PDE Tool Simulations- An example

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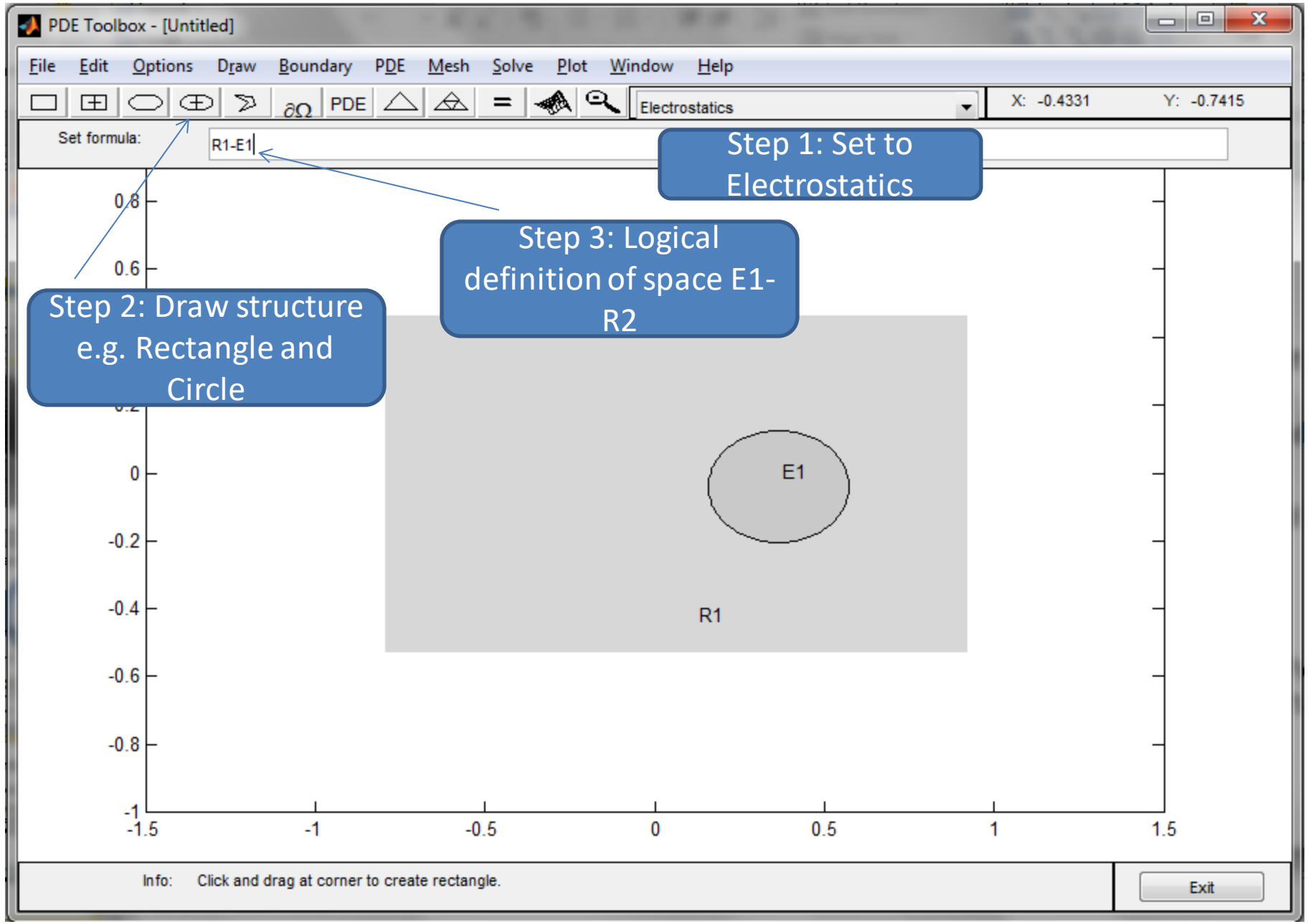
