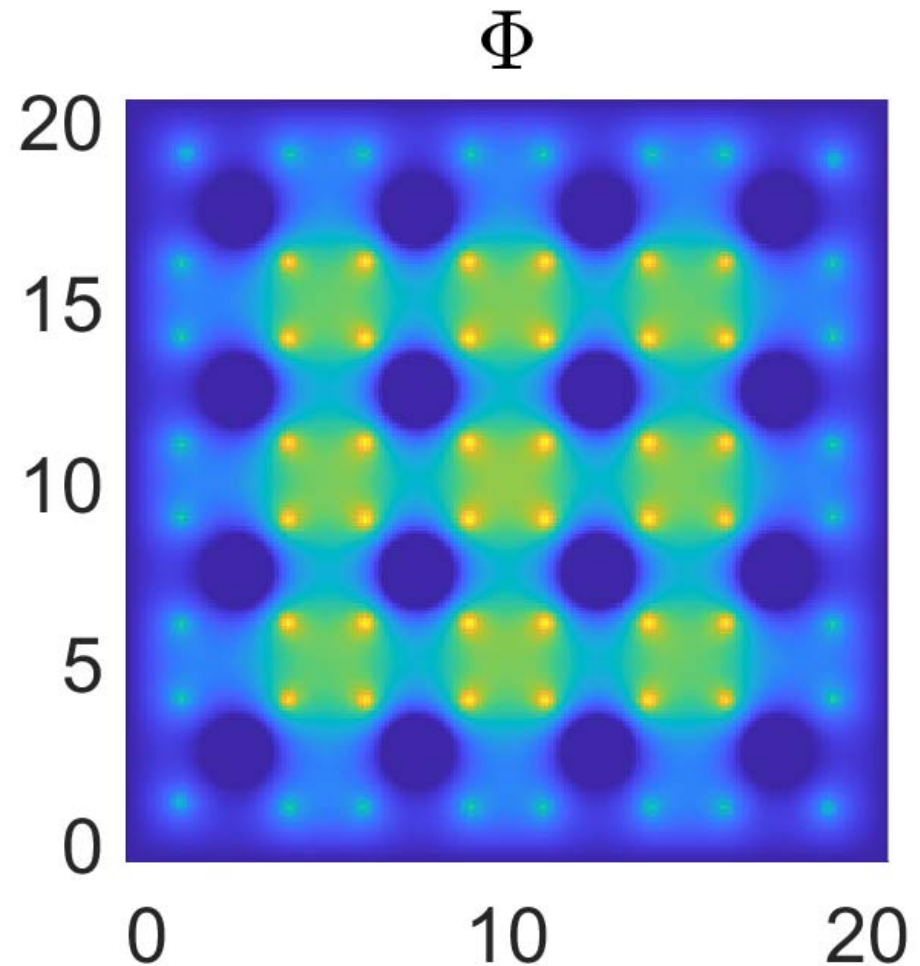


Overlapping Domain  
Decomposition Finite  
Element  
Method (FE-DDM) of  
Electrostatic Problem

TEAM 10

Junda Feng  
(jundaf2@illinois.edu)

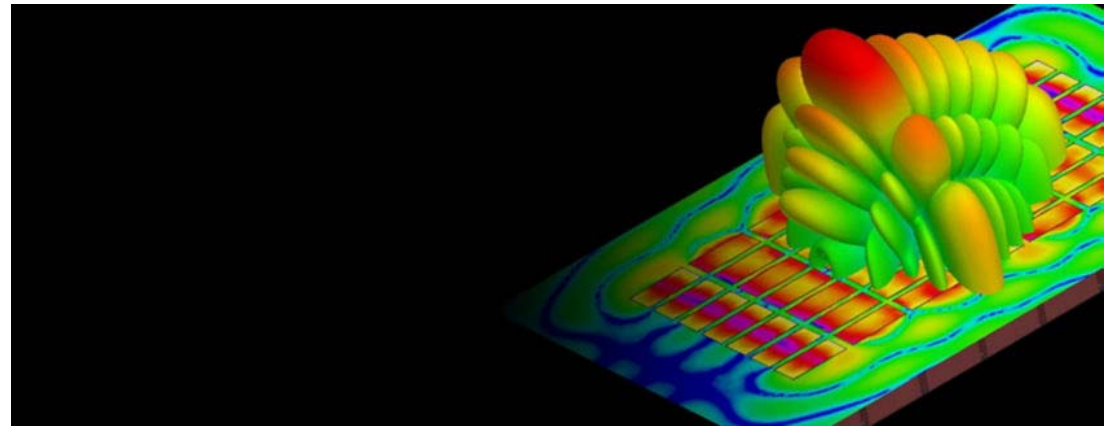
2021/5/8



# What is FEM?

The finite element method (FEM) is a widely used method for numerically solving partial differential equations (PDEs) arising in engineering and mathematical modeling.

-- Wikipedia



<https://www.ansys.com/products/electronics/ansys-hfss>

# Poisson Equation

The governing PDE of the electrostatic problem is Poisson equation.

$$-\nabla \cdot (\varepsilon(x, y) \nabla \Phi) = \rho_e(x, y)$$

# FEM Formulation

$$-\int_{\Omega} \omega_i [\nabla \cdot (\varepsilon(x, y) \nabla \Phi)] d\Omega = \int_{\Omega} \omega_i \rho_e(x, y) d\Omega \quad (3)$$

$$\int_{\Omega} \varepsilon(x, y) \nabla \omega_i \cdot \nabla \Phi d\Omega = \int_{\Omega} \omega_i \rho_e(x, y) d\Omega + \oint_{\Gamma_D} \hat{n} \cdot (\varepsilon(x, y) \nabla \Phi) \omega_i d\Gamma_D \quad (4)$$

$$\sum_{j=1}^N \phi_j \int_{\Omega} \varepsilon(x, y) \nabla N_i \cdot \nabla N_j d\Omega = \int_{\Omega} N_i \rho_e(x, y) d\Omega - \sum_{j=1}^{N_D} \phi_j^D \int_{\Omega} \varepsilon(x, y) \nabla N_i \cdot \nabla N_j^D d\Omega \quad (5)$$

$$\sum_{j=1}^N K_{ij} \phi_j = b_i, \quad i = 1, \dots, N \quad (6)$$

$$K_{ij} = \begin{cases} 1 & \text{if } i = j \text{ and node } j \text{ is on } \Gamma_D \\ \int_{\Omega} \varepsilon(x, y) \nabla N_i \cdot \nabla N_j d\Omega & \text{if } \phi_j \text{ is unknown} \end{cases} \quad (7)$$

$$b_i = \begin{cases} \int_{\Omega} N_i \rho_e(x, y) d\Omega - \sum_{j=1}^{N_D} \phi_j^D \int_{\Omega} \varepsilon(x, y) \nabla N_i \cdot \nabla N_j^D d\Omega & \text{if } \phi_i \text{ is unknown} \\ \phi_i^D - \sum_{j=1, j \neq i}^{N_D} \phi_j^D \int_{\Omega} \varepsilon(x, y) \nabla N_i \cdot \nabla N_j^D d\Omega & \text{if } \phi_i \text{ is prescribed (the potential of ground is zero)} \end{cases} \quad (8)$$

