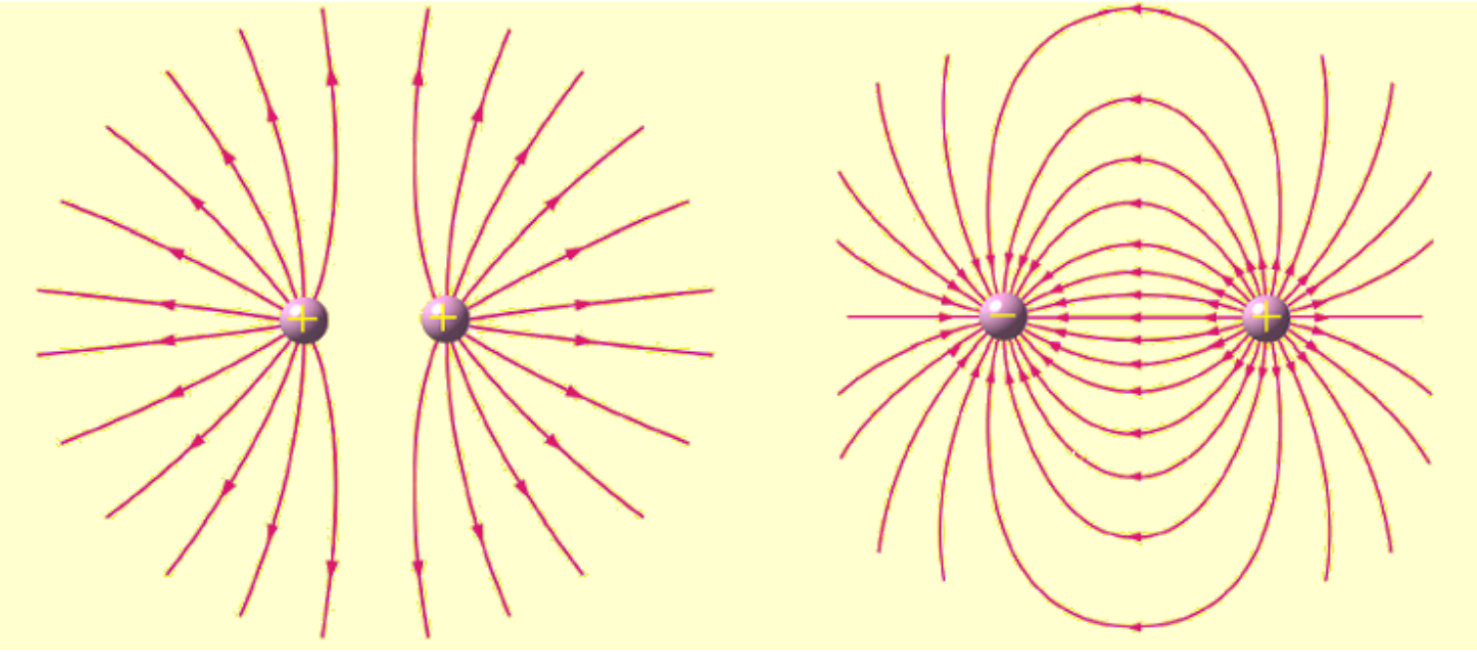
Electric field at **r** due to a **continuous charge distribution**:

$$\mathbf{E}(\mathbf{r}) = k \int d\mathbf{r}' \rho(\mathbf{r}') \frac{(\mathbf{r} - \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|^3}$$

- $d\mathbf{r}' = dx'dy'dz'$ is the three-dimensional volume element at $\mathbf{r}'$
- $\rho(\mathbf{r}') = \frac{\Delta q}{\Delta x \Delta y \Delta z}$ is the **charge density**, where Δq is the charge in a small volume $\Delta x \Delta y \Delta z$ at $\mathbf{r}'$

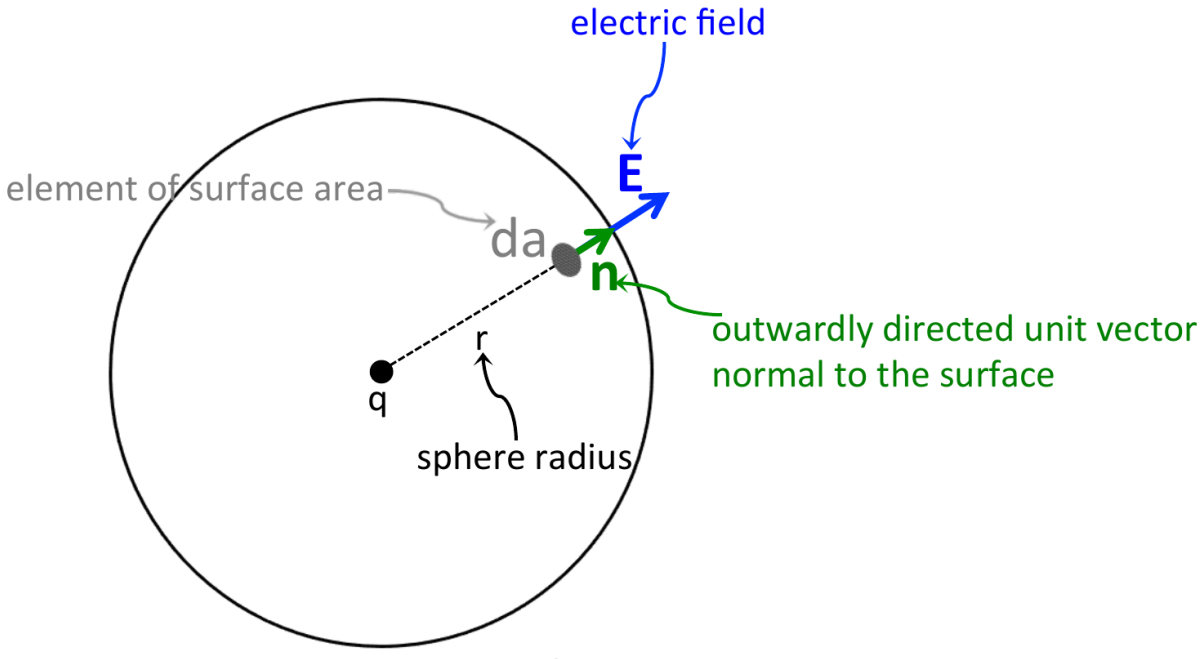
Electric field: electric field lines

- Directed lines whose tangent at every position is parallel to the electric field
- The density of lines at any location is proportional to the magnitude of the electric field at that point
- The electric field lines start at positive charges and end at negative charges



