MOLECULAR FOUNDRY

Making Figures and Movies with Code

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NCEM, Molecular Foundry, Lawrence Berkeley National Laboratory

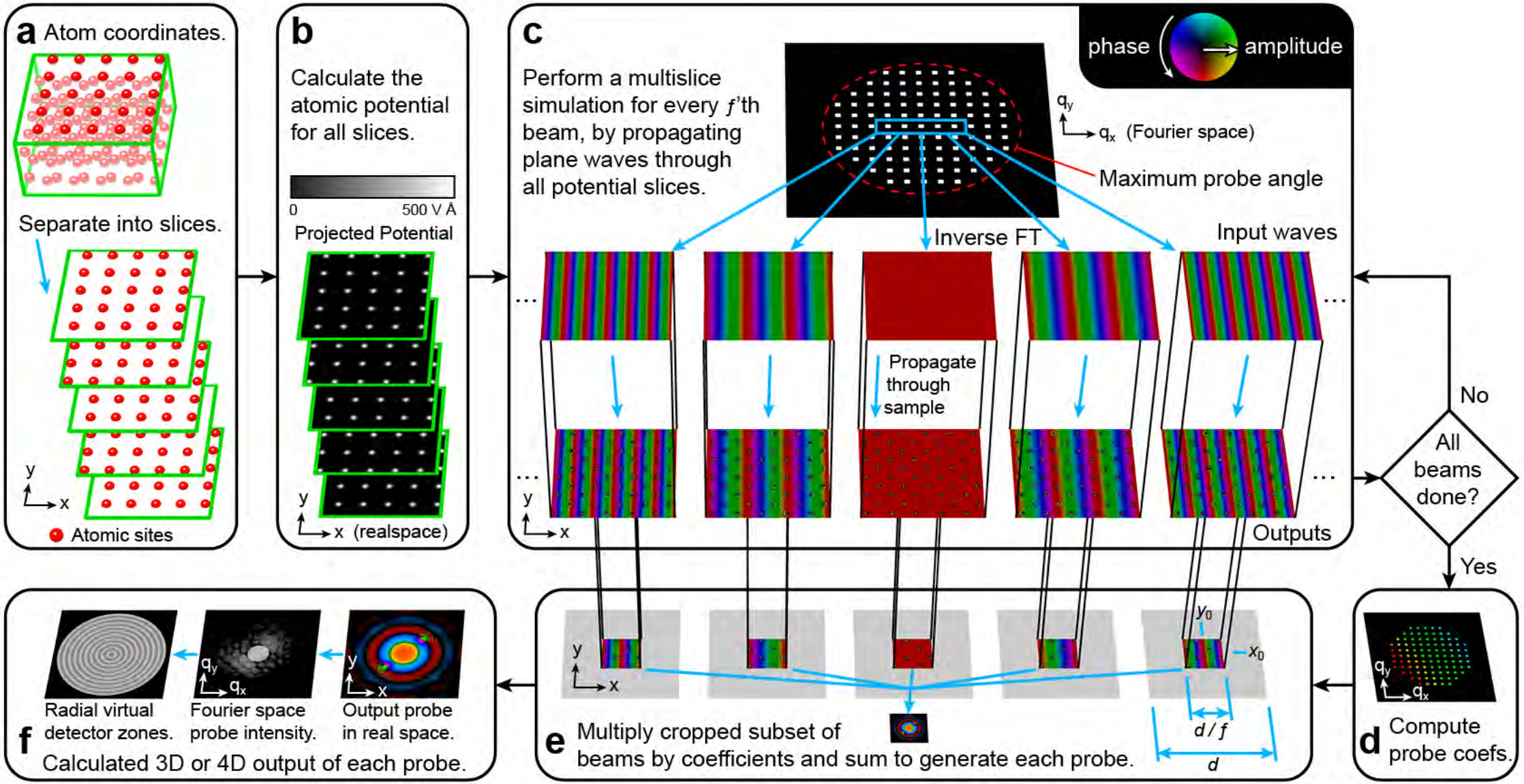
Tutorial 4 – Data Analysis and Modern Visualization
APS March Meeting – Pre-Meeting