Basis function

# Solution Process

(Simplified)

- Use the equations to formulate the linear sparse system.
- Solve it using conjugated gradient method for the coefficients of the corresponding basis functions.

$$\mathbf{K} \phi = \mathbf{b}$$

# Conjugated Gradient Method

Pseudo-code.

Many parallel versions studied  
in detail.

Simply using OpenMP.

---

**Algorithm 1** CG algorithm

---

```
1: Initialize  $\mathbf{r}_0 = \mathbf{b} - \mathbf{K}\phi_0$  and  $\mathbf{p}_0 = \mathbf{r}_0$ 
2: for  $k = 1, 2, \dots$  do
3:    $\rho_k = \|\mathbf{r}_k, \mathbf{r}_k\|_2$ 
4:    $\mathbf{q}_k = \mathbf{K}\mathbf{p}_k$ 
5:    $\alpha_k = \frac{\rho_k}{\|\mathbf{p}_k, \mathbf{q}_k\|_2^2}$ 
6:    $\phi_{k+1} = \phi_k + \alpha_k \mathbf{p}_k$ 
7:    $\mathbf{r}_{k+1} = \mathbf{r}_k - \alpha_k \mathbf{q}_k$ 
8:    $\mathbf{r}_{k+1} = \mathbf{M}^{-1} \mathbf{r}_{k+1}$ 
9:    $\rho_{k+1} = \|\mathbf{r}_{k+1}, \mathbf{r}_{k+1}\|_2^2$ 
10:   $\beta_{k+1} = \frac{\rho_{k+1}}{\rho_k}$ 
11:   $\mathbf{p}_{k+1} = \mathbf{r}_{k+1} + \beta_{k+1} \mathbf{p}_k$ 
12:  Check convergence status
13: end for
```

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- vector update (SAXPY)
- inner product
- matrix-vector multiplication

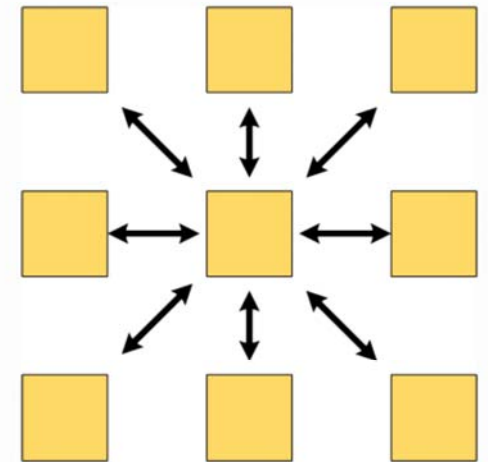
# Domain Decomposition

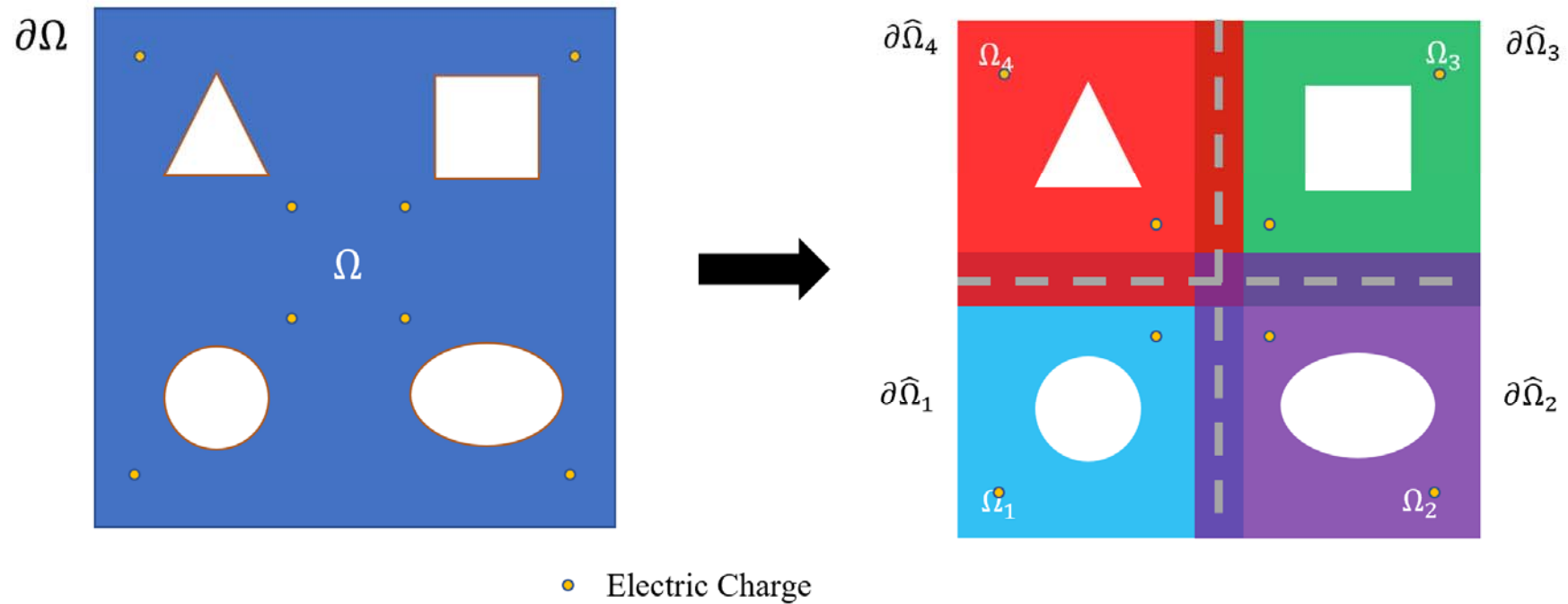
Some thing like this picture in  
the course slides.

