

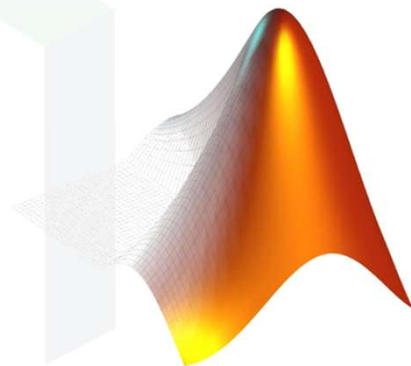


Computational Science:
Computational Methods in Engineering

Building Geometries into Data Arrays

Outline

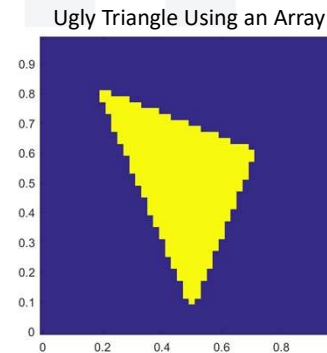
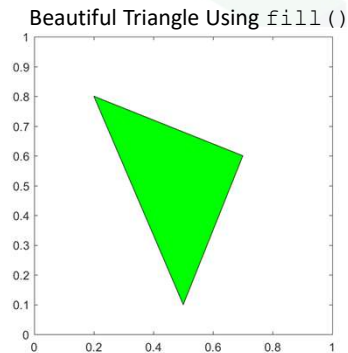
- Visualizing MATLAB Data and Arrays
- 3D \rightarrow 2D \rightarrow 1D
- Arrays, x and y in MATLAB
- Building Geometries in Arrays
 - Initializing arrays
 - Array indexing
 - Squares and rectangles
 - Simple triangles and arbitrary polygons
 - Circles and ellipses
 - Formed half-spaces
 - Linear half-spaces
 - Boolean operations
 - Scaling data in arrays



WARNING: Not Meant for Graphics!

This lecture teaches techniques that are NOT intended for generating graphics. See previous lecture if that is your purpose.

Instead, the techniques in this lecture are intended for you to build arrays containing different shapes and geometries so that you can do numerical computation on those shapes and geometries.



Visualizing MATLAB Data and Arrays

1D Data Arrays

Row Vectors

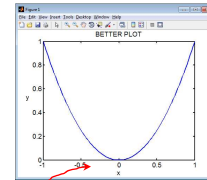
```
>> a = [1, 2, 3, 4, 5]
```

```
a =
```

```
1 2 3 4 5
```

Row vectors are most commonly used to store one-dimensional data. They can be used to label axes on grids, store functions, and more. Row vectors are used in some matrix algorithms, but less frequently.

```
x = linspace(-1, 1, 100);
y = x.^2;
```



Column Vectors

```
>> a = [1; 2; 3; 4; 5]
```

```
a =
```

```
1
2
3
4
5
```

Column vectors can be used the same way as row vectors, but column vectors are used more commonly in linear algebra and matrix manipulation.

$$\begin{bmatrix} 0.8 & 0.6 & 1.0 & 1.0 \\ 0.9 & 0.1 & 1.0 & 0.5 \\ 0.1 & 0.3 & 0.2 & 0.8 \\ 0.9 & 0.5 & 1.0 & 0.1 \end{bmatrix} \begin{bmatrix} 0.4 \\ 0.9 \\ 0.8 \\ 1.0 \end{bmatrix} = \begin{bmatrix} 2.66 \\ 1.75 \\ 1.27 \\ 1.71 \end{bmatrix}$$

Column vectors

2D Data Arrays

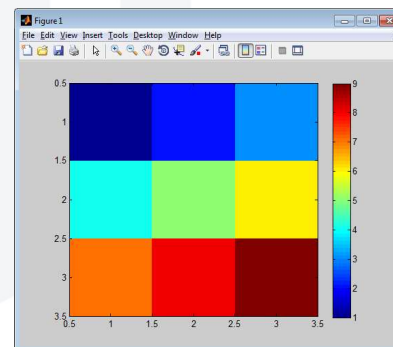
```
>> A = [ 1 2 3 ; 4 5 6 ; 7 8 9 ]
```

```
A =
```

```
1 2 3
4 5 6
7 8 9
```

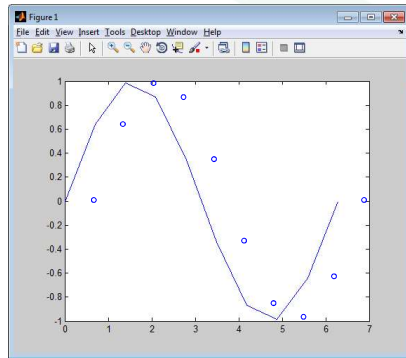
A 2D array could be a matrix, a JPEG image, a 2D set of data, or many other things. MATLAB does not differentiate between these and treats them the same. It is up to you to know the difference and stay consistent in your code.

```
>> imagesc(A); colorbar
```

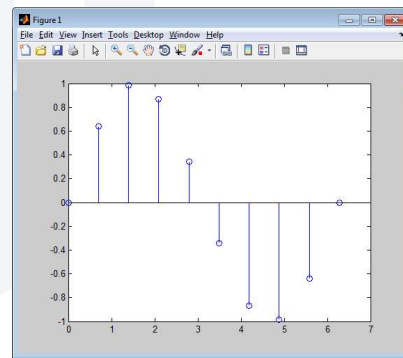


Visualizing 1D Arrays

```
>> phi = linspace(0,2*pi,10);
>> y = sin(phi);
>> plot(phi,y);
```