All files and updated slides available at – github.com/cophus/Programmatic_Figures_Tutorial

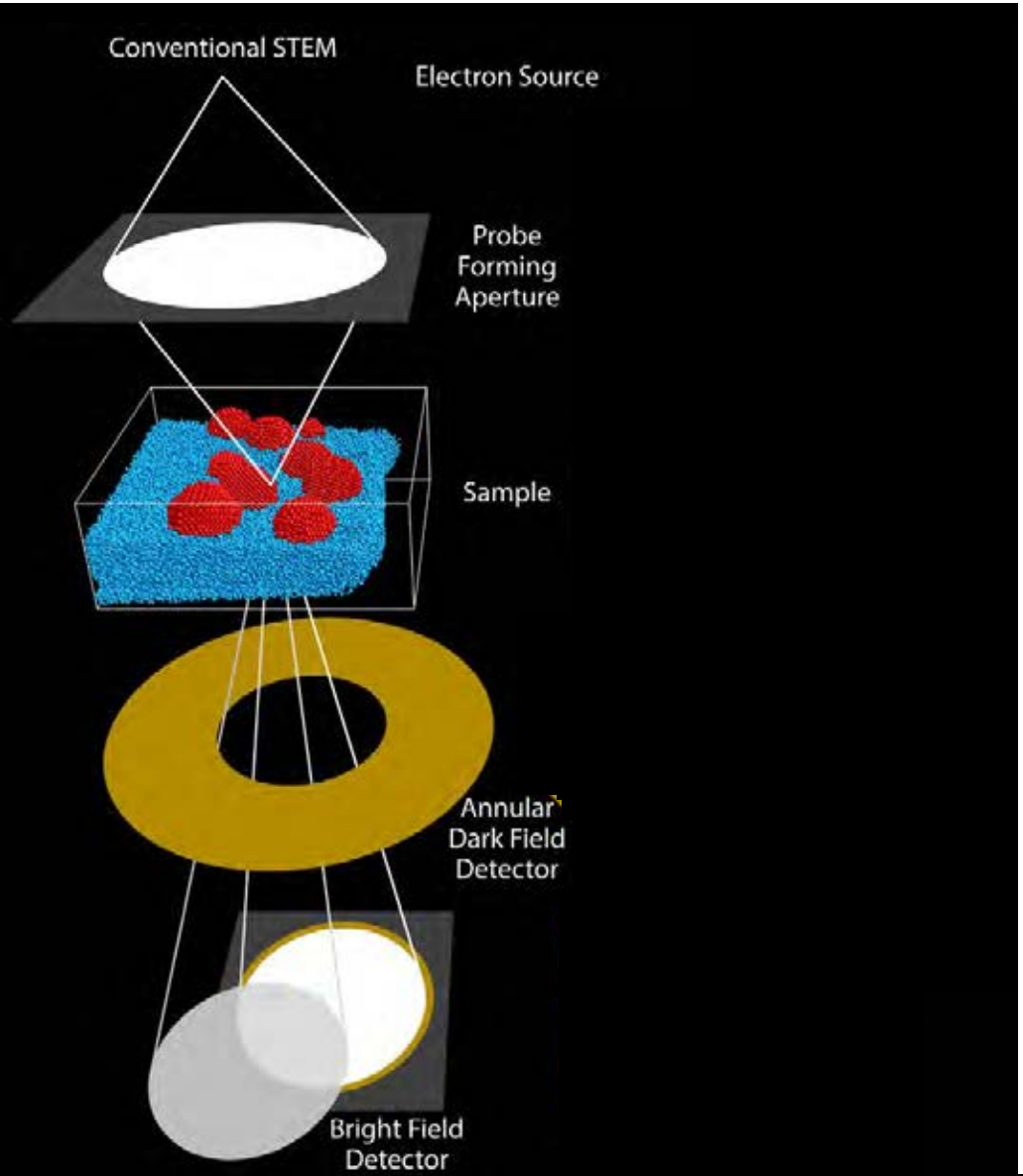
Molecular Foundry – Proposals due Mar 31 2021 – foundry.lbl.gov