Using MPI between ranks.

## Spatial Decomposition

- ▶ Atoms distributed to cubes based on their location
  - ▶ Relatively uniform atom density
- ▶ Size of each cube
  - ▶ Just a bit larger than cut-off radius
  - ▶ Communicate only with neighbors
  - ▶ Work: for each pair of neighbor objects
- ▶ Communication to computation ratio:  $O(1)$ 
  - ▶ E.g. imagine 1 cube per process
- ▶ However:
  - ▶ Load imbalance
  - ▶ Limited parallelism



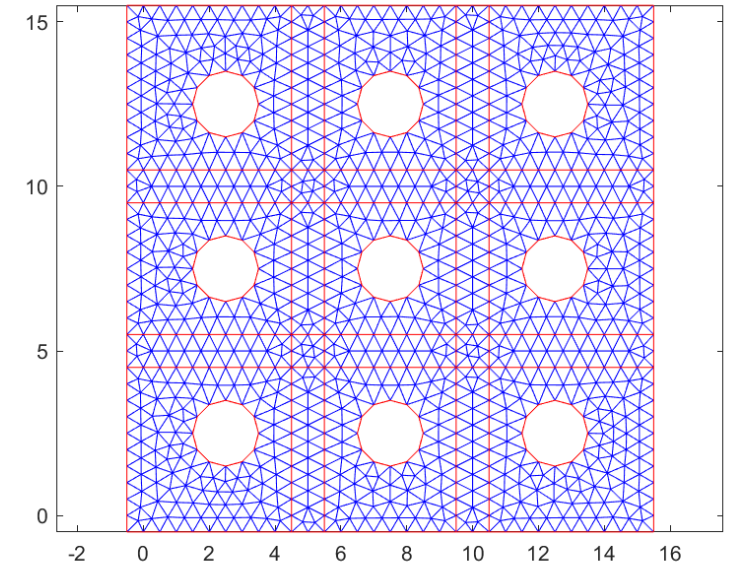
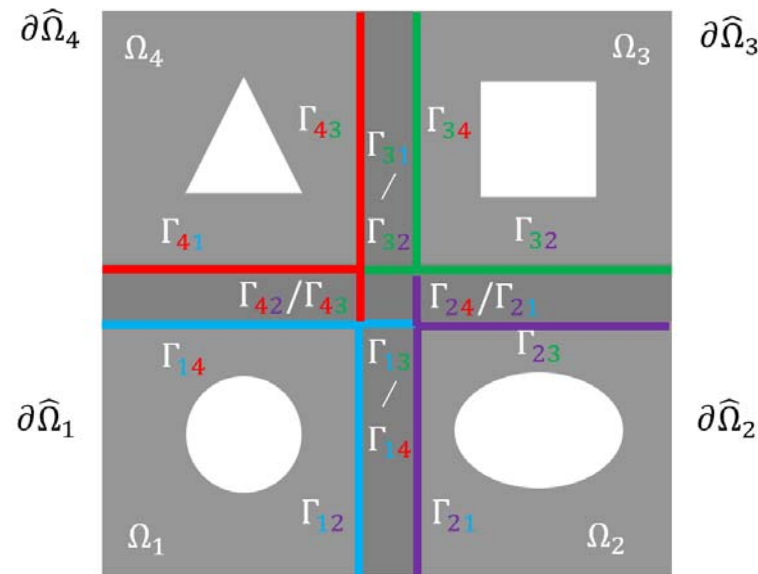
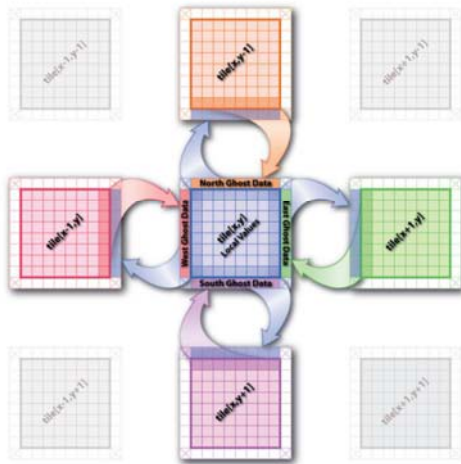


# Domain Decomposition

To be more specific (as an example).  
Divide the original domain into 2x2 sub-region.