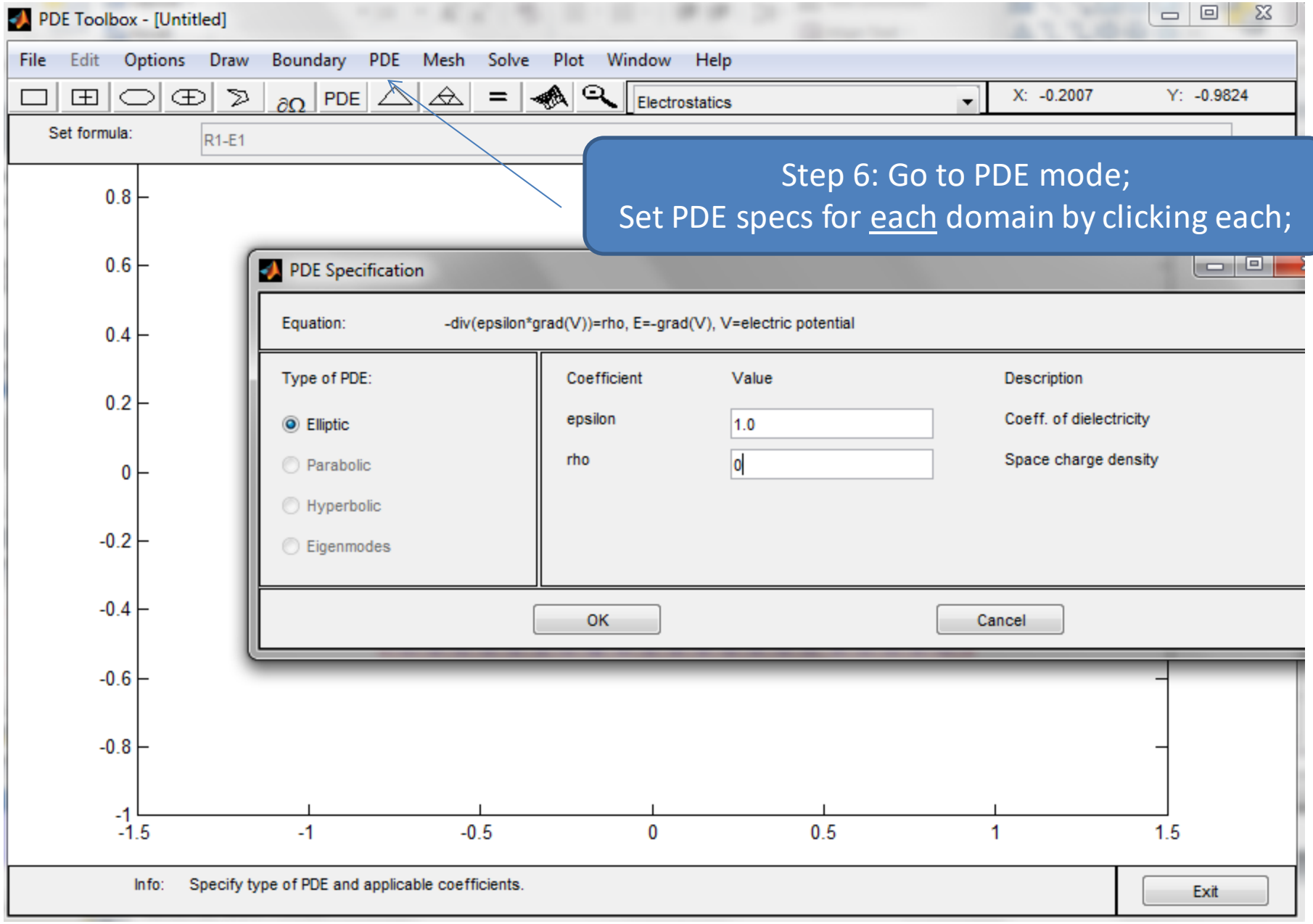
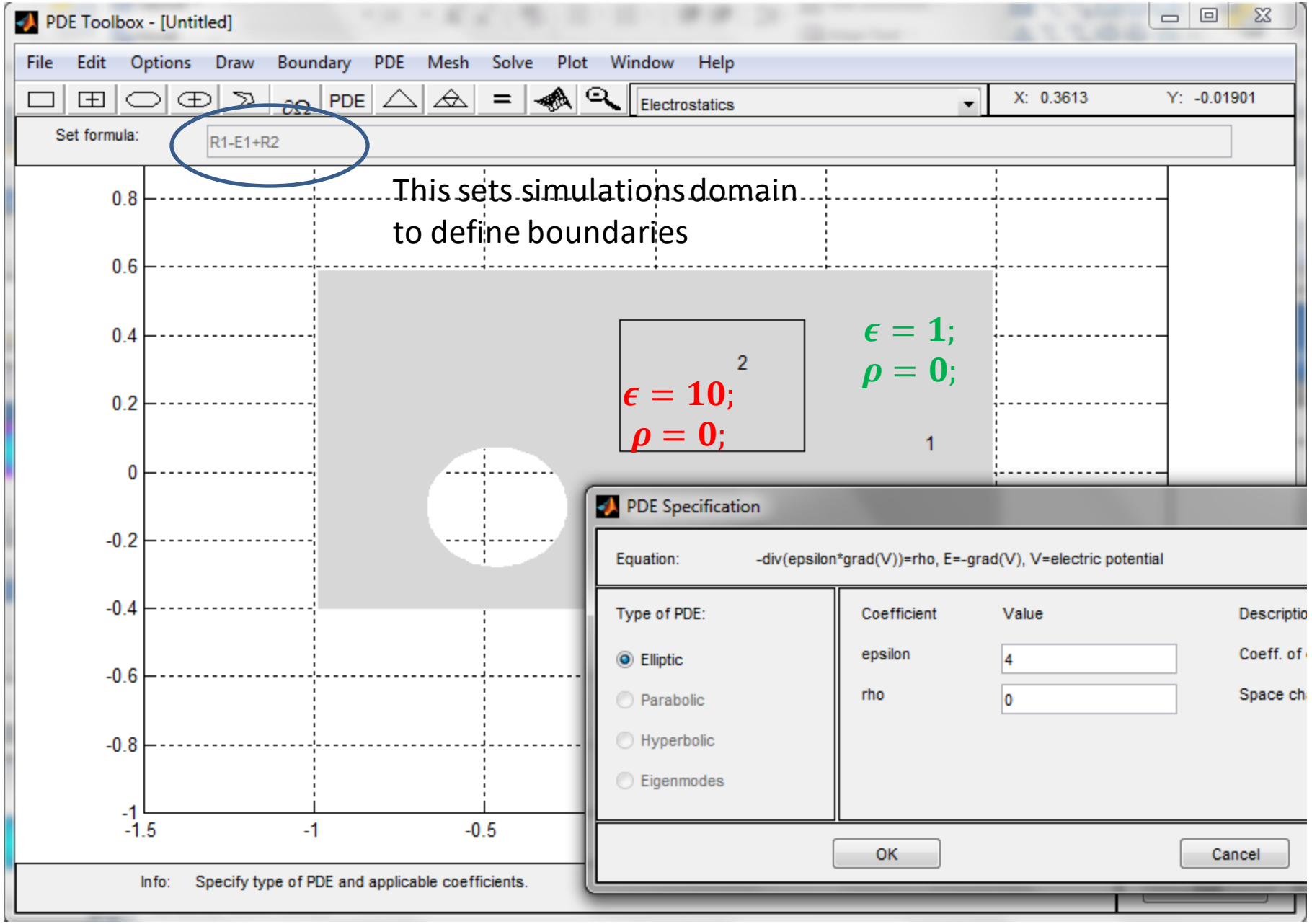
Simulations steps