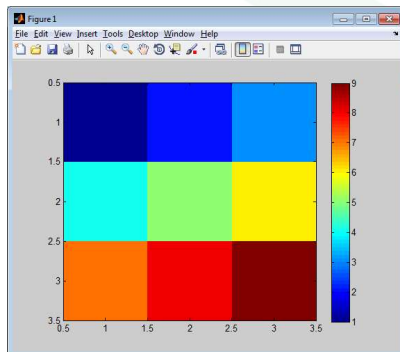


```
>> phi = linspace(0,2*pi,10);
>> y = sin(phi);
>> stem(phi,y);
```

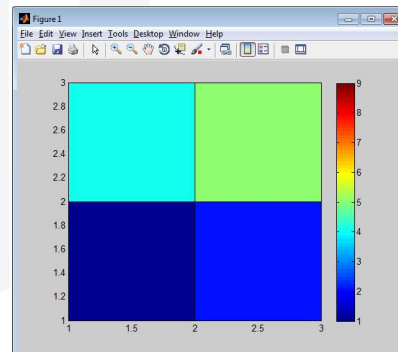


Visualizing 2D Arrays

```
A = [1 2 3 ; 4 5 6 ; 7 8 9 ];
imagesc(A);
colorbar;
```



```
A = [1 2 3 ; 4 5 6 ; 7 8 9 ];
pcolor(A);
colorbar;
```



linspace() vs. [a:Δ:b]

Linspace

```
xa = linspace(0,10,10);
```

```
xa = 0 1.11 2.22 3.33 4.44 5.55 6.66 7.77 8.88 10.00
```



- Easier to control number of points
- Easier to control position of end points.
- More difficult to control step size.

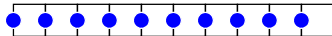
DIRECT ARRAY

```
Nx = 10;
```

```
dx = 1;
```

```
xa = [0:Nx-1]*dx;
```

```
xa = 0 1 2 3 4 5 6 7 8 9
```

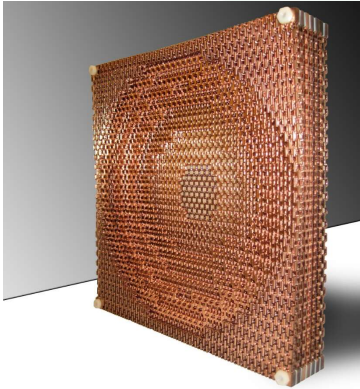


- Easier to control step size.
- More difficult to control number of points.
- More difficult to control position of last point.

3D → 2D → 1D

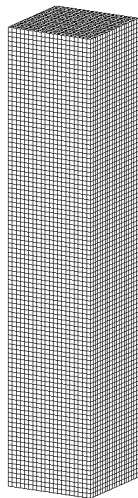
3D

All physical devices are three-dimensional.



Numerical Complexity

Typical grid required to model a 3D device.



$$\begin{aligned} N_x &= 20 \\ N_y &= 20 \\ N_z &= 100 \end{aligned}$$

Size of 3D Problem

$$20 \times 20 \times 100 = 40,000 \text{ points}$$

Size of 2D Problem

$$20 \times 100 = 2,000 \text{ points}$$

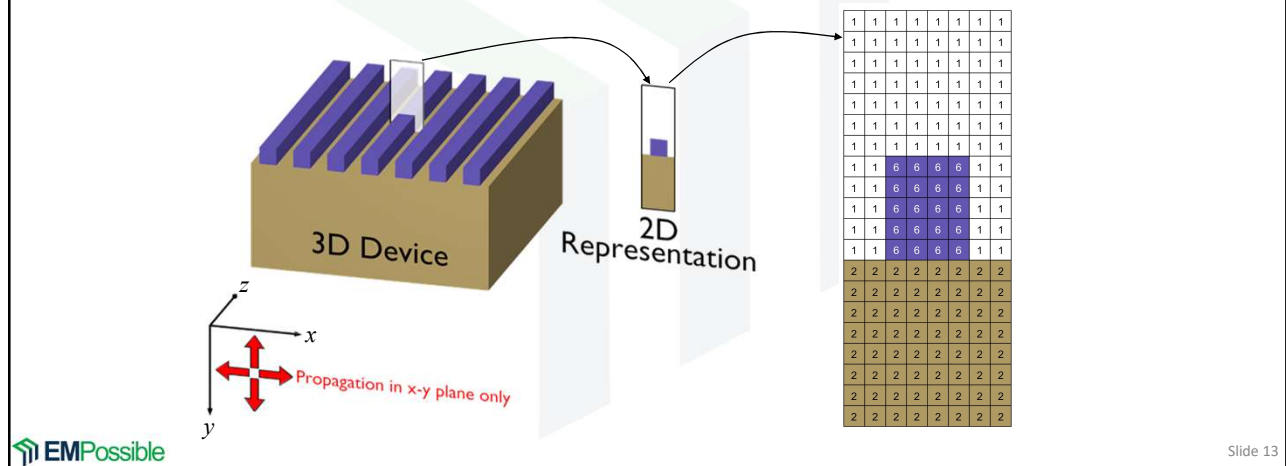
Size of 1D Problem

$$100 \text{ points}$$

Can we simulate 3D devices in one or two dimensions?

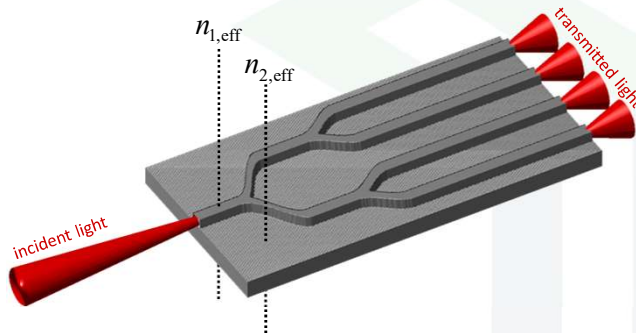
3D → 2D (Exact)

Sometimes it is possible to describe a physical device using just two dimensions. Doing so dramatically reduces the numerical complexity of the problem and is ALWAYS GOOD PRACTICE.