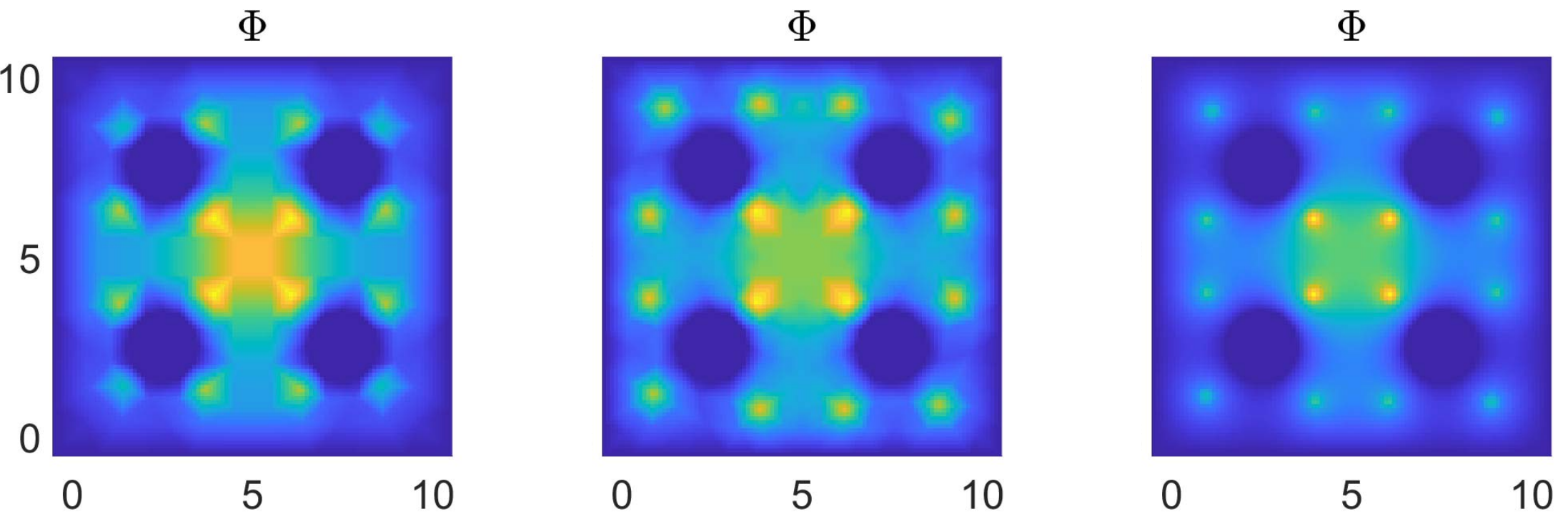
## 5 Point Stencil



## Artificial boundary (ghost boundary)

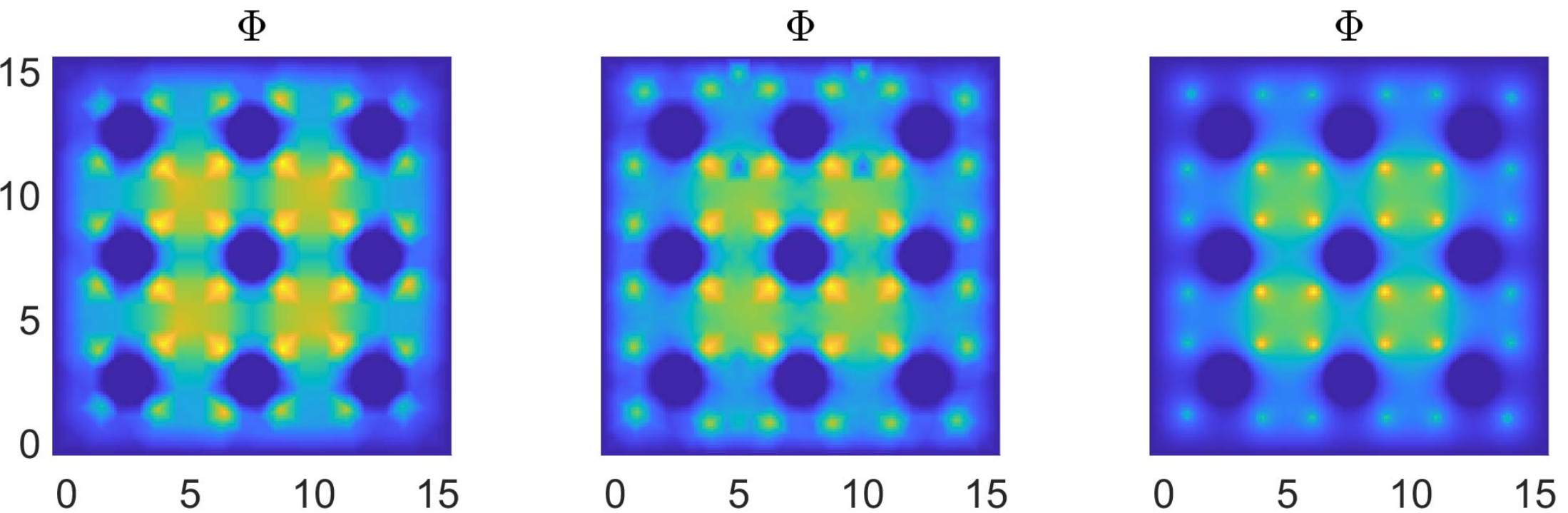
But this time the ghost is in the interior region of its nearby sub-regions.

If some sub-region is not on the outer boundary, it may have 8 adjacent sub-regions.