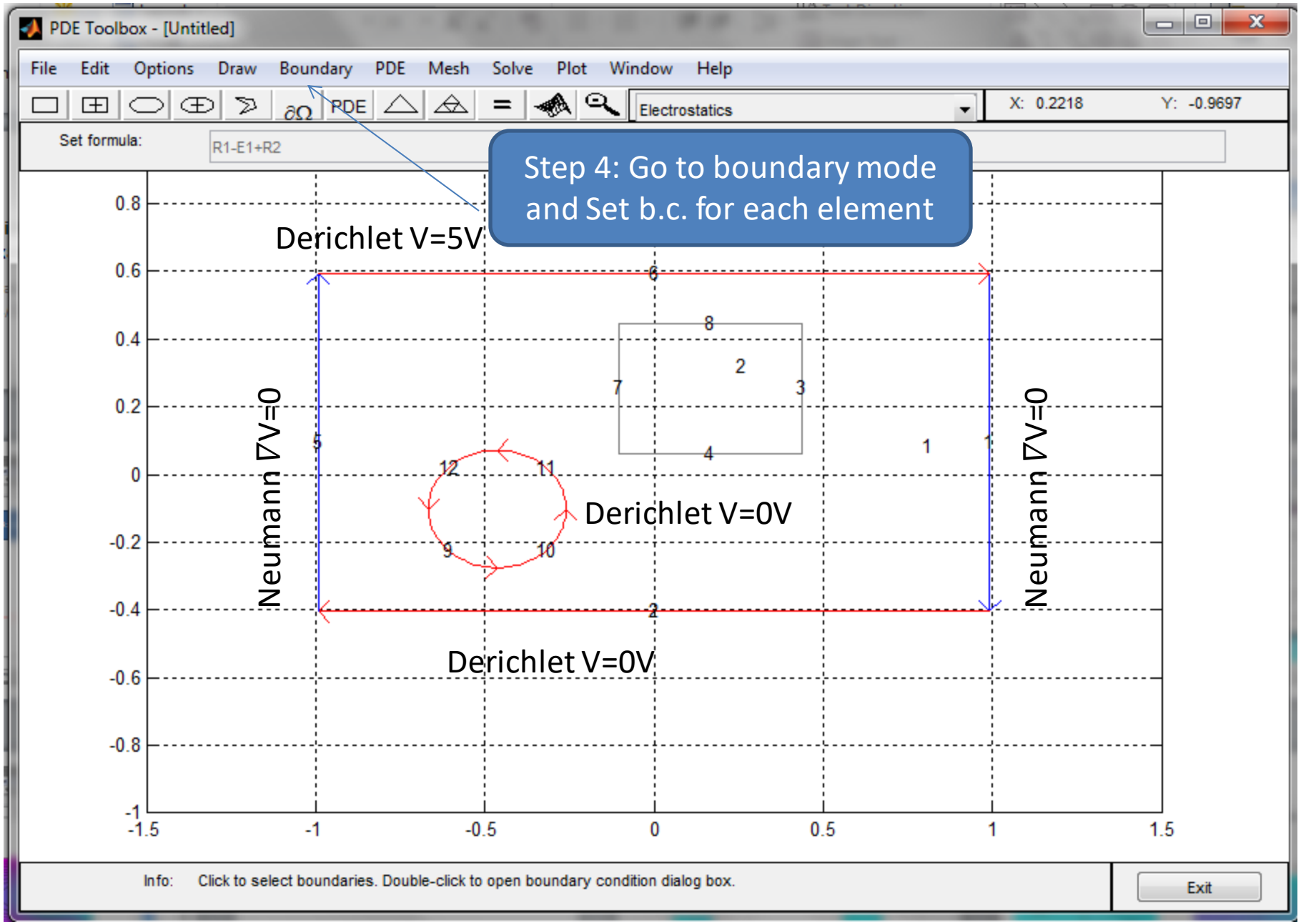
- Set Options/grid to x :-1.5: 0.5:1.5 y:-1:0.5:1;
- Set Options/snap to grid
  - This makes drawings regular and not based on your dexterity
- Choose “Electrostatics”
- Draw shapes
- Set simulations domain lo
- Set PDE mode and set materials parameters in sub-domain (e.g. ρ and ϵ)
- Choose b.c. (Neumann or Derichlet)
- Define mesh fine enough (see next slide)
- Simulate and plot; write observation and conclusion for each plot