Gauss's law: integral form (Gaussian units)

Case 1: Spherical surface enclosing a single static point charge

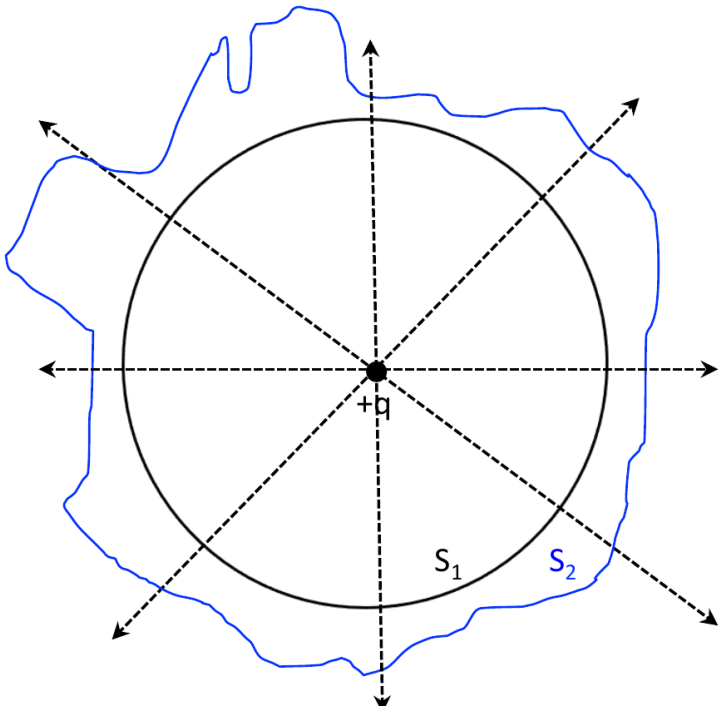


$$\oint_S \mathbf{E} \cdot \mathbf{n}\, da = \frac{q}{r^2} \oint_S da = \frac{q}{r^2}(4\pi r^2) = 4\pi q$$

where $\oint_S$ is an integral over a closed surface S and $\mathbf{E} = q\mathbf{r}/r^3$ (point charge q is located at the origin of coordinates)

Gauss's law: integral form (Gaussian units)

Case 2: Irregular surface enclosing a single static point charge



$$\oint_{S_1} \mathbf{E} \cdot \mathbf{n}\, da = \oint_{S_2} \mathbf{E} \cdot \mathbf{n}\, da = 4\pi q$$

The same number of field lines pass through surface S_1 as surface S_2

Gauss's law: integral form (Gaussian units)

Case 3: Many static charges in some region of space

$$\begin{aligned} \oint_S \mathbf{E} \cdot \mathbf{n}\, da &= \sum_i \oint_S \mathbf{E}_i \cdot \mathbf{n}\, da \\ &= 4\pi \sum_i q_i \end{aligned}$$

where we use the **superposition principle** (first equality) and **Gauss's law for each single static point charge** (second equality)

Case 4: Gauss's law in terms of the charge density

$$\oint_S \mathbf{E} \cdot \mathbf{n}\, da = 4\pi \int_V \rho(\mathbf{r}) d\mathbf{r}$$

where V is the volume enclosed by the surface S

Gauss's law: differential form (Gaussian units)

- **Divergence theorem**:

$$\oint_S \mathbf{E} \cdot \mathbf{n}\, da = \int_V \nabla \cdot \mathbf{E}\, d\mathbf{r}$$

  where $\nabla \cdot \mathbf{E} = \frac{\partial E_x}{\partial x} + \frac{\partial E_y}{\partial y} + \frac{\partial E_z}{\partial z}$ is the divergence of the electric field (cartesian coordinates)

- **Gauss's law**: (previous slide)

$$\oint_S \mathbf{E} \cdot \mathbf{n}\, da = 4\pi \int_V \rho(\mathbf{r}) d\mathbf{r}$$

- Combining both:

$$\int_V \left[\nabla \cdot \mathbf{E}(\mathbf{r}) - 4\pi\rho(\mathbf{r})\right]\, d\mathbf{r} = 0$$

  which implies

$$\boxed{\nabla \cdot \mathbf{E}(\mathbf{r}) = 4\pi\rho(\mathbf{r})}$$

Electric potential: definition

Electric field (a vector) is derived from a scalar (i.e., electric potential) by the gradient operation

$$\mathbf{E}(\mathbf{r}) = -\nabla V(\mathbf{r})$$

$$\mathbf{E}(\mathbf{r}) = -\frac{\partial V(\mathbf{r})}{\partial x}\mathbf{u}_x - \frac{\partial V(\mathbf{r})}{\partial y}\mathbf{u}_y - \frac{\partial V(\mathbf{r})}{\partial z}\mathbf{u}_z$$

where $\mathbf{u}_x$, $\mathbf{u}_y$ and $\mathbf{u}_z$ are unit vectors in the x, y and z directions