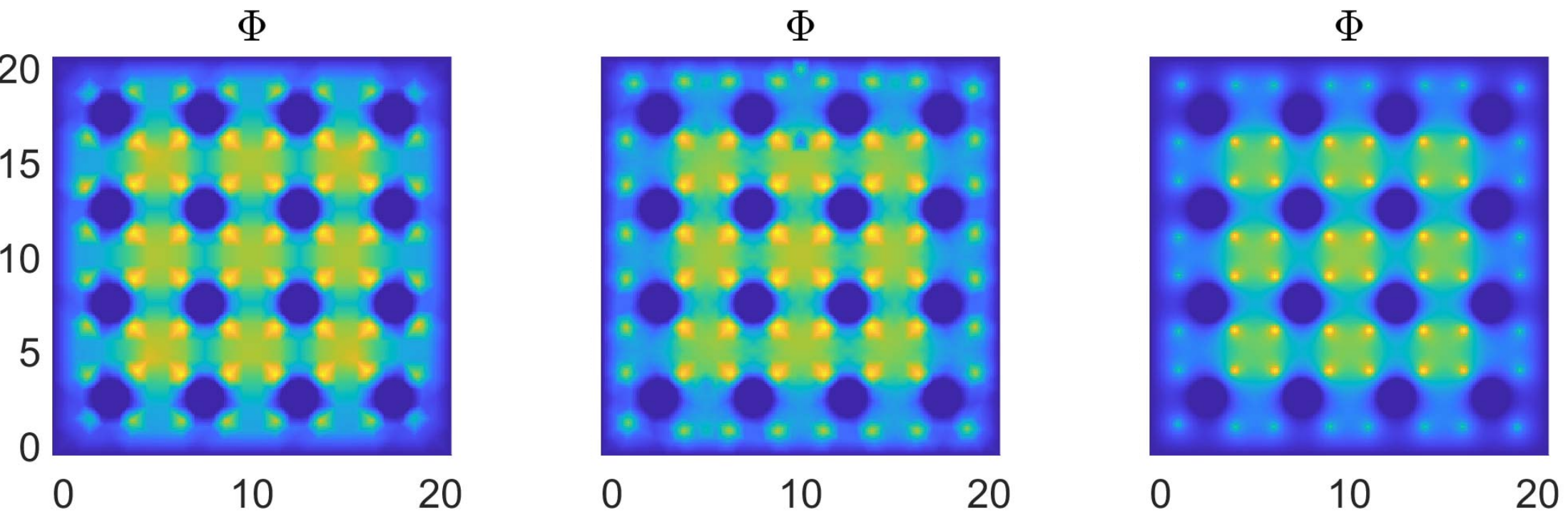
Electric potential visualization

2 by 2



Electric potential visualization

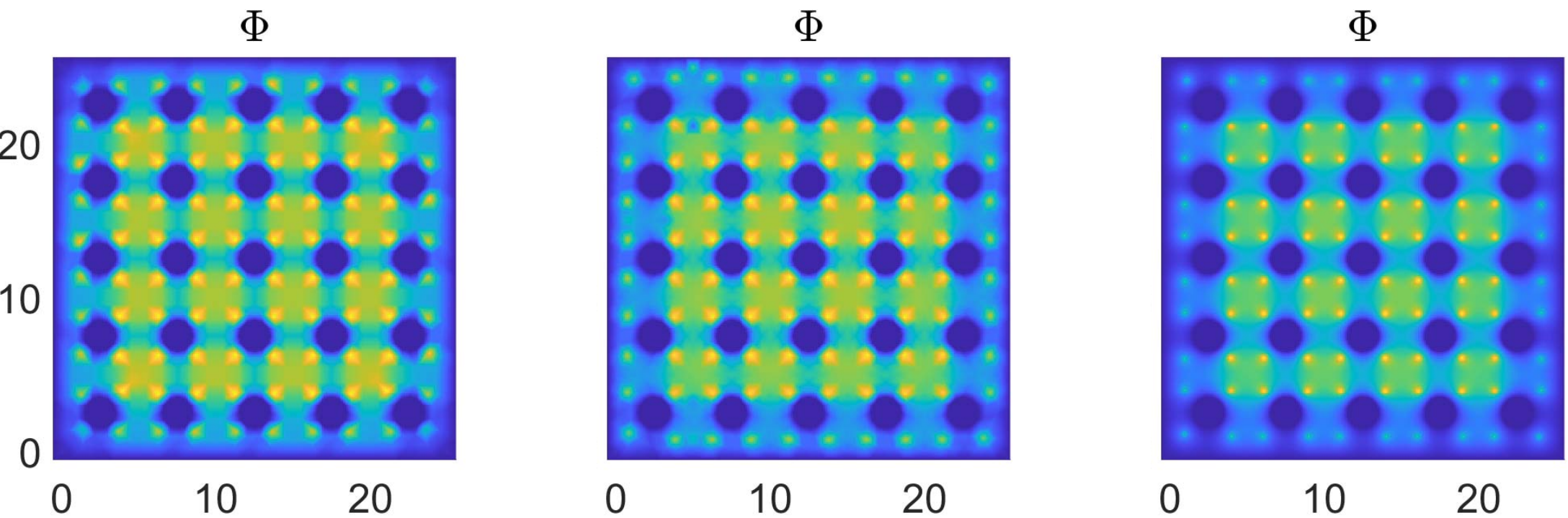
3 by 3



Electric potential visualization

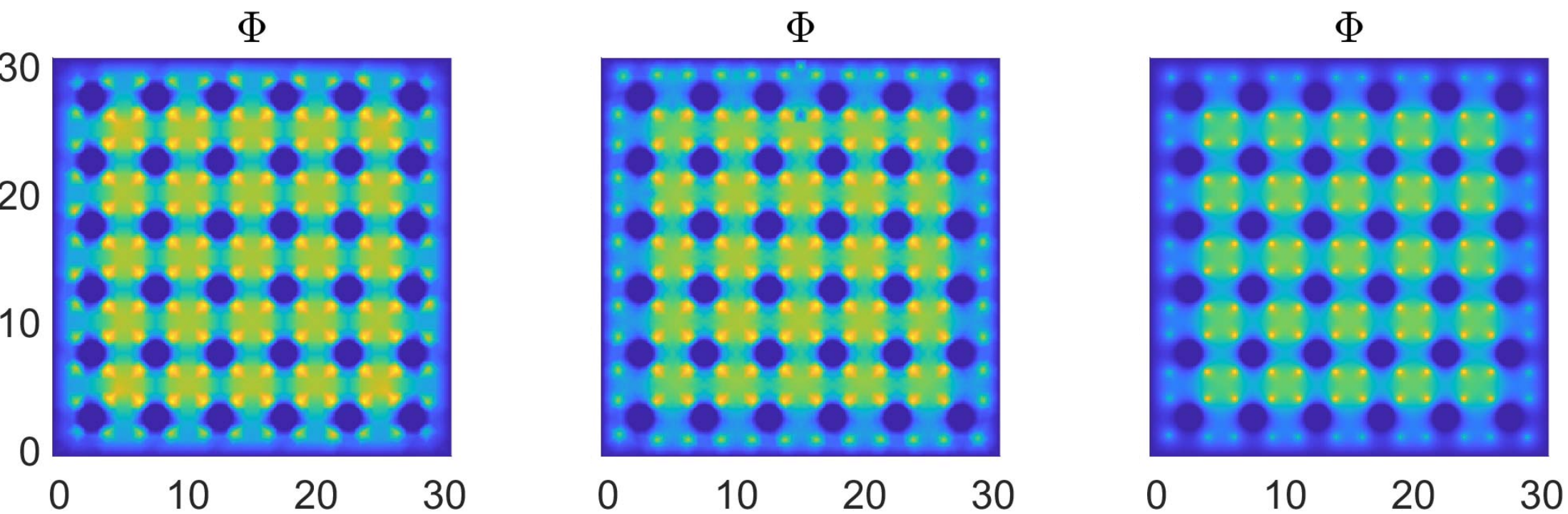
4 by 4





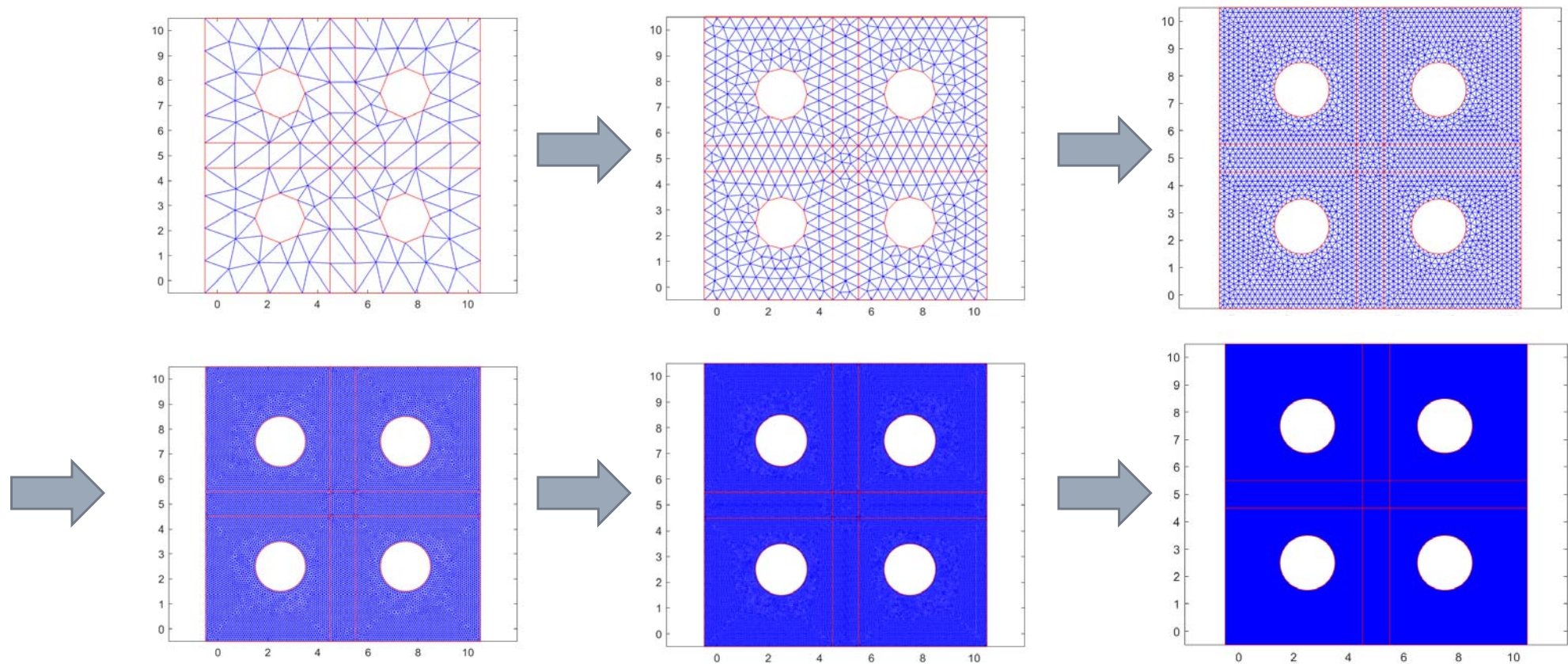
Electric potential visualization