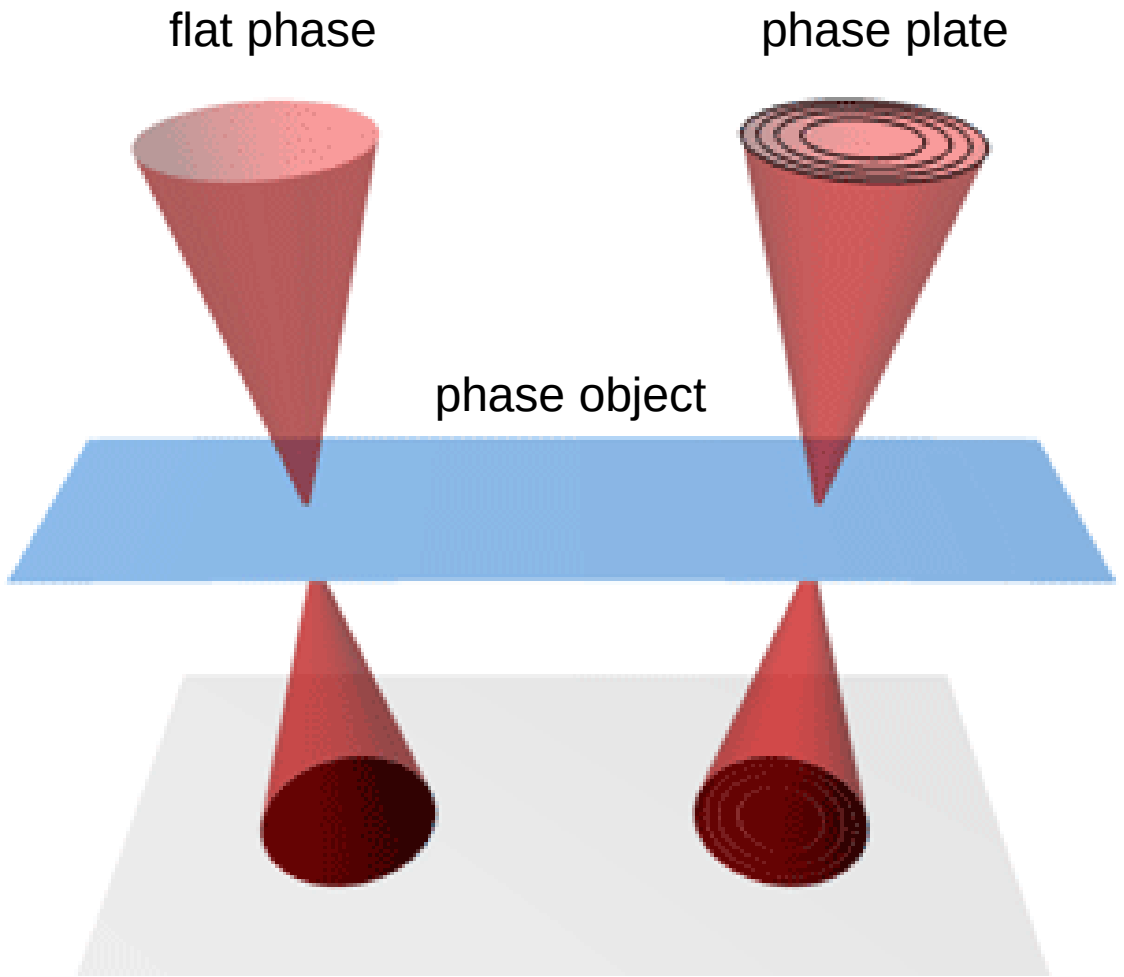
- We are a **user facility** at the Berkeley Lab, operated by the US Department of Energy.
- **Anyone** can submit a proposal (including for **computation**, **simulation** or **analysis**!).
- If accepted by independent review board, access to microscopes and staff is **free**.