Proof:

$$\begin{aligned}\mathbf{E}(\mathbf{r}) &= k\int d\mathbf{r}'\rho(\mathbf{r}')\frac{(\mathbf{r}-\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|^3} \\ &= -\nabla k\int d\mathbf{r}'\frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} \\ &= -\nabla V(\mathbf{r})\end{aligned}$$

where

$$V(\mathbf{r}) = k\int d\mathbf{r}'\frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}$$

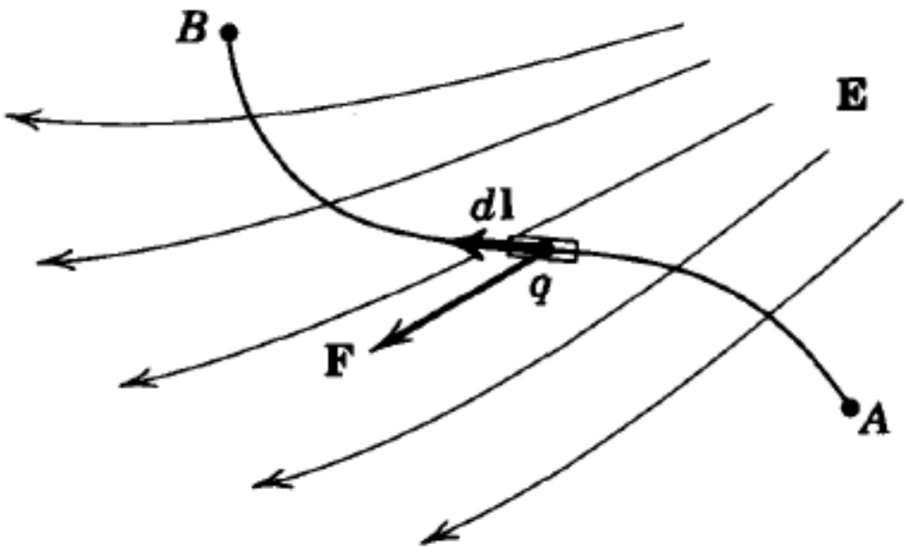
is the **electric potential** and we use the relation

$$\frac{(\mathbf{r}-\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|^3} = -\nabla\left(\frac{1}{|\mathbf{r}-\mathbf{r}'|}\right)$$

Electric potential: physical interpretation

The work done on test charge q in transporting it from one point A to another point B in the presence of an electric field $\mathbf{E}(\mathbf{r})$ is given by

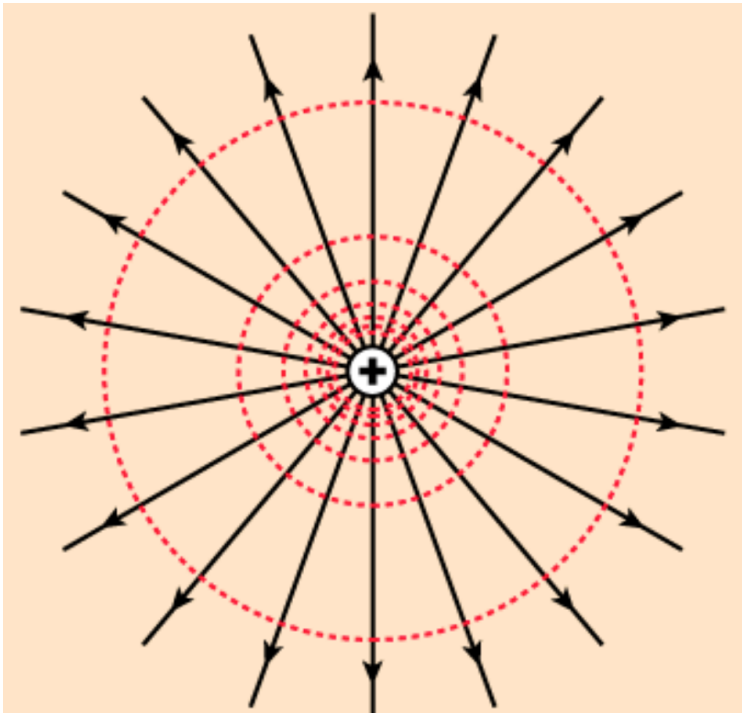
$$
\begin{aligned}
W &= -\int_A^B \mathbf{F} \cdot d\mathbf{l} \\
&= -q \int_A^B \mathbf{E} \cdot d\mathbf{l} \\
&= q \int_A^B \nabla V \cdot d\mathbf{l} \\
&= q \int_A^B dV = q(V_B - V_A)
\end{aligned}
$$



qV can be interpreted as the **potential energy** of the test charge in the electric field

Electric potential: equipotential lines

- Equipotential lines are like contour lines on a map which trace lines of equal electric potential
- They are always perpendicular to the electric field
- In 3D, the lines form equipotential surfaces
- Movement along an equipotential surface requires no work because such movement is always perpendicular to the electric field



Poisson's and Laplace's equations

- We have seen that the Gauss's law implies that $\nabla \cdot \mathbf{E}(\mathbf{r}) = 4\pi\rho(\mathbf{r})$
- We have seen that $\mathbf{E}$ can be written as the gradient of V, i.e., $\mathbf{E}(\mathbf{r}) = -\nabla V(\mathbf{r})$
- Combining both we get a **partial differential equation** of elliptic type:

$$\nabla^2 V(\mathbf{r}) = \frac{\partial^2 V(x,y,z)}{\partial x^2} + \frac{\partial^2 V(x,y,z)}{\partial y^2} + \frac{\partial^2 V(x,y,z)}{\partial z^2} = -4\pi\rho(x,y,z)$$

  which is known as **Poisson's equation**

- In regions of space where there is no charge density, we get the **Laplace's equation** $\nabla^2 V(\mathbf{r}) = 0$