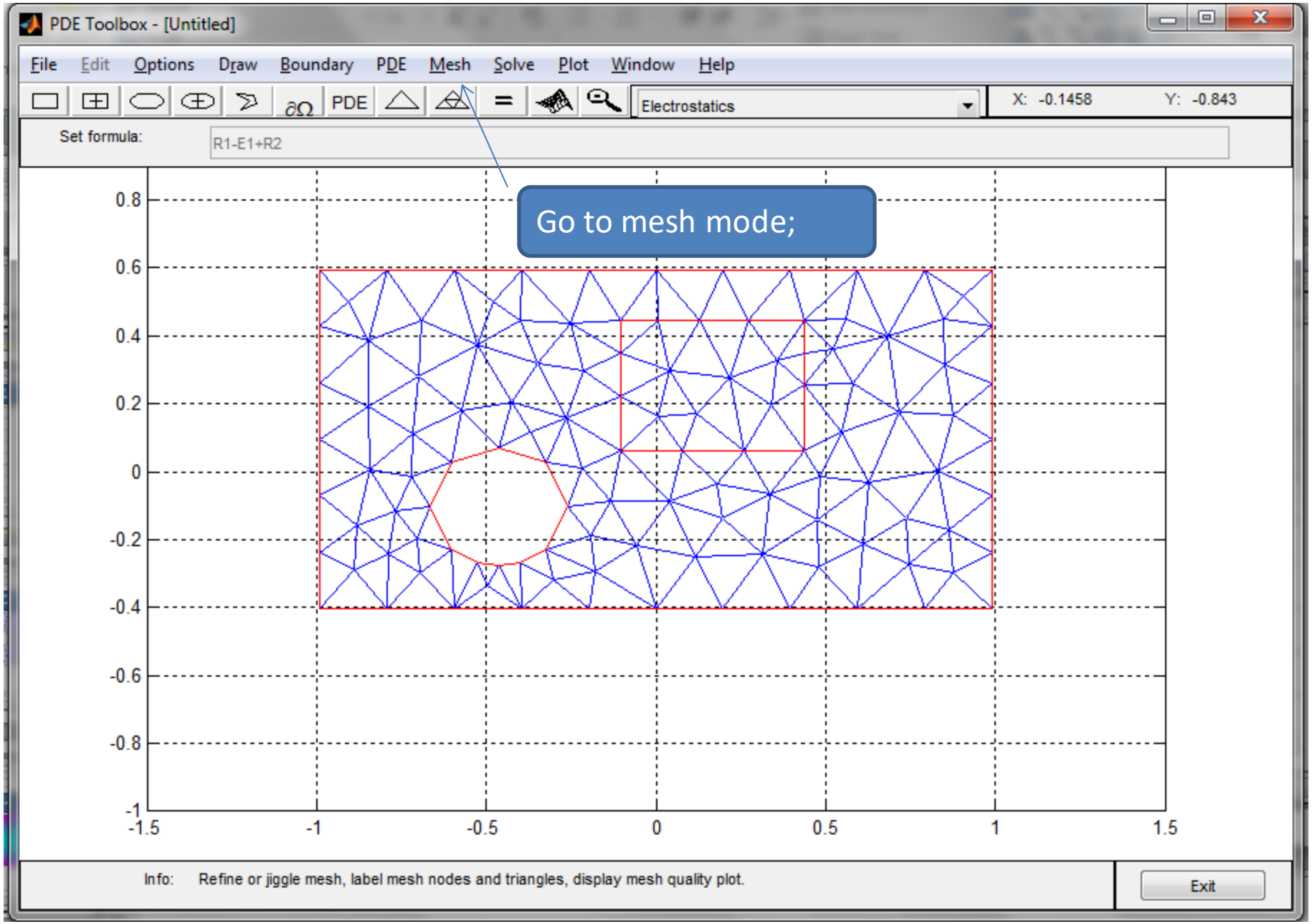

PDE Toolbox - [Untitled]
File Edit Options Draw Boundary PDE Mesh Solve Plot Window Help
Electrostatics
X: -0.4331 Y: -0.7415
Set formula: R1-E1
Step 1: Set to Electrostatics
Step 2: Draw structure e.g. Rectangle and Circle
Step 3: Logical definition of space E1-R2
E1
R1
0.8
0.6
0
-0.2
-0.4
-0.6
-0.8
-1
-1.5
-1
-0.5
0
0.5
1
1.5
Info: Click and drag at corner to create rectangle.
Exit

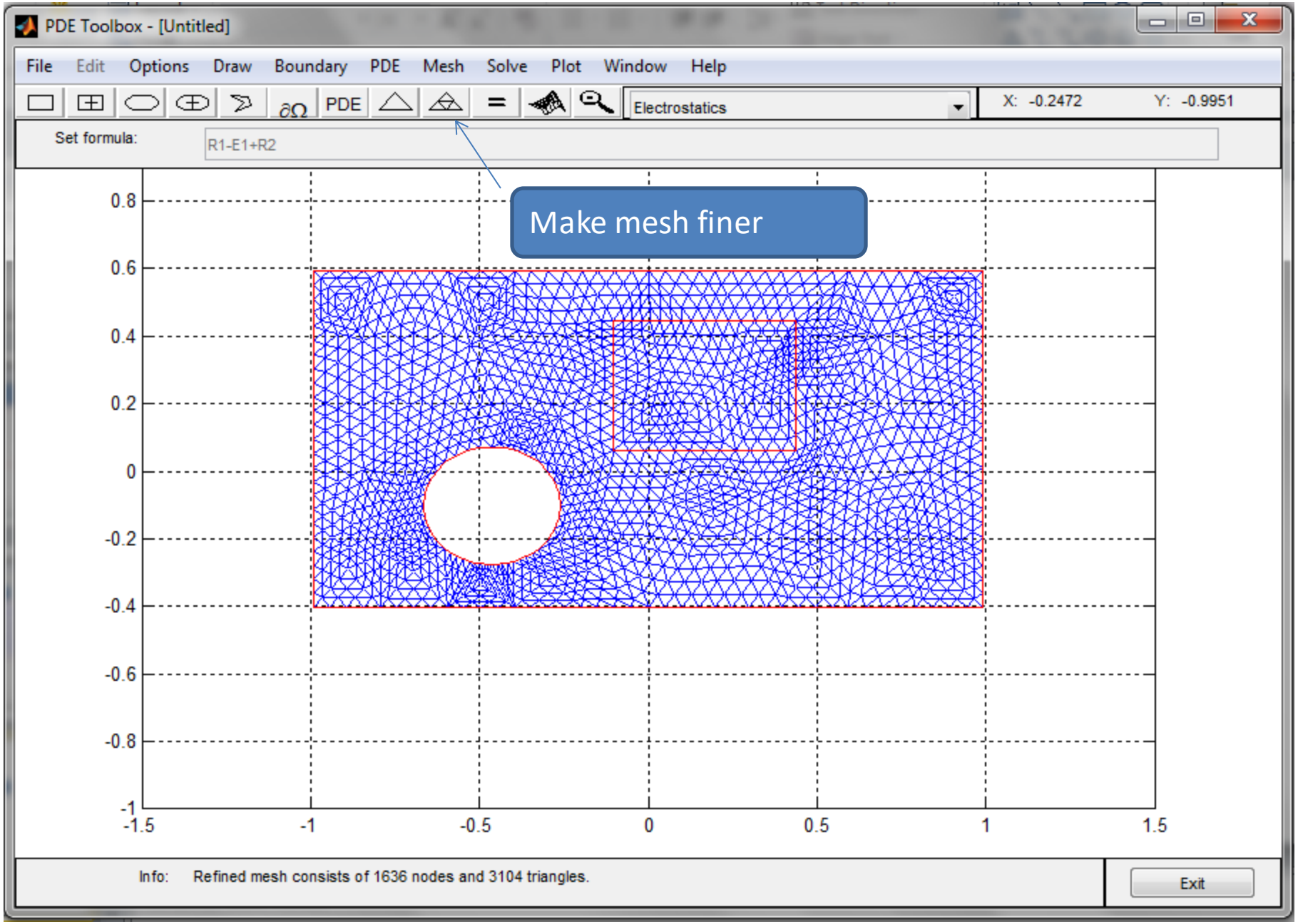

PDE Toolbox - [Untitled]
File Edit Options Draw Boundary PDE Mesh Solve Plot Window Help
PDE
Electrostatics
X: -0.2007 Y: -0.9824
Set formula:
R1-E1
Step 6: Go to PDE mode;
Set PDE specs for each domain by clicking each;
PDE Specification
Equation: -div(epsilon*grad(V))=rho, E=-grad(V), V=electric potential
Type of PDE:
Elliptic
Parabolic
Hyperbolic
Eigenmodes
Coefficient
Value
Description
epsilon
1.0
Coeff. of dielectricity
rho
0
Space charge density
OK
Cancel
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
-1
-1.5
-1
-0.5
0
0.5
1
1.5
Info: Specify type of PDE and applicable coefficients.
Exit