Programmatic Visualization Examples



Programmatic Visualization Examples

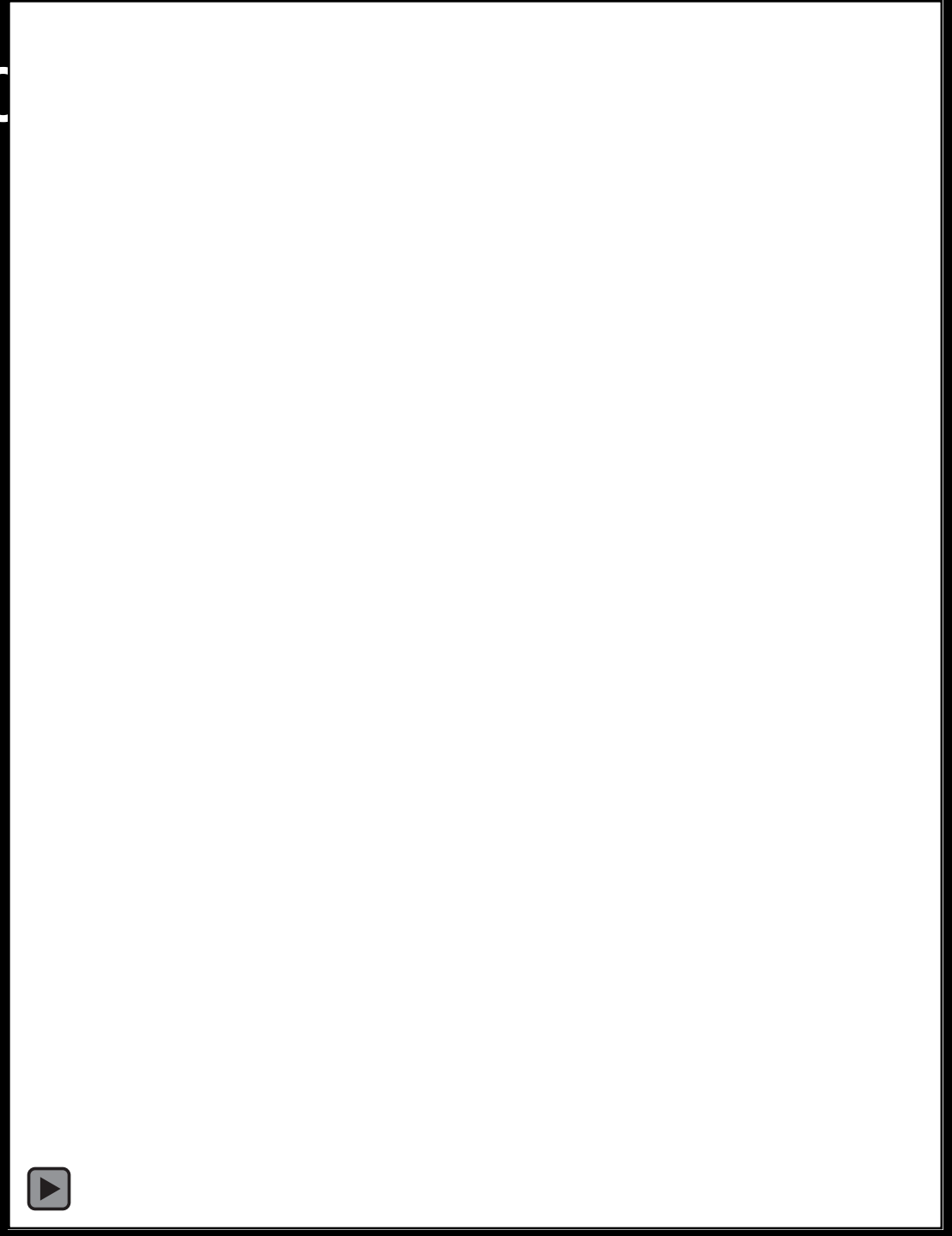




Phase plate interference pattern can generate linear interference.