Outline

Poisson's equation: goal and boundary conditions

- **Partial differential equation** on some domain $\Omega = [x_{min}, x_{max}] \times [y_{min}, y_{max}] \times [z_{min}, z_{max}]$:

$$\frac{\partial^2 V(x,y,z)}{\partial x^2} + \frac{\partial^2 V(x,y,z)}{\partial y^2} + \frac{\partial^2 V(x,y,z)}{\partial z^2} = -4\pi\rho(x,y,z)$$

- Goal: Determine $V(x,y,z)$ for $(x,y,z) \in \Omega$ using **numerical methods**
- **Boundary value problem**: Poisson's equation is an ill-posed problem and, therefore, **boundary conditions** (BC) are required:
  - **Dirichlet BC**. Specification of V values on a closed boundary surface
  - **Neumann BC**. Specification of $E = -\nabla V$ values on a closed boundary surface
  - **Periodic BC**. $V(x_{min}, y, z) = V(x_{max}, y, z)$, $V(x, y_{min}, z) = V(x, y_{max}, z)$ and $V(x, y, z_{min}) = V(x, y, z_{max})$

Finite-difference method: discretization in 2D

- **Poisson's equation** (Gaussian units):

$$\frac{\partial^2 V(x,y,z)}{\partial x^2} + \frac{\partial^2 V(x,y,z)}{\partial y^2} = -4\pi\rho(x,y)$$

- We define a **mesh grid** covering the region of interest $\Omega = [x_0, x_I] \times [y_0, y_J]$:

$$\begin{aligned} x_i &= x_0 + ih,\ i = 0, \ldots, I \\ y_i &= y_0 + jh,\ j = 0, \ldots, J \end{aligned}$$

- For convenience, we take the **grid spacing** h to be uniform and equal in both directions

Finite-difference method: discretization in 2D

- Taylor expansion:

$$V(x_i + h, y_j) = V(x_i, y_j) + h\frac{\partial V(x_i, y_j)}{\partial x} + \frac{h^2}{2}\frac{\partial^2 V(x_i, y_j)}{\partial x^2} + \frac{h^3}{6}\frac{\partial^3 V(x_i, y_j)}{\partial x^3} + O(h^4)$$

+

$$V(x_i - h, y_j) = V(x_i, y_j) - h\frac{\partial V(x_i, y_j)}{\partial x} + \frac{h^2}{2}\frac{\partial^2 V(x_i, y_j)}{\partial x^2} - \frac{h^3}{6}\frac{\partial^3 V(x_i, y_j)}{\partial x^3} + O(h^4)$$

$$\frac{\partial^2 V(x_i, y_j)}{\partial x^2} = \frac{V(x_i + h, y_j) + V(x_i - h, y_j) - 2V(x_i, y_j)}{h^2} + O(h^2)$$ ← discretization error

If h small ➡ $$\boxed{\frac{\partial^2 V(x_i, y_j)}{\partial x^2} \approx \frac{V(x_i + h, y_j) + V(x_i - h, y_j) - 2V(x_i, y_j)}{h^2}}$$

Similarly ➡ $$\boxed{\frac{\partial^2 V(x_i, y_j)}{\partial y^2} \approx \frac{V(x_i, y_j + h) + V(x_i, y_j - h) - 2V(x_i, y_j)}{h^2}}$$

Finite-difference method: discretization in 2D

- For simplicity, we use the notation $V_{i,j} \equiv V(x_i, y_j)$ and $\rho_{i,j} \equiv \rho(x_i, y_j)$:

$$\frac{V_{i+1,j} + V_{i-1,j} - 2V_{i,j}}{h^2} + \frac{V_{i,j+1} + V_{i,j-1} - 2V_{i,j}}{h^2} = -4\pi\rho_{i,j}$$

$$V_{i+1,j} + V_{i-1,j} + V_{i,j+1} + V_{i,j-1} - 4V_{i,j} = -4\pi h^2 \rho_{i,j}$$

- This equation holds only at the **interior points**, which satisfy:

$$\begin{aligned} i &= 1, \ldots, I-1 \\ j &= 1, \ldots, J-1 \end{aligned}$$

- V or its derivative should be specified at the **boundary points**, which satisfy:

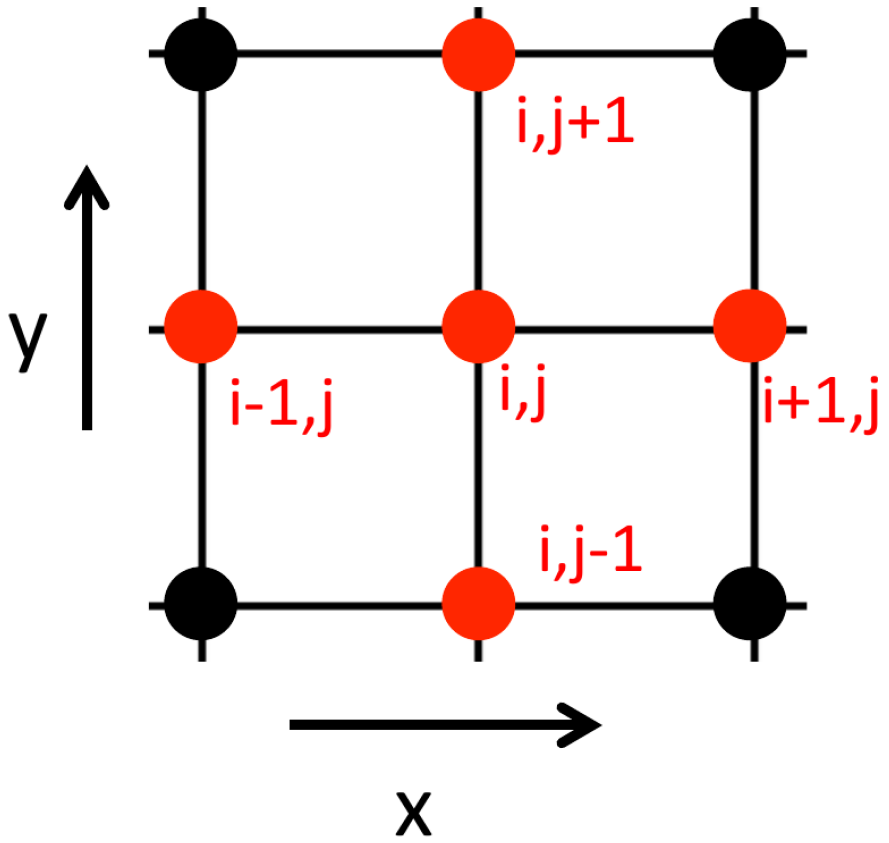
$$\begin{aligned} i &= 0, I \\ j &= 0, J \end{aligned}$$