For each of the multiple domains (1&2), the PDE specs (ρ, ϵ) needs to be set


PDE Toolbox - [Untitled]
File Edit Options Draw Boundary PDE Mesh Solve Plot Window Help
Electrostatics
X: 0.2218 Y: -0.9697
Set formula:
R1-E1+R2
Step 4: Go to boundary mode and Set b.c. for each element
Derichlet V=5V
Neumann ∇V=0
Derichlet V=0V
Neumann ∇V=0
Derichlet V=0V
Info: Click to select boundaries. Double-click to open boundary condition dialog box.
Exit


PDE Toolbox - [Untitled]
File Edit Options Draw Boundary PDE Mesh Solve Plot Window Help
PDE
Electrostatics
X: -0.1458 Y: -0.843
Set formula:
R1-E1+R2
Go to mesh mode;
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
-1
-1.5
-1
-0.5
0
0.5
1
1.5
Info: Refine or jiggle mesh, label mesh nodes and triangles, display mesh quality plot.
Exit

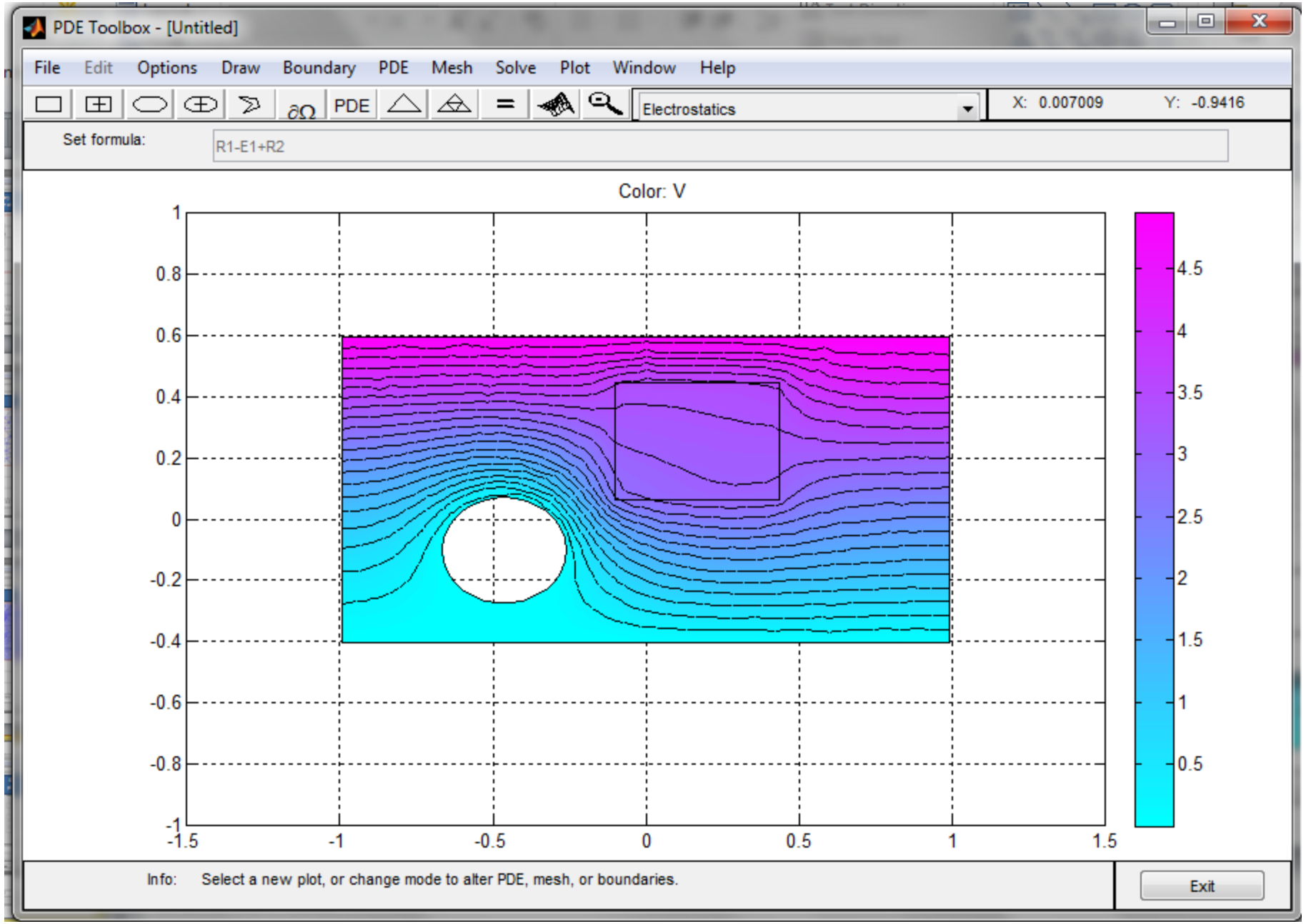

PDE Toolbox - [Untitled]
File Edit Options Draw Boundary PDE Mesh Solve Plot Window Help
PDE
Electrostatics
X: -0.2472 Y: -0.9951
Set formula:
R1-E1+R2
Make mesh finer
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
-1
-1.5
-1
-0.5
0
0.5
1
1.5
Info: Refined mesh consists of 1636 nodes and 3104 triangles.
Exit