3D → 2D (Approximate)

Many times it is possible to approximate a 3D device in two dimensions. It is very good practice to at least perform the initial simulations in 2D and only moving to 3D to verify the final design.



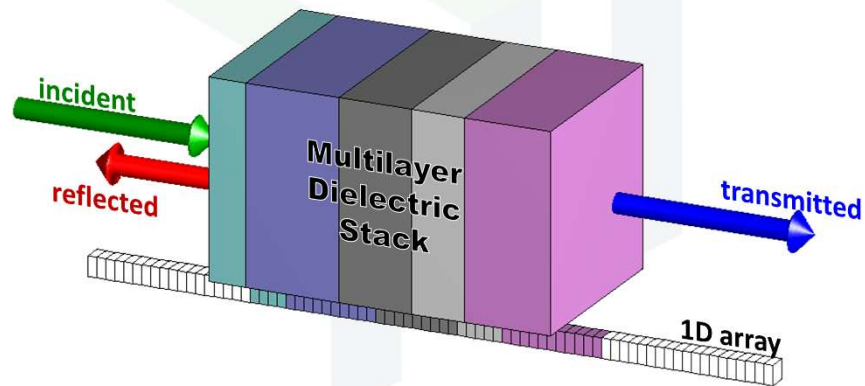
Effective indices are best computed by modeling the vertical cross section as a slab waveguide.

A simple average index can also produce good results.



3D \rightarrow 1D (Exact)

Sometimes it is possible to describe a physical device using just one dimension. Doing so dramatically reduces the numerical complexity of the problem and is ALWAYS GOOD PRACTICE.



Arrays, x and y in MATLAB

How MATLAB Indexes Arrays

MATLAB uses matrix notation for indexing arrays.

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} \quad \begin{array}{l} a_{mn} \\ m \text{ is the row number} \\ n \text{ is the column number} \end{array}$$

In MATLAB notation, a_{mn} is indexed as $A(m, n)$.

In this sense, the first number is the vertical position and the second number is the horizontal position. This is like $f(y, x)$ and so it is awkward for us to think about when the array is not a matrix.

To be consistent with matrix notation, the index of the first element in an array is 1, not zero like in other programming languages like C or Fortran.

A More Intuitive Way of Indexing Arrays

Experience suggests that one of the most challenging tasks in numerical modeling is representing devices on a grid.

To be more intuitive, we would like the first argument when indexing an array to be the horizontal position and the second to be the vertical position so that it looks like $f(x, y)$ instead of $f(y, x)$.

For this reason, we will treat the first argument of an array as the horizontal position and the second as the vertical position. This is consistent with the standard $f(x, y)$ notation.

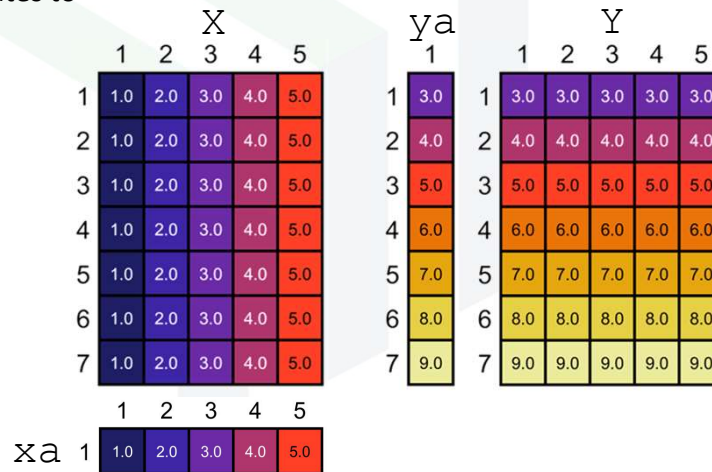
Think $A(nx, ny)$ instead of $A(m, n)$.

This is fine, but MATLAB still treats the array otherwise. We only need to consider how MATLAB handles things when using the `meshgrid()` command or when using plotting commands.

meshgrid()

The `meshgrid()` command allows complex equations involving grid coordinates to be typed directly into MATLAB without the need of using for loops to iterate across the grid.

```
% GENERATE MESHGRID
xa = [1:5];
ya = [3:9];
[Y,X] = meshgrid(ya,xa);
```



Revised Use of meshgrid()

MATLAB Standard Use of `meshgrid()`

```
xa = [0:Nx-1]*dx;
ya = [0:Ny-1]*dy;
[X,Y] = meshgrid(xa,ya);
```

Revised Use of `meshgrid()`

```
xa = [0:Nx-1]*dx;
ya = [0:Ny-1]*dy;
[Y,X] = meshgrid(ya,xa);
```

We will do it this way.

Revised Plot Commands

MATLAB Standard Use of `imagesc()`

```
imagesc(xa, ya, A);
```

← This fails to properly convey our sense of x and y.