5 by 5



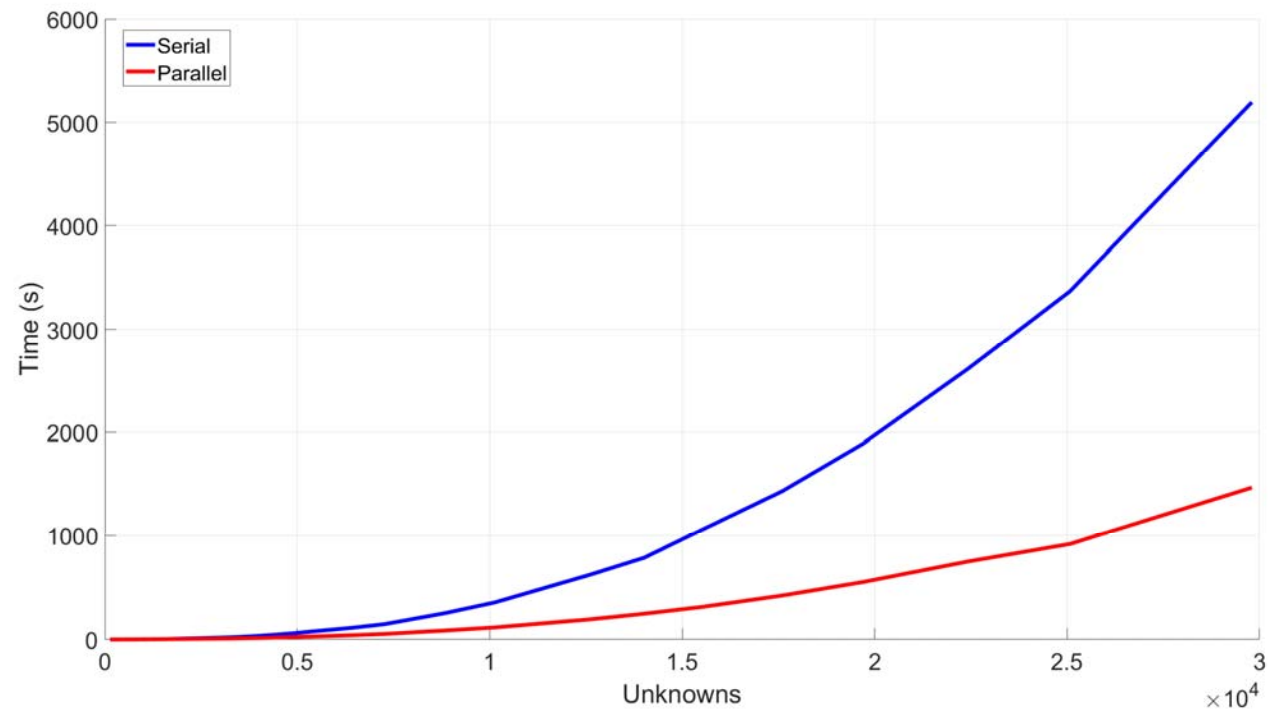
Electric potential visualization

6 by 6



Benchmarking: Increase the number of unknowns  
4 by 4

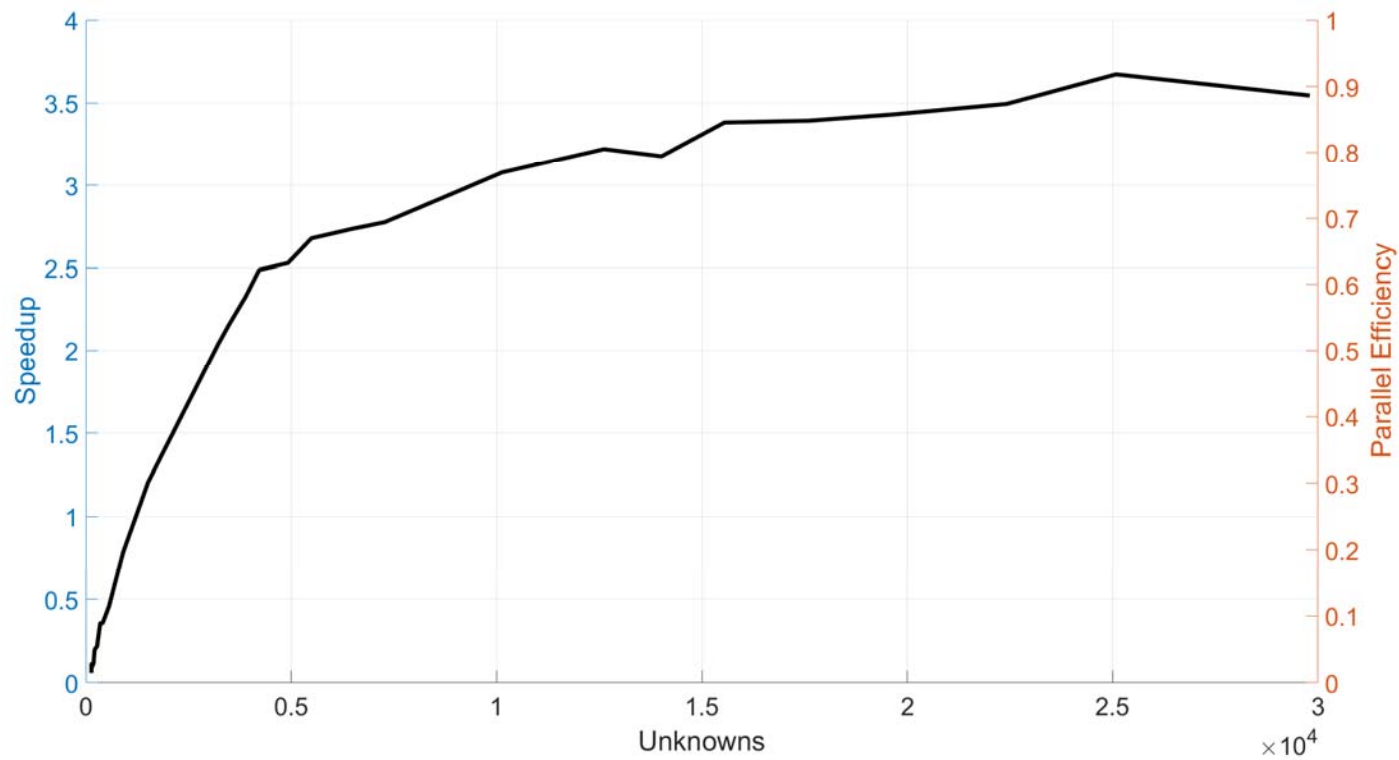




# Comparison of time consumption

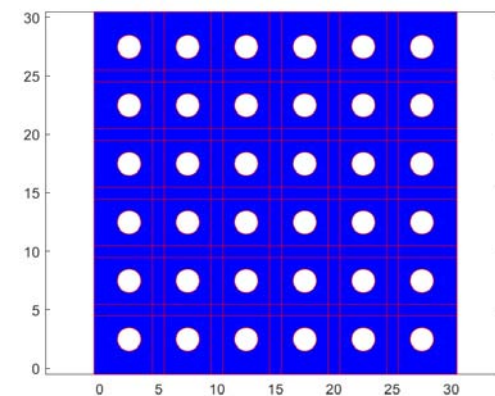
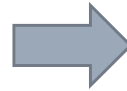