Grid Coarse vs fine

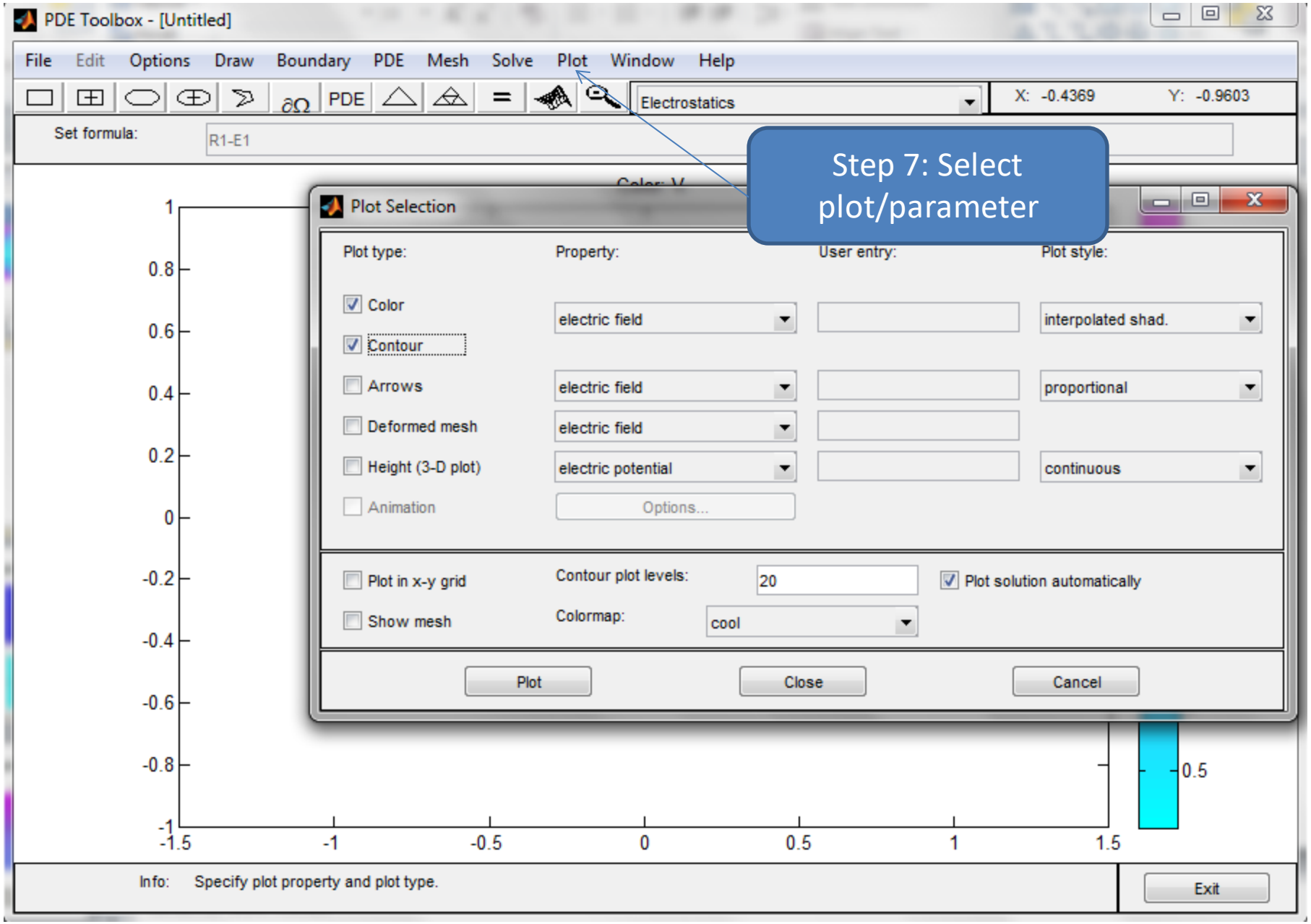
- Do coarse vs fine grid
- Is there a difference in the quality of solution