Revised Use of `imagesc()`

```
imagesc(xa, ya, A.');
```

```
>> A = zeros(4,4);
>> A(2,3) = 1;
>> A
```

A =

```
0 0 0 0
0 0 1 0
0 0 0 0
0 0 0 0
```

```
>> A. '
```

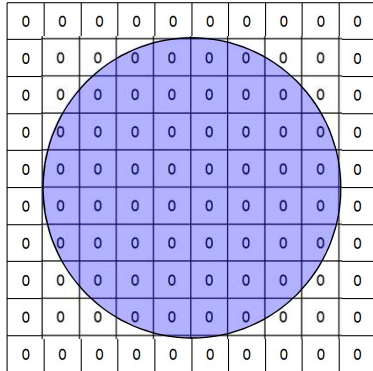
ans =

```
0 0 0 0
0 0 0 0
0 1 0 0
0 0 0 0
```

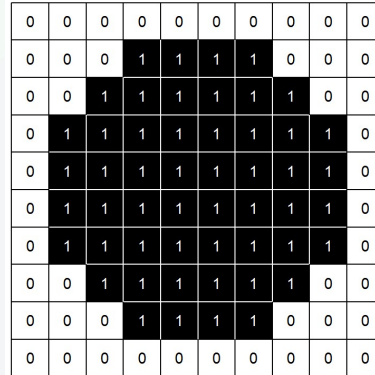
Building Geometries into Data Arrays

Building a Geometry?

A geometry is “built” into an array when you can visualize the array and see the desired geometry.



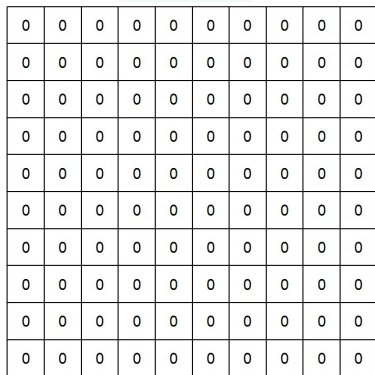
Suppose we wish to “build” a circle into this array.



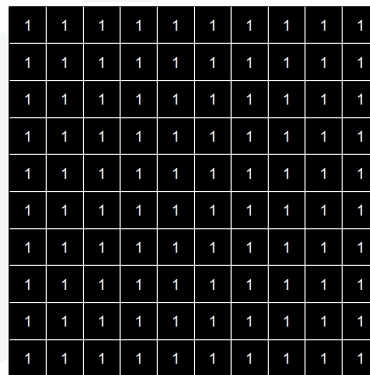
We fill in our array so that when the array is plotted we see our circle.

Initializing Data Arrays

```
Nx = 10;
Ny = 10;
A = zeros (Nx, Ny);
```



```
Nx = 10;
Ny = 10;
A = ones (Nx, Ny);
```

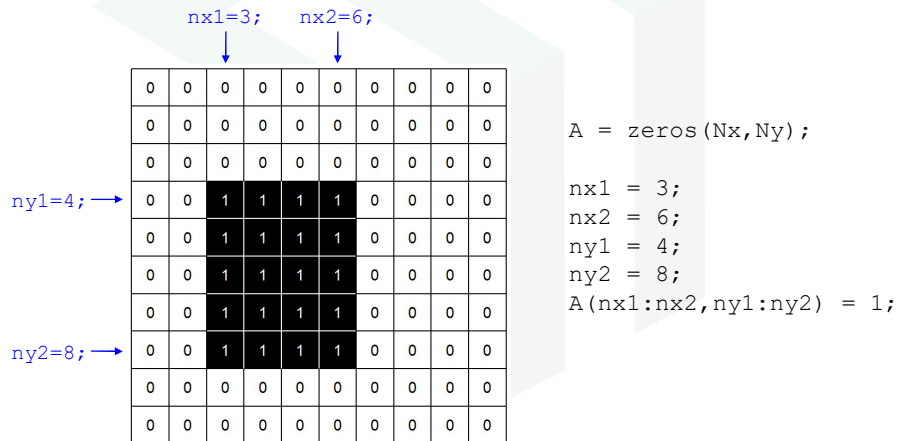


You can initialize an array with any number:

```
A = 3.1 * ones (Nx, Ny);
```

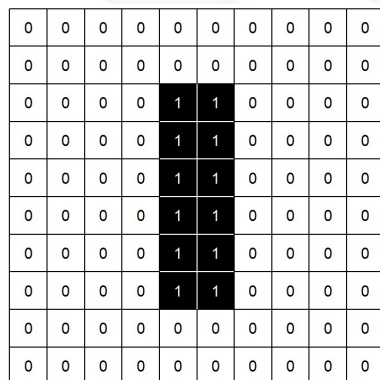
Adding Rectangles to an Array

Consider adding rectangles by first computing the start and stop indices in the array, then filling in the array.



Centering a Rectangle

It is often necessary to center a rectangle type structure in an array.



```

% DEFINE GRID
Sx = 1;      %physical size along x
Sy = 1;      %physical size along y
Nx = 10;     %number of cells along x
Ny = 10;     %number of cells along y

% DEFINE RECTANGLE SIZE
wx = 0.2;
wy = 0.6;

% COMPUTE POSITION INDICES
dx = Sx/Nx;
nx = round(wx/dx);
nx1 = 1 + floor((Nx - nx)/2);
nx2 = nx1 + nx - 1;

dy = Sy/Ny;
ny = round(wy/dy);
ny1 = 1 + floor((Ny - ny)/2);
ny2 = ny1 + ny - 1;

% CREATE A
A = zeros(Nx,Ny);
A(nx1:nx2,ny1:ny2) = 1;