C Ophus et al., Nature Communications 7, 10719 (2016)

Programmatic Visualization Examples

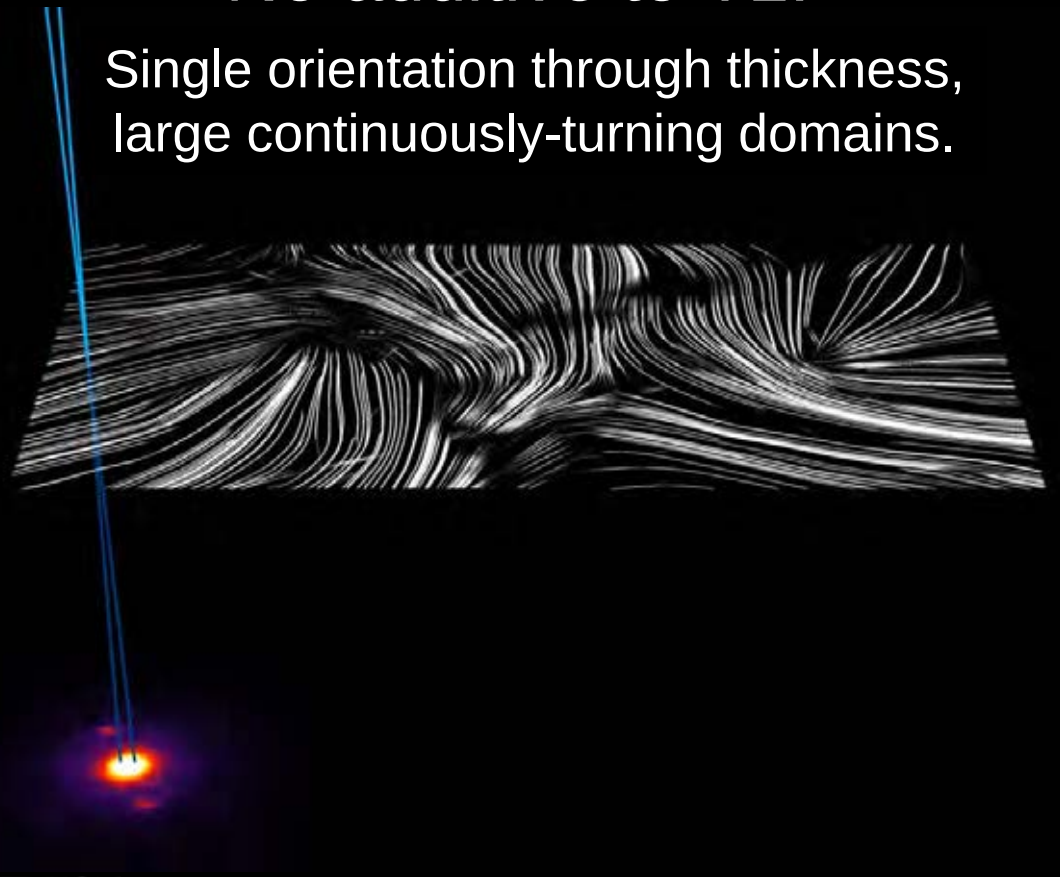


Programmatic Visualization Examples

Visualization of the two morphologies:

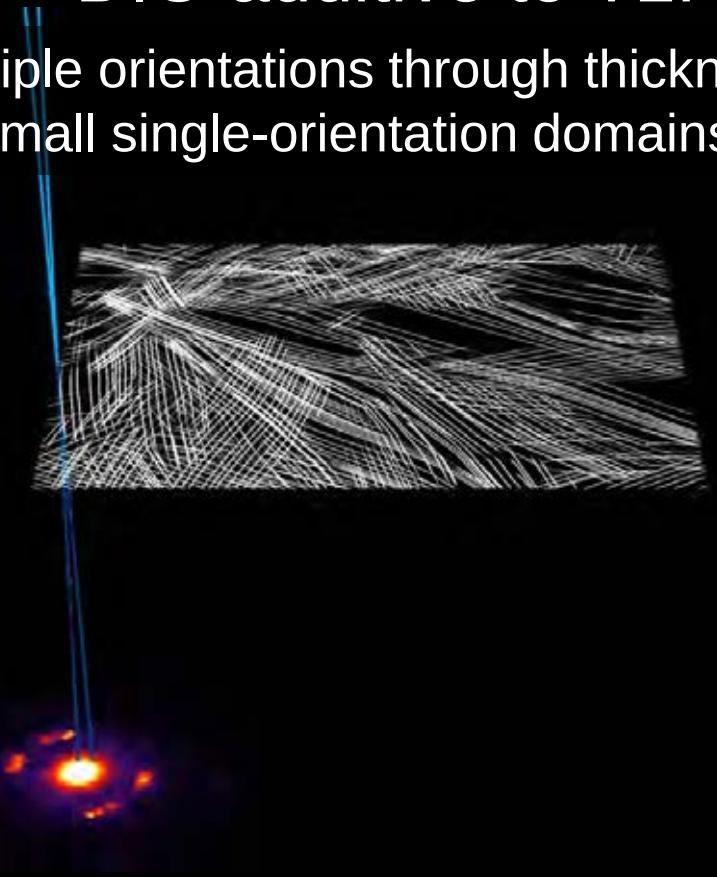
No additive to T1:

Single orientation through thickness,
large continuously-turning domains.



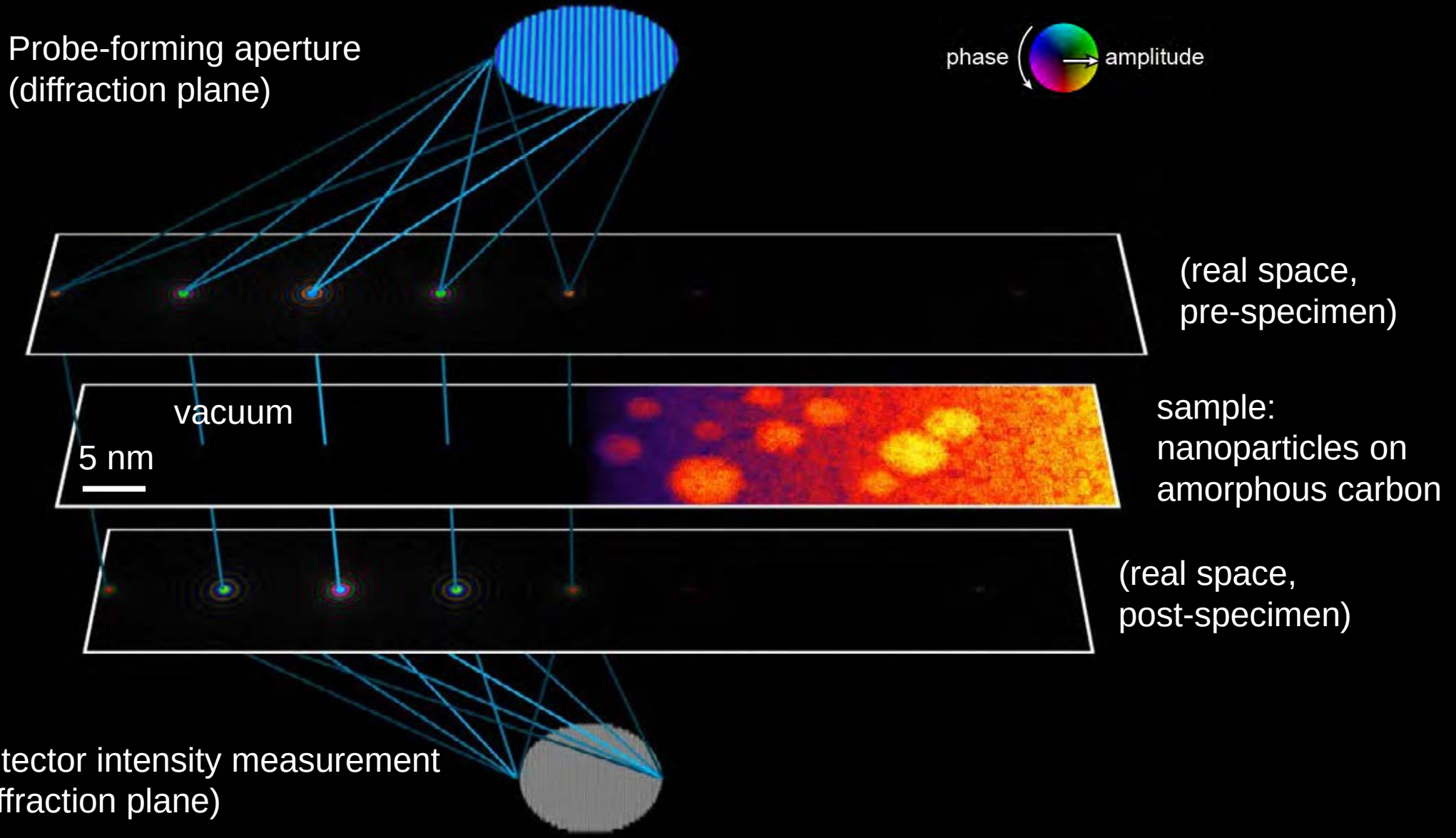
DIO additive to T1:

Multiple orientations through thickness,
small single-orientation domains.



C Ophus*, O Panova* et al., Nature Materials 18, 860 (2019)

Programmatic Visualization Examples



Progr
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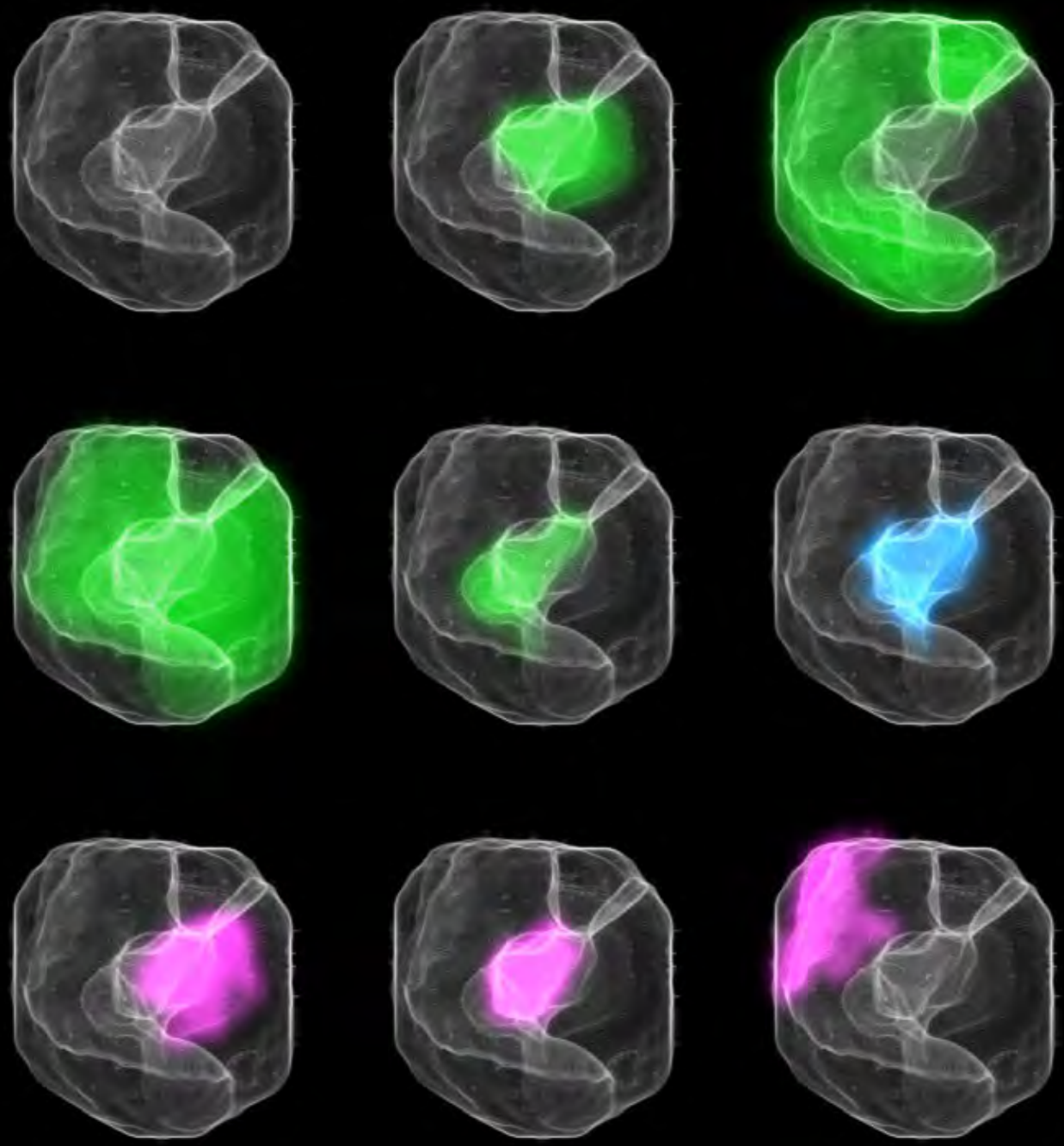
Programmatic Visualization Examples