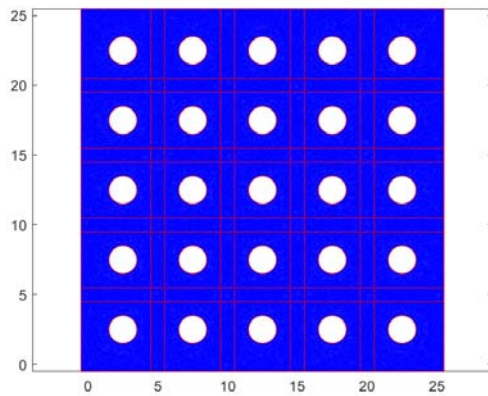
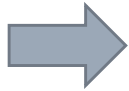
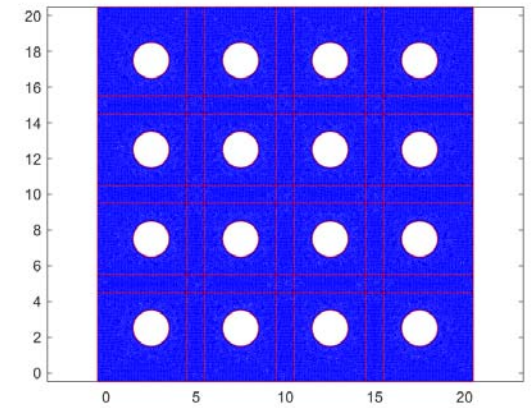
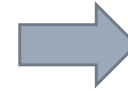
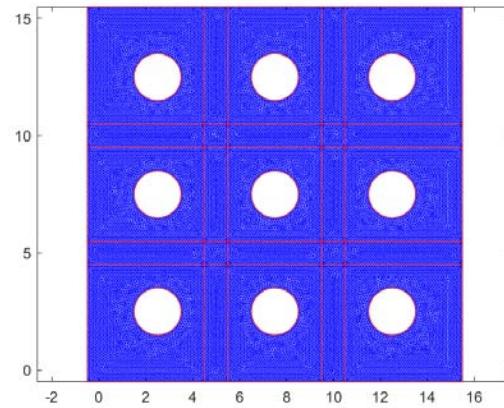
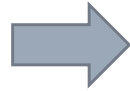
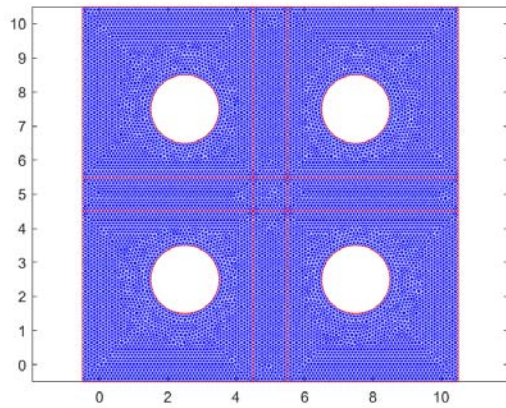
Serial version vs Parallel version