```

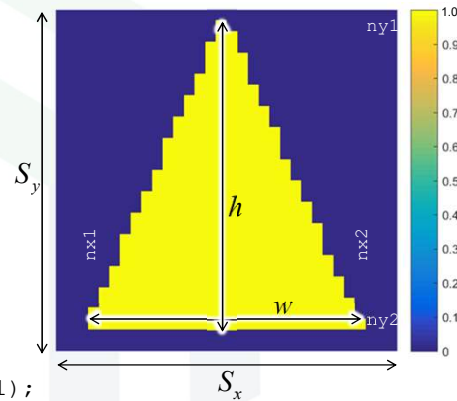
A Simple Centered Triangle

```

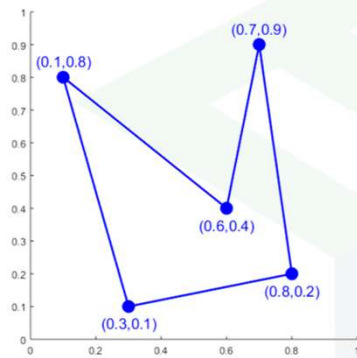
% TRIANGLE
w = 0.8*Sx;
h = 0.9*Sy;

% CREATE CENTERED TRIANGLE
ER = zeros(Nx,Ny);
ny = round(h/dy);
ny1 = 1 + floor((Ny - ny)/2);
ny2 = ny1 + ny - 1;
for ny = ny1 : ny2
    f = (ny - ny1 + 1)/(ny2 - ny1 + 1);
    nx = round(f*w/dx);
    nx1 = 1 + floor((Nx - nx)/2);
    nx2 = nx1 + nx - 1;
    ER(nx1:nx2,ny) = 1;
end

```



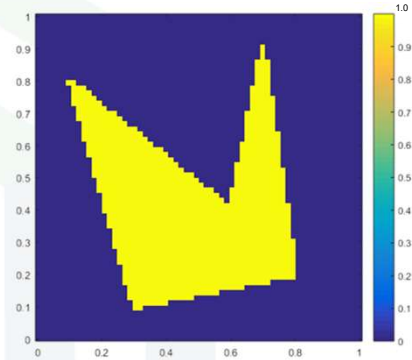
Creating Arbitrary Polygons



```

% DEFINE VERTICES OF POLYGON
p1 = [ 0.3 ; 0.1 ];
p2 = [ 0.8 ; 0.2 ];
p3 = [ 0.7 ; 0.9 ];
p4 = [ 0.6 ; 0.4 ];
p5 = [ 0.1 ; 0.8 ];
P = [ p1 p2 p3 p4 p5 ];

```



```

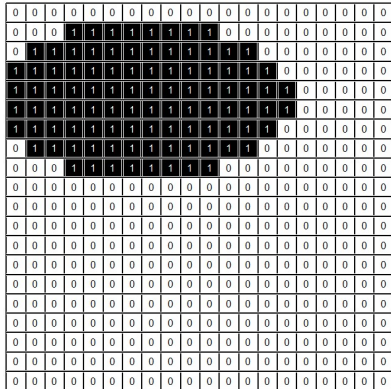
% CALL POLYFILL() TO FILL
% POLYGON IN ARRAY A
A = polyfill(xa, ya, P);

```

Get `polyfill()` from course website.

Offset Ellipses

Ellipses and circles can be placed anywhere on the grid.



```

% DEFINE GRID
Sx = 1;      %physical size along x
Sy = 1;      %physical size along y
Nx = 20;     %number of cells along x
Ny = 20;     %number of cells along y

% GRID ARRAYS
dx = Sx/Nx;
xa = [0:Nx-1]*dx;
xa = xa - mean(xa);

dy = Sy/Ny;
ya = [0:Ny-1]*dy;
ya = ya - mean(ya);

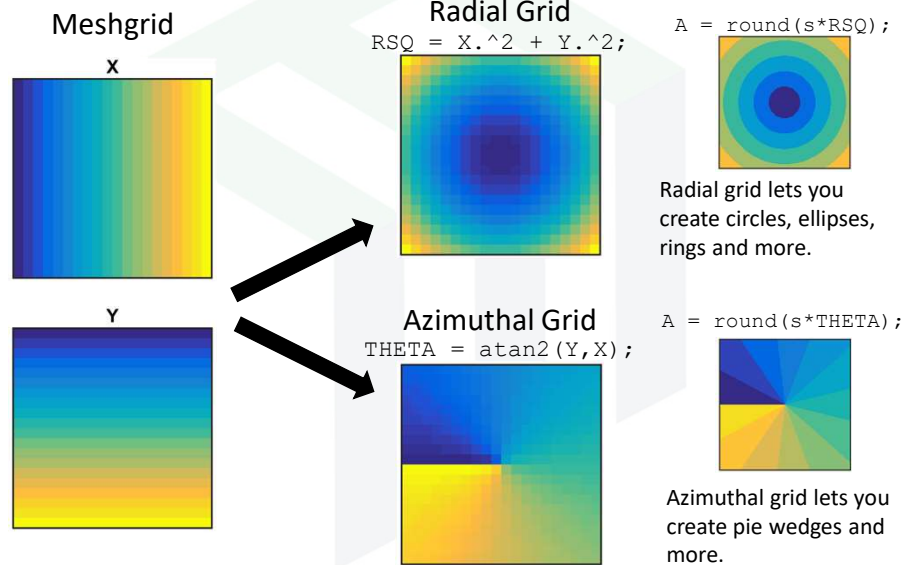
[Y,X] = meshgrid(ya,xa);

% CREATE ELLIPSE
xc = -0.15;
yc = +0.25;
rx = 0.4;
ry = 0.2;
A = ( ((X - xc)/rx).^2 + ...
      ((Y - yc)/ry).^2 ) <= 1;
    
```