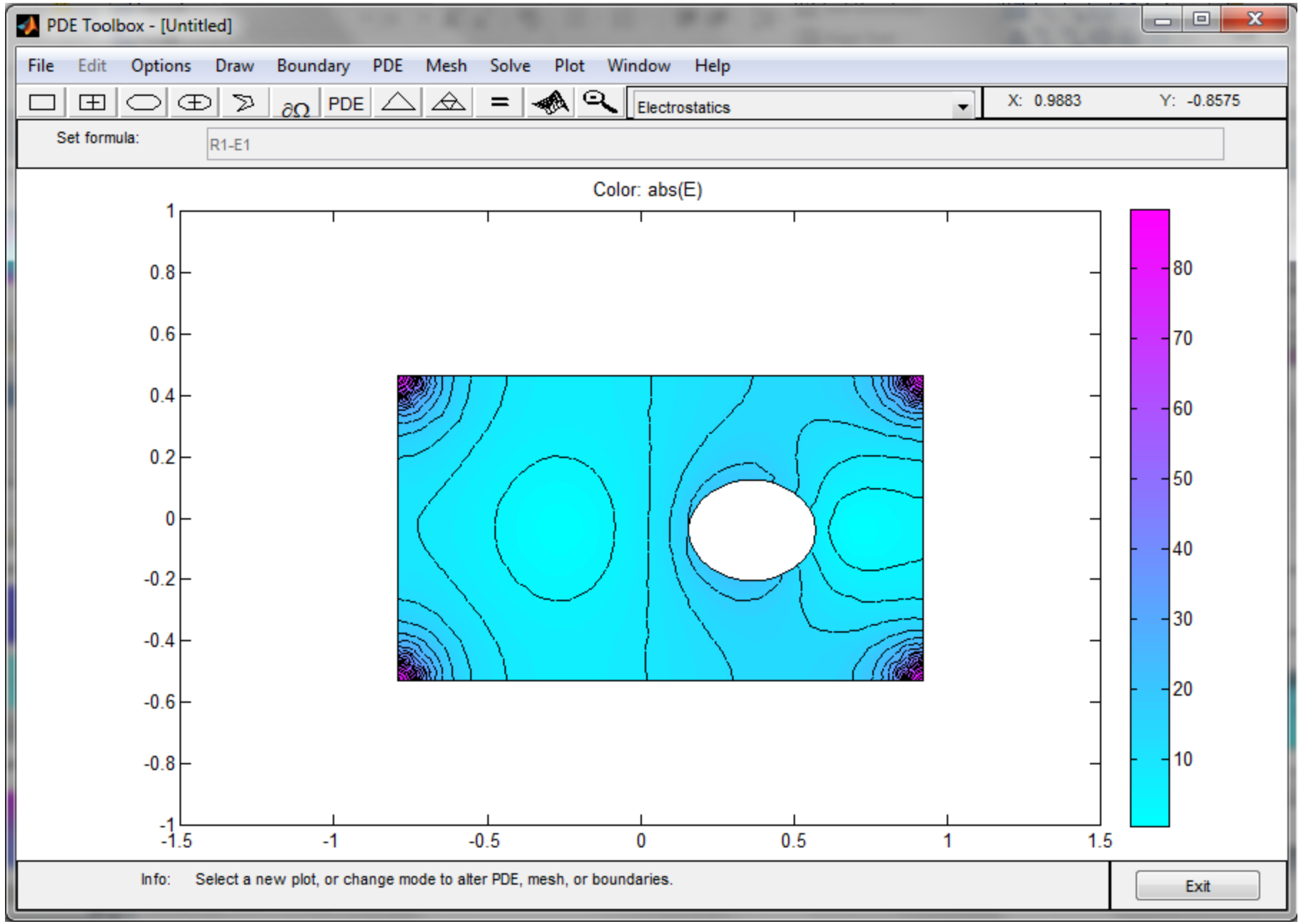
Exercise

- Guess the potential profile – write down reasons (2 mins)
  - Draw equipotential lines
  - Draw E field lines
  - write down points.
- Check after simulation if this was close
  - Same equipotential lines, E-lines
  - Note differences with your guess
- Write down reasons for difference of Simulation with 1st Guess

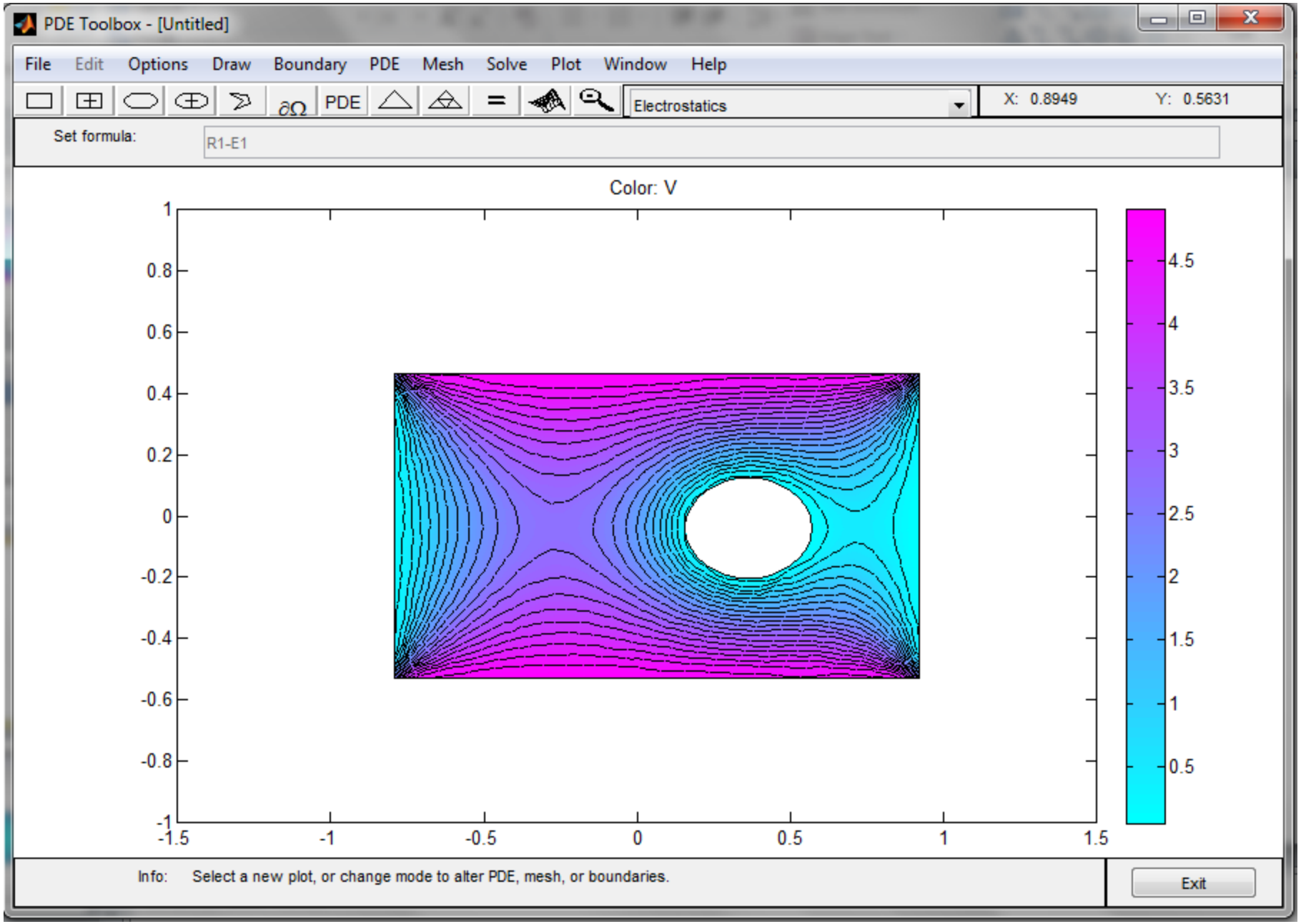


Go to plot mode and play with the parameter section;


PDE Toolbox - [Untitled]
File Edit Options Draw Boundary PDE Mesh Solve Plot Window Help
Electrostatics
X: -0.4369 Y: -0.9603
Set formula:
R1-E1
Step 7: Select plot/parameter
Plot Selection
Plot type:
Property:
User entry:
Plot style:
Color
electric field
interpolated shad.
Contour
Arrows
electric field
proportional
Deformed mesh
electric field
Height (3-D plot)
electric potential
continuous
Animation
Options...
Plot in x-y grid
Contour plot levels:
20
Plot solution automatically
Show mesh
Colormap:
cool
Plot
Close
Cancel
Info: Specify plot property and plot type.
Exit