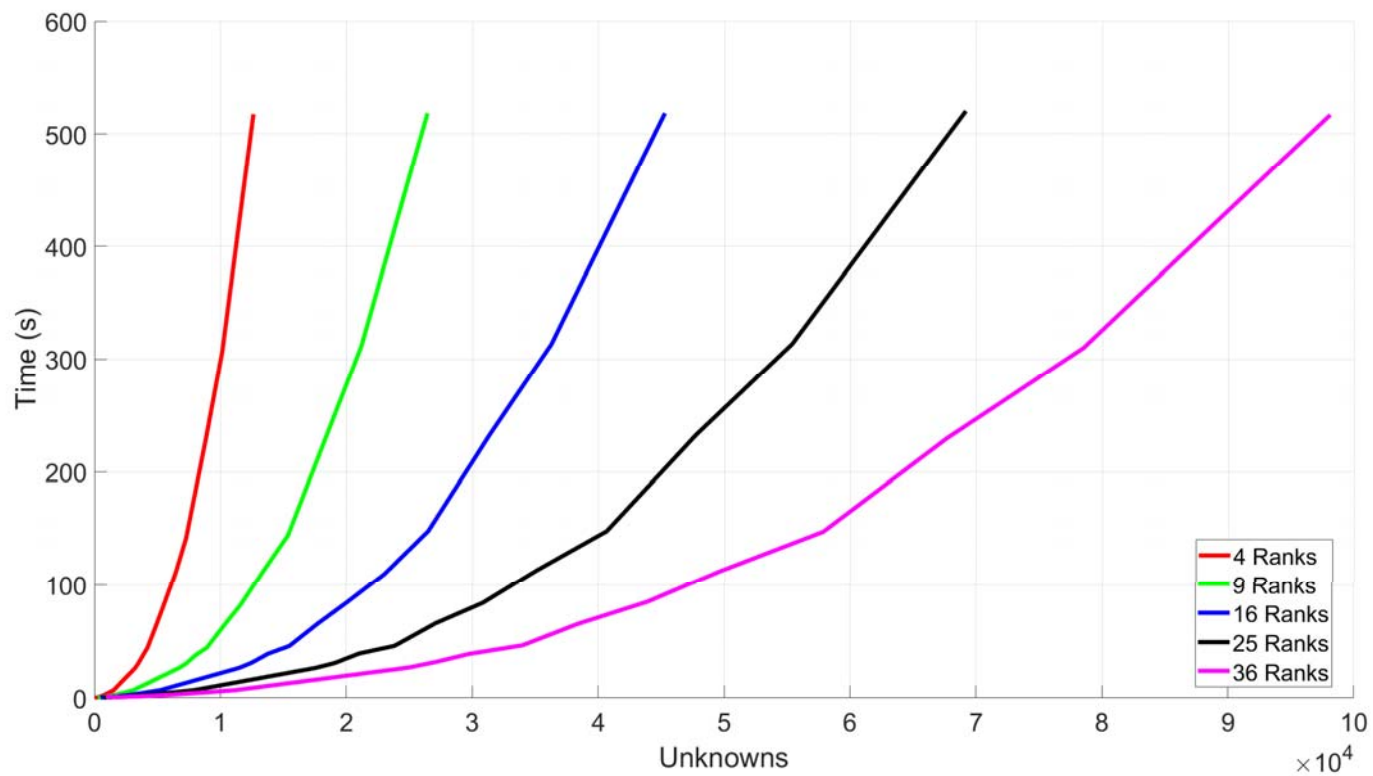


# Speed up and parallel efficient

According to the definition.



Benchmarking: Scaling  
Increase decomposition, more sub-regions



## Scaling Result (Weak & Strong)

Increasing number of ranks (different color)

# Code Demonstration

Let me open the VS Code if needed.



main.cpp



Parallel\_CGM  
M.cpp



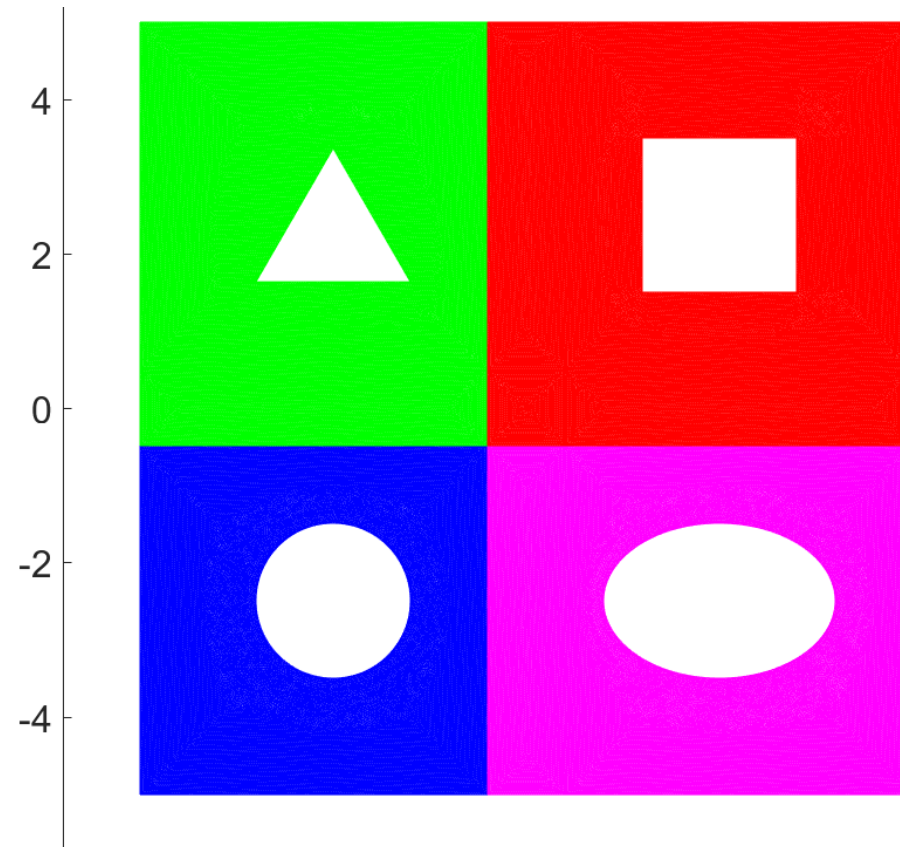
Parallel\_CGM  
M.h



Serial\_CGM  
.cpp



Serial\_CGM  
.h



*Q&A Session*