Slide 31

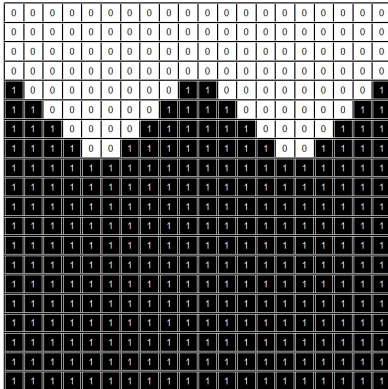
Radial & Azimuthal Geometries



Slide 32

Formed Half-Spaces

We can “fill in” half the grid under an arbitrary function like this...



```
% DEFINE GRID
Sx = 1;      %physical size along x
Sy = 1;      %physical size along y
Nx = 20;     %number of cells along x
Ny = 20;     %number of cells along y

% GRID ARRAYS
dx = Sx/Nx;
xa = [0:Nx-1]*dx;
xa = xa - mean(xa);

dy = Sy/Ny;
ya = [0:Ny-1]*dy;
ya = ya - mean(ya);

% CALCULATE SURFACE
y = 0.2 + 0.1*cos(4*pi*xa/Sx);

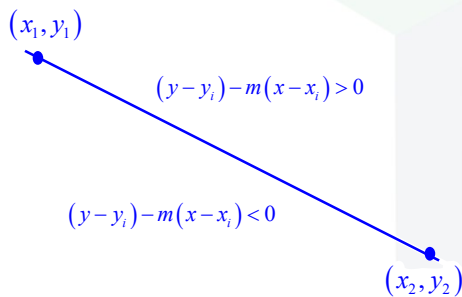
% FILL HALF SPACE
A = zeros(Nx,Ny);
for nx = 1 : Nx
    ny = round((y(nx) + Sy/2)/dy);
    A(nx,1:ny) = 1;
end
```

Linear Half-Spaces (1 of 2)

Given two points (x_1, y_1) and (x_2, y_2) ,
an equation for the line passing
through these two points is:

$$(y - y_i) = m(x - x_i)$$

$$m = \frac{y_2 - y_1}{x_2 - x_1} \quad i = 1 \text{ or } 2$$



This equation can be rearranged as

$$(y - y_i) - m(x - x_i) = 0$$

The space on one half of this line is
called a half-space. It is defined as:

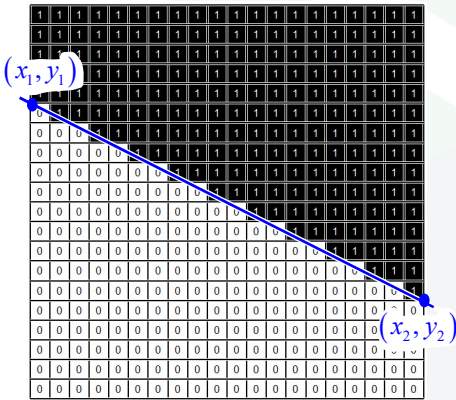
$$(y - y_i) - m(x - x_i) > 0$$

or

$$(y - y_i) - m(x - x_i) < 0$$

Linear Half-Spaces (2 of 2)

A half-space can be filled anywhere on the grid.



```
% DEFINE GRID
Sx = 1; %physical size along x
Sy = 1; %physical size along y
Nx = 20; %number of cells along x
Ny = 20; %number of cells along y

% GRID ARRAYS
dx = Sx/Nx;
xa = [0:Nx-1]*dx;
xa = xa - mean(xa);

dy = Sy/Ny;
ya = [0:Ny-1]*dy;
ya = ya - mean(ya);

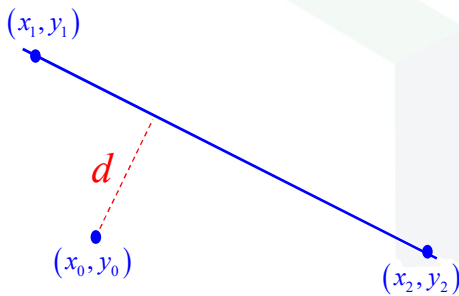
[Y,X] = meshgrid(ya,xa);

% DEFINE TWO POINTS
x1 = -0.50;
y1 = +0.25;
x2 = +0.50;
y2 = -0.25;

% FILL HALF SPACE
m = (y2 - y1)/(x2 - x1);
A = (Y - y1) - m*(X - x1) > 0;
```

Creating Linear Gradients (1 of 2)

The distance from a point to a line is calculated as



Two Dimensions

$$d = \frac{|(y_2 - y_1)x_0 - (x_2 - x_1)y_0 + x_2y_1 - x_1y_2|}{\sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2}}$$

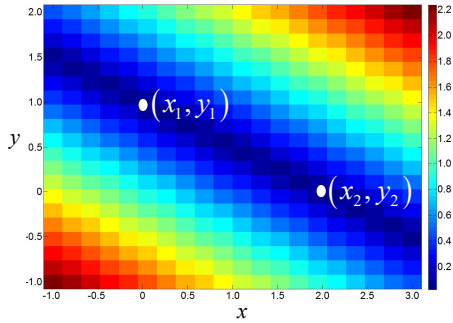
$$d = \frac{|ax_0 + by_0 + c|}{\sqrt{a^2 + b^2}} \quad ax_0 + by_0 + c = 0$$

Three Dimensions

$$d = \frac{|(\vec{r}_2 - \vec{r}_1) \times (\vec{r}_1 - \vec{r}_0)|}{|\vec{r}_2 - \vec{r}_1|}$$

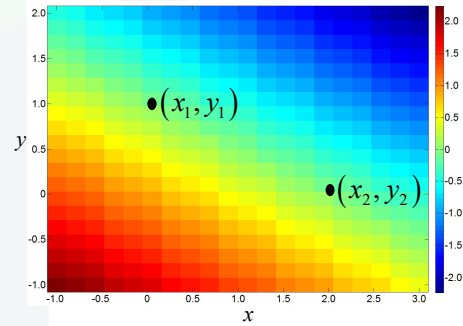
Creating Linear Gradients (2 of 2)

$$d = \frac{|(y_2 - y_1)x_0 - (x_2 - x_1)y_0 + x_2y_1 - x_1y_2|}{\sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2}}$$



```
x1 = 0;    y1 = 1;
x2 = 2;    y2 = 0;
D = (y2 - y1)*X - (x2 - x1)*Y + x2*y1 - x1*y2;
D = abs(D)/sqrt((y2 - y1)^2 + (x2 - x1)^2);
```