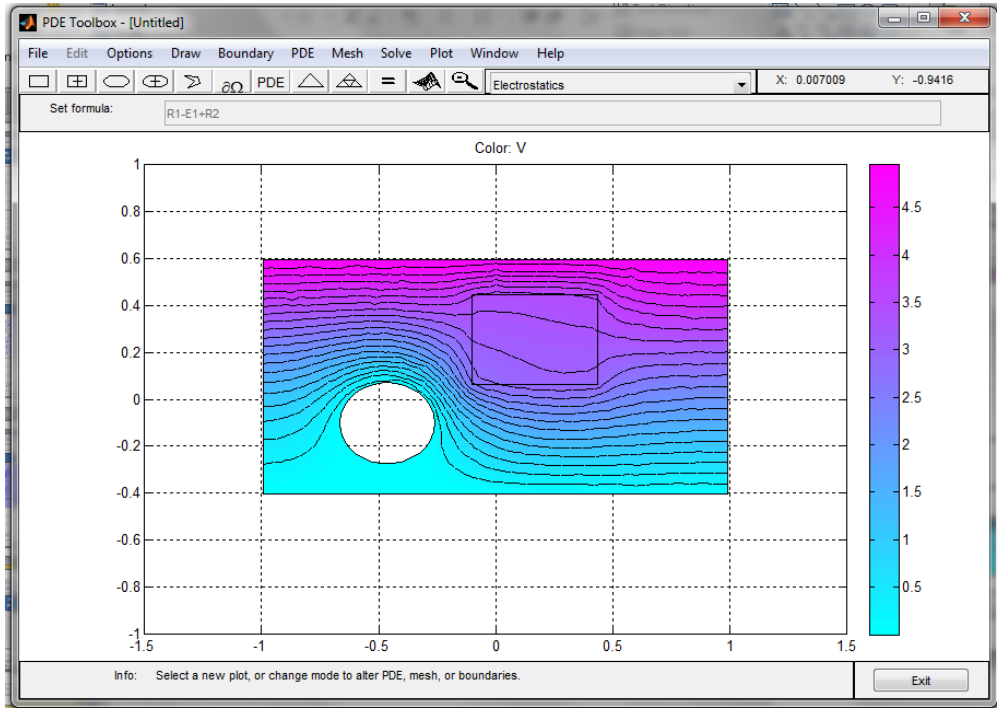
E field and contour lines plotted



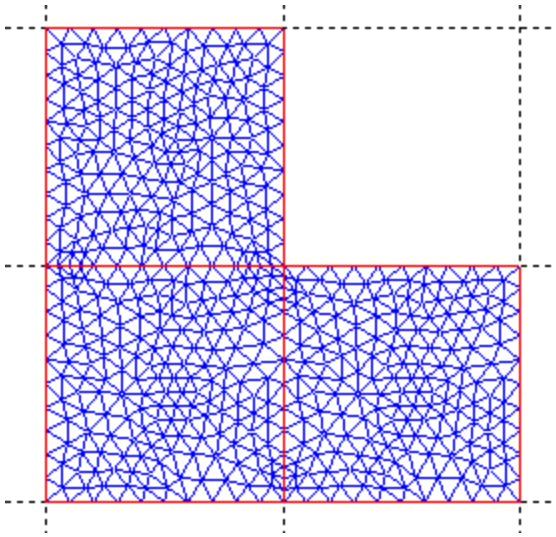
Potential with contour

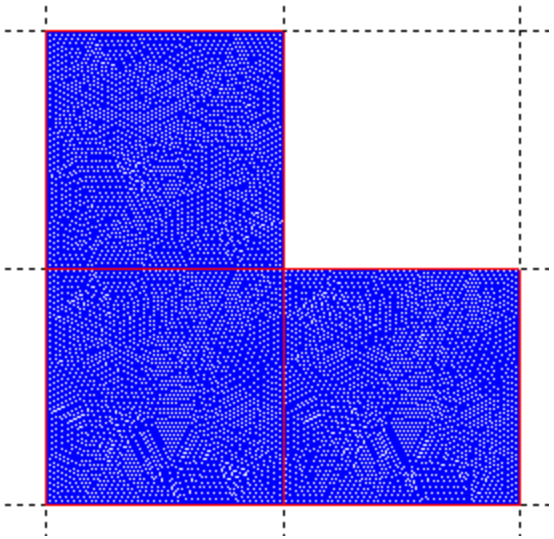
Exercise

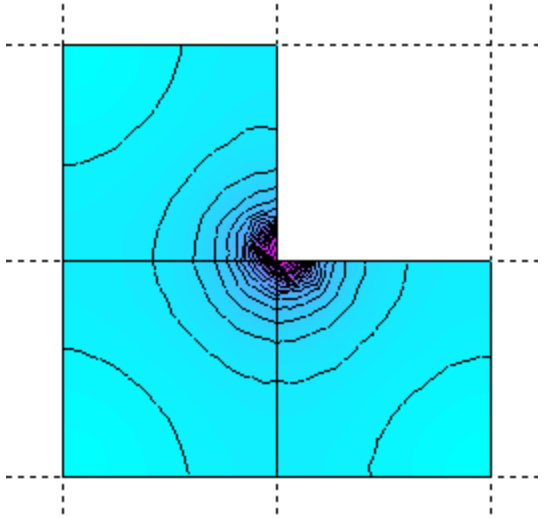
- Simulate the following-
- Between two parallel plates there is a dielectric of k=1. Embedded in this, there is a metal nanocrystal circle and a semiconductor square “k=10”

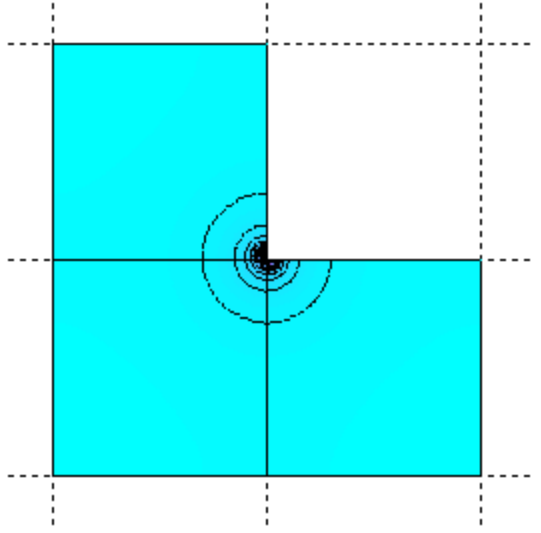


Poor Mesh vs sufficient mesh









Circles are nicely resolved