Finite-difference method: discretization in 2D

System of linear equations (Gaussian units):

$$V_{i+1,j} + V_{i-1,j} + V_{i,j+1} + V_{i,j-1} - 4V_{i,j} = -4\pi h^2 \rho_{i,j}$$

- Each grid point is connected to 4 nearest neighbors:



Finite-difference method: discretization in 2D

System of linear equations (Gaussian units):

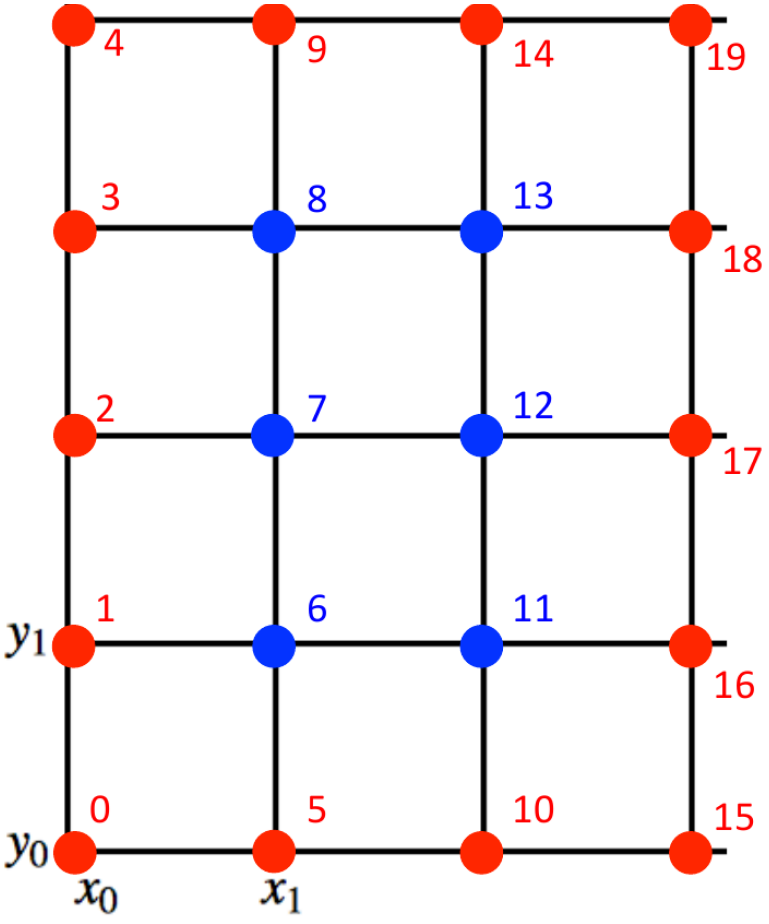
$$V_{i+1,j} + V_{i-1,j} + V_{i,j+1} + V_{i,j-1} - 4V_{i,j} = -4\pi h^2 \rho_{i,j}$$

To write the system of linear equations in matrix form we need to make a vector out of V. Let us number the two dimensions of grid points in a single one-dimensional sequence by defining $n \equiv i(J+1) + j$ for $i = 0, \ldots, I$ and $j = 0, \ldots, J$. Thus, the linear equations can be rewritten as:

$$V_{n+J+1} + V_{n-(J+1)} + V_{n+1} + V_{n-1} - 4V_n = -4\pi h^2 \rho_n$$

Finite-difference method: discretization in 2D

Example: $I = 3$, $J = 4$, Dirichlet BC

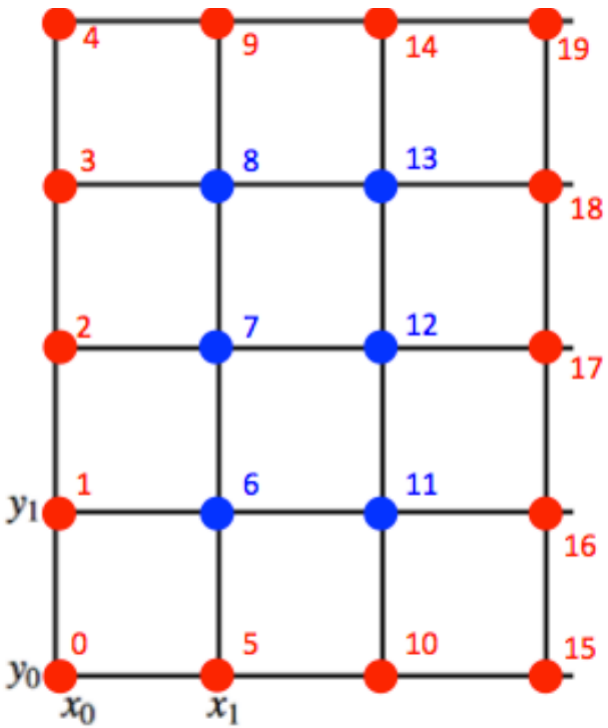


Boundary points

Interior points

Finite-difference method: discretization in 2D

Example: $I = 3$, $J = 4$, Dirichlet BC



$$-4V_6 + V_7 + 0 + V_{11} + 0 + 0 = -4\pi h^2\rho_6 - V_1 - V_5$$

$$V_6 - 4V_7 + V_8 + 0 + V_{12} + 0 = -4\pi h^2\rho_7 - V_2$$

$$0 + V_7 - 4V_8 + 0 + 0 + V_{13} = -4\pi h^2\rho_8 - V_3 - V_9$$

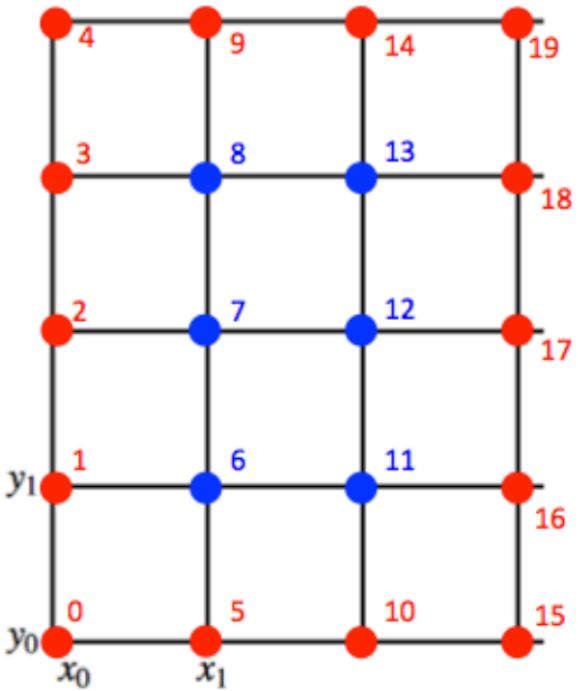
$$V_6 + 0 + 0 - 4V_{11} + V_{12} + 0 = -4\pi h^2\rho_{11} - V_{10} - V_{16}$$

$$0 + V_7 + 0 + V_{11} - 4V_{12} + 0 = -4\pi h^2\rho_{12} - V_{17}$$

$$0 + 0 + V_8 + 0 + V_{12} - 4V_{13} = -4\pi h^2\rho_{13} - V_{14} - V_{18}$$

Finite-difference method: discretization in 2D

Example: $I = 3$, $J = 4$, Dirichlet BC



Matrix notation $\mathbf{Ax} = \mathbf{b}$

$$\mathbf{x} = \begin{pmatrix} V_6 \\ V_7 \\ V_8 \\ V_{11} \\ V_{12} \\ V_{13} \end{pmatrix} \qquad \mathbf{b} = \begin{pmatrix} -4\pi h^2 \rho_6 - V_1 - V_5 \\ -4\pi h^2 \rho_7 - V_2 \\ -4\pi h^2 \rho_8 - V_3 - V_9 \\ -4\pi h^2 \rho_{11} - V_{10} - V_{16} \\ -4\pi h^2 \rho_{12} - V_{17} \\ -4\pi h^2 \rho_{13} - V_{14} - V_{18} \end{pmatrix}$$

$$\mathbf{A} = \left(\begin{array}{ccc:ccc} -4 & 1 & 0 & 1 & 0 & 0 \\ 1 & -4 & 1 & 0 & 1 & 0 \\ 0 & 1 & -4 & 0 & 0 & 1 \\ \hdashline 1 & 0 & 0 & -4 & 1 & 0 \\ 0 & 1 & 0 & 1 & -4 & 1 \\ 0 & 0 & 1 & 0 & 1 & -4 \end{array}\right)$$

tridigonal matrix with fringes

Finite-difference method: discretization in 3D

- **Poisson's equation** (Gaussian units):

$$\frac{\partial^2 V(x,y,z)}{\partial x^2} + \frac{\partial^2 V(x,y,z)}{\partial y^2} + \frac{\partial^2 V(x,y,z)}{\partial z^2} = -4\pi\rho(x,y,z)$$

- We define a **mesh grid** covering the region of interest $\Omega = [x_0, x_I] \times [y_0, y_J] \times [z_0, z_K]$:

$$\begin{aligned} x_i &= x_0 + ih, \ i = 0, \ldots, I \\ y_i &= y_0 + jh, \ j = 0, \ldots, J \\ z_i &= z_0 + kh, \ k = 0, \ldots, K \end{aligned}$$

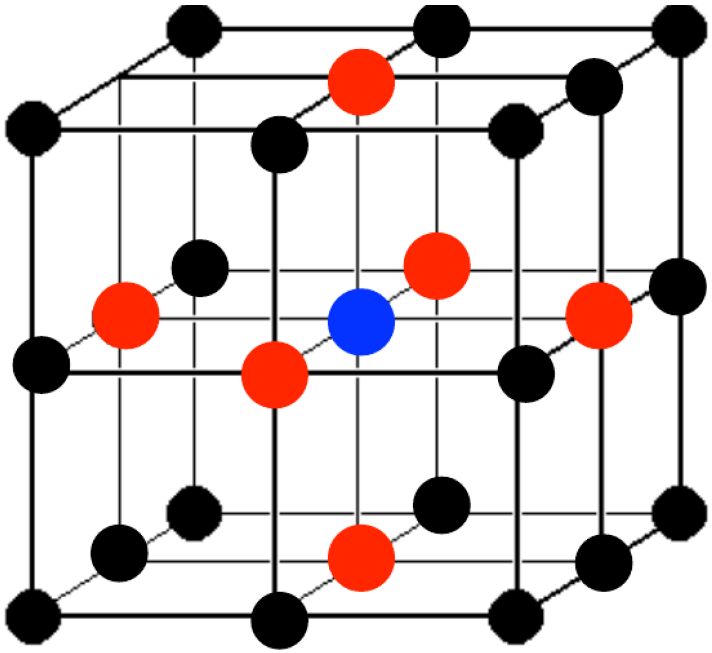
- **Discretization**:

$$V_{i+1,j,k} + V_{i-1,j,k} + V_{i,j+1,k} + V_{i,j-1,k}$$

$$+ V_{i,j,k+1} + V_{i,j,k-1} - 6V_{i,j,k} = -4\pi h^2 \rho_{i,j,k}$$

where $V_{i,j,k} \equiv V(x_i, y_j, z_k)$ and $\rho_{i,j,k} = \rho(x_i, y_j, z_k)$

Finite-difference method: discretization in 3D



Each grid point is connected to 6 nearest neighbors

Finite-difference method: discretization in 3D

- **Matrix form**:

$$V_{n+J(K+1)+1} + V_{n-[J(K+1)+1]} + V_{n+K+1} + V_{n-(K+1)}$$

$$+V_{n+1} + V_{n-1} - 6V_n = -4\pi h^2 \rho_n$$

or, equivalently,

$$\mathbf{Ax} = \mathbf{b}$$

where $n \equiv i(J+1)(K+1) + j(K+1) + k$ for $i = 0, \ldots, I$, $j = 0, \ldots, J$ and $k = 0, \ldots, K$

Approaches to solve the system of linear equations

1. **Direct matrix methods**:
   - Attempt to solve the equation directly
   - It is not applicable for large grids
2. **Relaxation methods**:
   - Because most of the elements of **A** vanish (it is sparse), one can use efficient iterative techniques
3. **Random walk solutions**:
   - Applied to find a local solution (i.e., at a given interior point)

Relaxation methods: Jacobi's iterative method

We rewrite the Poisson's equation as a **diffusion equation**:

$$\frac{\partial V(\mathbf{r},t)}{\partial t} = \nabla^2 V(\mathbf{r},t) + 4\pi\rho(\mathbf{r}) = 0$$

- An initial distribution V relaxes to an equilibrium solution as $t \to \infty$
- This equilibrium has all time derivatives vanishing and, thus, it is the solution of the original Poisson's equation

Relaxation methods: Jacobi's iterative method

Finite-difference method (2D):

- $t_n = t_0 + n\Delta t$, where $n = 0, \ldots, T$ and Δt is the timestep
- Taylor expansions:

$$V(x_i, y_j, t_n + \Delta t) = V(x_i, y_j, t_n) + \Delta t \frac{\partial V(x_i, y_j, t_n)}{\partial t} + O(\Delta t^2)$$

$$\frac{\partial^2 V(x_i, y_j, t_n)}{\partial x^2} = \frac{V(x_i + h, y_j, t_n) + V(x_i - h, y_j, t_n) - 2V(x_i, y_j, t_n)}{h^2} + O(h^2)$$

$$\frac{\partial^2 V(x_i, y_j, t_n)}{\partial y^2} = \frac{V(x_i, y_j + h, t_n) + V(x_i, y_j - h, t_n) - 2V(x_i, y_j, t_n)}{h^2} + O(h^2)$$

- If Δt and h are small:

$$\frac{\partial V(x_i, y_j, t_n)}{\partial t} \approx \frac{V(x_i, y_j, t_n + \Delta t) - V(x_i, y_j, t_n)}{\Delta t}$$

$$\frac{\partial^2 V(x_i, y_j, t_n)}{\partial x^2} \approx \frac{V(x_i + h, y_j, t_n) + V(x_i - h, y_j, t_n) - 2V(x_i, y_j, t_n)}{h^2}$$

$$\frac{\partial^2 V(x_i, y_j, t_n)}{\partial y^2} \approx \frac{V(x_i, y_j + h, t_n) + V(x_i, y_j - h, t_n) - 2V(x_i, y_j, t_n)}{h^2}$$

Relaxation methods: Jacobi's iterative method

Finite-difference method (2D):

- For simplicity, we use the notation $V_{i,j}^n = V(x_i, y_j, t_n)$ and $\rho_{i,j} = \rho(x_i, y_j)$:

$$V_{i,j}^{n+1} = V_{i,j}^n + \frac{\Delta t}{h^2}\left(V_{i+1,j}^n + V_{i-1,j}^n + V_{i,j+1}^n + V_{i,j-1}^n - 4V_{i,j}^n + 4\pi h^2 \rho_{i,j}\right)$$

- The differencing is stable only if $\frac{\Delta t}{h^2} \leq \frac{1}{4}$. If we take the largest possible time step $\Delta t = \frac{h^2}{4}$:

$$V_{i,j}^{n+1} = \frac{1}{4}\left(V_{i+1,j}^n + V_{i-1,j}^n + V_{i,j+1}^n + V_{i,j-1}^n + 4\pi h^2 \rho_{i,j}\right)$$

Relaxation methods: Jacobi's iterative method

$$V_{i,j}^{n+1} = \frac{1}{4}\left(V_{i+1,j}^{n} + V_{i-1,j}^{n} + V_{i,j+1}^{n} + V_{i,j-1}^{n} + 4\pi h^2 \rho_{i,j}\right)$$

Algorithm:

- **Step 1**: Initial values (guess) $V_{i,j}^{0}$
- **Step 2**: Calculate $V_{i,j}^{n+1}$ for iteration $n+1$, where $n = 0, 1, \ldots$
- Repeat **Step 2** until convergence. **Convergence criteria**: there is not significant change in the electric potential from one to next iteration