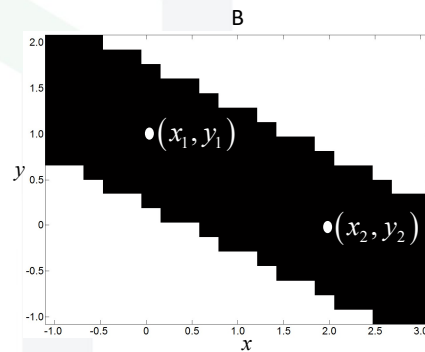
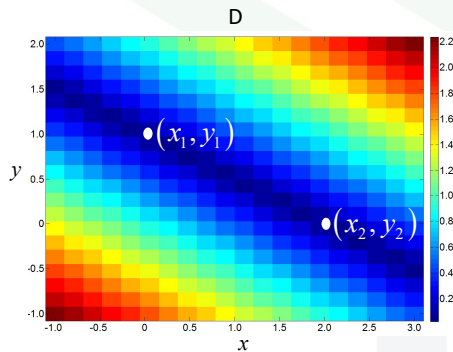
$$d = \frac{(y_2 - y_1)x_0 - (x_2 - x_1)y_0 + x_2y_1 - x_1y_2}{\sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2}}$$



```
x1 = 0;    y1 = 1;
x2 = 2;    y2 = 0;
D = (y2 - y1)*X - (x2 - x1)*Y + x2*y1 - x1*y2;
D = D./sqrt((y2 - y1)^2 + (x2 - x1)^2);
```

Creating Thick Bars

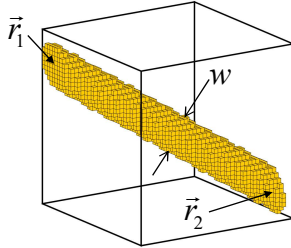
We can use the linear gradients to create thick bars through our grid with any thickness and orientation.



```
x1 = 0;    y1 = 1;
x2 = 2;    y2 = 0;
D = (y2 - y1)*X - (x2 - x1)*Y + x2*y1 - x1*y2;
D = abs(D)/sqrt((y2 - y1)^2 + (x2 - x1)^2);
```

```
B = D < 0.7;
```

Creating Thick Bars on 3D Grids



```
% DEFINE TWO POINTS ALONG BAR AND WIDTH
w = 0.1;
r1 = [ 0.1 ; 0 ; 0.8 ];
r2 = [ 0.8 ; 1 ; 0.1 ];

% CALCULATE DISTANCE FUNCTION
d = r2 - r1;
d = d/norm(d);
D = sqrt( (d(2)*(r1(3) - Z) - d(3)*(r1(2) - Y)).^2 + ...
          (d(3)*(r1(1) - X) - d(1)*(r1(3) - Z)).^2 + ...
          (d(1)*(r1(2) - Y) - d(2)*(r1(1) - X)).^2 );

% CALCULATE BAR
ER = (D <= w);
```

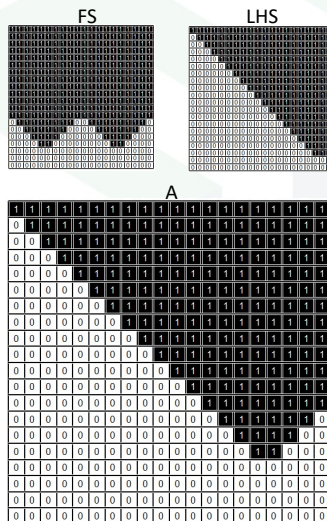
$$\hat{\delta} = \frac{\vec{r}_2 - \vec{r}_1}{|\vec{r}_2 - \vec{r}_1|}$$

$$d = \left| \hat{\delta} \times (\vec{r}_1 - \vec{r}_0) \right|$$

$$= \left| \left[\delta_y(z_1 - z) - \delta_z(y_1 - y) \right] \hat{a}_x + \left[\delta_z(x_1 - x) - \delta_x(z_1 - z) \right] \hat{a}_y + \left[\delta_x(y_1 - y) - \delta_y(x_1 - x) \right] \hat{a}_z \right|$$

$$= \sqrt{\left[\delta_y(z_1 - z) - \delta_z(y_1 - y) \right]^2 + \left[\delta_z(x_1 - x) - \delta_x(z_1 - z) \right]^2 + \left[\delta_x(y_1 - y) - \delta_y(x_1 - x) \right]^2}$$

Masking and Boolean Operations



The figure below is the formed surfaced masked by a linear half-space.

```
% DEFINE GRID
Sx = 1; %physical size along x
Sy = 1; %physical size along y
Nx = 20; %number of cells along x
Ny = 20; %number fo cells along y

% GRID ARRAYS
dx = Sx/Nx;
xa = [0:Nx-1]*dx;
xa = xa - mean(xa);

dy = Sy/Ny;
ya = [0:Ny-1]*dy;
ya = ya - mean(ya);

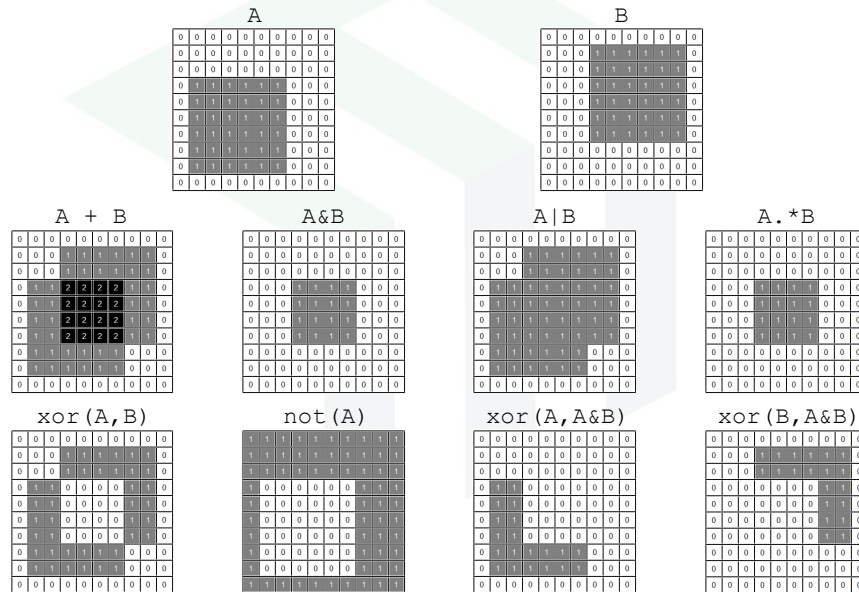
[Y,X] = meshgrid(ya,xa);

% CREATE A FORMED SURFACE
y = -0.2 + 0.1*cos(4*pi*xa/Sx);
FS = zeros(Nx,Ny);
dy = Sy/Ny;
for nx = 1 : Nx
    ny = round((y(nx) + Sy/2)/dy);
    FS(nx,ny:Ny) = 1;
end

% CREATE A LINEAR HALF SPACE
x1 = -0.5;
y1 = +0.5;
x2 = +0.5;
y2 = -0.5;
m = (y2 - y1)/(x2 - x1);
LHS = (Y - y1) - m*(X - x1) > 0;

% COMBINE ABOVE GEOMETRIES
A = FS .* LHS;
```

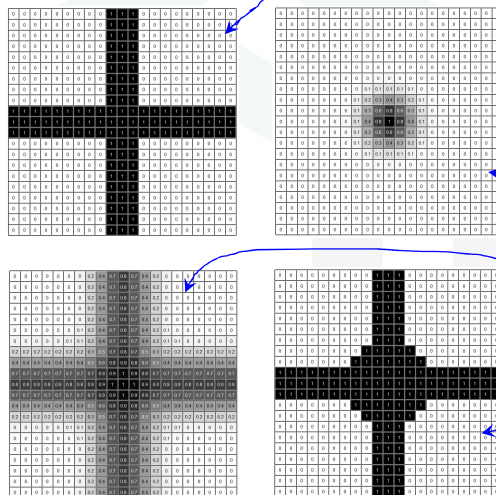
Comparison of Boolean Operations



Slide 41

Blurring Geometries

Blurring is used to resolve surfaces that slice through the middle of cells or to build more realistic device geometries.



```

% DEFINE GRID
Sx = 1; %physical size along x
Sy = 1; %physical size along y
Nx = 21; %number of cells along x
Ny = 21; %number of cells along y

% GRID ARRAYS
dx = Sx/Nx;
xa = [0:Nx-1]*dx;
xa = xa - mean(xa);
dy = Sy/Ny;
ya = [0:Ny-1]*dy;
ya = ya - mean(ya);
[Y,X] = meshgrid(ya, xa);

% CREATE A CROSS
ER = abs(X)<=0.075 | abs(Y)<=0.075;

% CREATE BLUR FUNCTION
B = exp(-(X.^2 + Y.^2)/0.1^2);

% PERFORM BLUR OPERATION
ER = fft2(ER) .* fft2(B)/sum(B(:));
ER = ifftshift(real(ifft2(ER)));

% PERFORM THRESHOLD OPERATION
ER = ER > 0.4;
    
```



Slide 42

Scaling the Values of the Data

Eventually, we need to build devices on a grid. This is done by a dielectric constant to specific geometries in the array. Typically, the background will be air with a dielectric constant of 1.0.

```
er1 = 1.0;
er2 = 2.4;
A   = er1*(1-A) + er2*A;
A   = er1 + (er2 - er1)*A;
```

0	0	0	0	0	0	0	0	0	0
0	0	0	0	1	1	0	0	0	0
0	0	1	1	1	1	1	1	0	0
0	0	1	1	1	1	1	1	0	0
0	1	1	1	1	1	1	1	1	0
0	1	1	1	1	1	1	1	1	0
0	0	1	1	1	1	1	1	0	0
0	0	1	1	1	1	1	1	0	0
0	0	0	0	1	1	0	0	0	0
0	0	0	0	0	0	0	0	0	0

1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
1.0	1.0	1.0	1.0	2.4	2.4	1.0	1.0	1.0	1.0
1.0	1.0	2.4	2.4	2.4	2.4	2.4	2.4	1.0	1.0
1.0	1.0	2.4	2.4	2.4	2.4	2.4	2.4	1.0	1.0
1.0	2.4	2.4	2.4	2.4	2.4	2.4	2.4	2.4	1.0
1.0	2.4	2.4	2.4	2.4	2.4	2.4	2.4	2.4	1.0
1.0	1.0	2.4	2.4	2.4	2.4	2.4	2.4	1.0	1.0
1.0	1.0	2.4	2.4	2.4	2.4	2.4	2.4	1.0	1.0
1.0	1.0	1.0	1.0	2.4	2.4	1.0	1.0	1.0	1.0
1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0