Jacobi's method is not practical because it converges too slowly. However, it is the basis for understanding the modern methods, which are always compared with it

Relaxation methods: Gauss-Seidel method

- Modification of Jacobi's method which converges a little faster
- If we are proceeding along the arrows, incrementing i for fixed j, we have for the $n+1$ iteration:

$$V_{i,j}^{n+1} = \frac{1}{4}\left(V_{i+1,j}^{n} + V_{i-1,j}^{n+1} + V_{i,j+1}^{n} + V_{i,j-1}^{n+1} + 4\pi h^2 \rho_{i,j}\right)$$

  where $V_{i-1,j}^{n+1}$ and $V_{i,j-1}^{n+1}$ are neighbors already updated
- The average is done *in place* instead of being *copied* from an earlier iteration to a later one. Thus, the most *current* values of electric potential are use in each iteration

Relaxation methods: sucessive overrelaxation method

- If we are proceeding along the arrows, incrementing i for fixed j, we have for the $n+1$ iteration:

$$V_{i,j}^{n+1} = (1-\omega)V_{i,j}^{n} + \frac{\omega}{4}\left(V_{i+1,j}^{n} + V_{i-1,j}^{n+1} + V_{i,j+1}^{n} + V_{i,j-1}^{n+1} + 4\pi h^2 \rho_{i,j}\right)$$

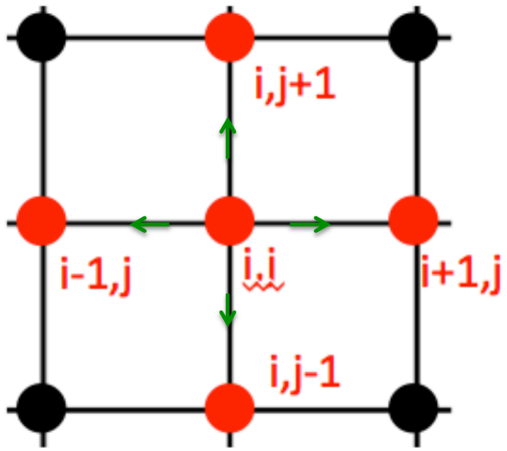
  where the **relaxation parameter** ω can be tuned to optimize the convergence (**overrelaxation** means $\omega > 1$, **underrelaxation** means $\omega < 1$)
- The following theorems can be proved:
  - The method converges only for $0 < \omega < 2$
  - Under certain restrictions generally satisfied by matrices arising from finite differencing, only **overrelaxation** ($1 < \omega < 2$) can give faster convergence than the Gauss-Seidel method
  - The *optimal* choice for ω on $l \times l$ square grid is given by $\omega \simeq \frac{2}{1+\frac{\pi}{l}}$

Relaxation methods: convergence estimation

- For a $l \times l$ squared grid with Dirichlet BC, the **number of iterations** r required to reduce the overall error by a factor 10^{-p} is:
  - Jacobi's iterative method: $r \approx pl^2/2$
  - Gauss-Seidel method: $r \approx pl^2/4$
  - Successive overrelaxation method: $r \approx pl/\omega$ for *optimal* ω
- Example: 50×50 squared grid with Dirichlet BC, r required to reduce the overall error by a factor 10^{-3} is:
  - Jacobi's iterative method: $r \approx 3750$
  - Gauss-Seidel method: $r \approx 1875$
  - Successive overrelaxation method: $r \approx 50$

Random walk solution: definition and discrete random walkers

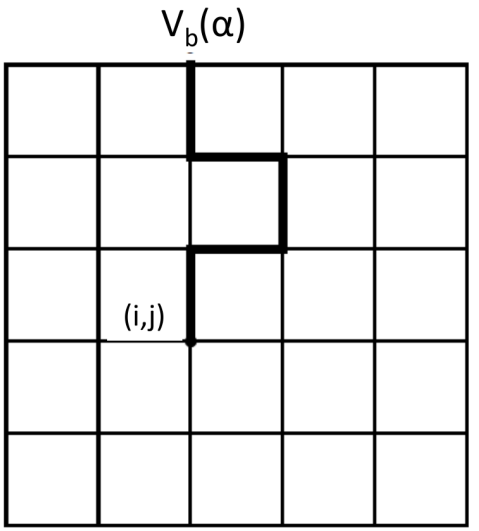
- **Relaxation method**
  - **Global method**. A global solution of the electric potential is obtained by solving a system of linear equations
- **Random walk solution**
  - **Local method**. The electric potential is calculated only at a desired single point
  - It can be applied with **Dirichlet** and **Neumann BC**
- A **discrete random walker** at a point (x_i, y_j) (or (x_i, y_j, z_k)) is able to jump to one of its 4 (or 6) nearest neighbors with equal probability $p = 1/4$ (or $p = 1/6$)



Random walk solution: algorithm

Algorithm (2D and Dirichlet BC):

1. Begin with a discrete walker at desired point (x_i, y_j)
2. Take steps until walker reaches a boundary point
3. Record the electric potential at the boundary point $V_b(\alpha)$ and the charge density visited by the walker $\rho(x_{k\alpha}, y_{k\alpha})$, where α labels the walker and k labels the points visited by the walker α
4. Repeat steps 1, 2 and 3 n times
5. The electric potential at desired point (x_i, y_j) is given by



$$V(x_i, y_j) = \frac{1}{n}\sum_{\alpha=1}^{n} V_b(\alpha) + \frac{\pi h^2}{n}\sum_{\alpha=1}^{n}\sum_{k} \rho(x_{k\alpha}, y_{k\alpha})$$

Random walk solution: limitations

Main disadvantage: Random walk solution requires many walkers to obtain a good estimate of the electric potential