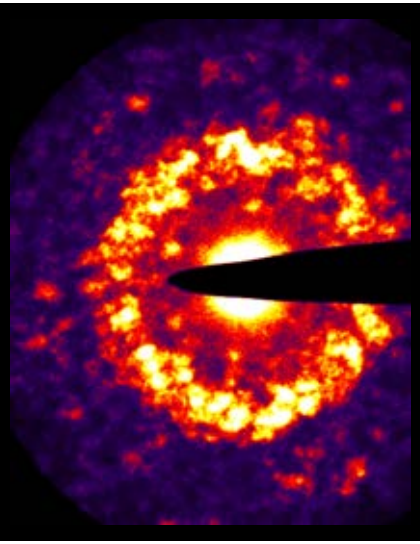
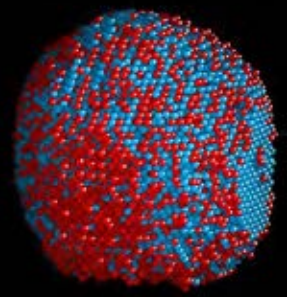
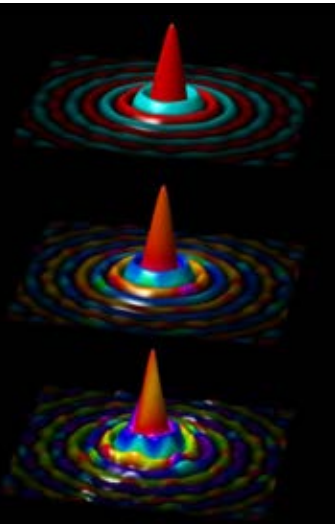
- Same data as previous slide, but visualized in a completely different way – grains become volumetric renders.

Programmatic Visualization Examples

Each of these visualizations was generated almost entirely from code –

and not very much code either!

Outline

1

Basic concepts when making figures and movies – raster vs vector.

2

Scaling, coloring and saving scalar and vector **imaging data**.

3

Plotting **points in 3D**, highlight internal features – e.g. atomic coordinates.

4

Animating 3D points, making **movies** – e.g. atomic coordinates.

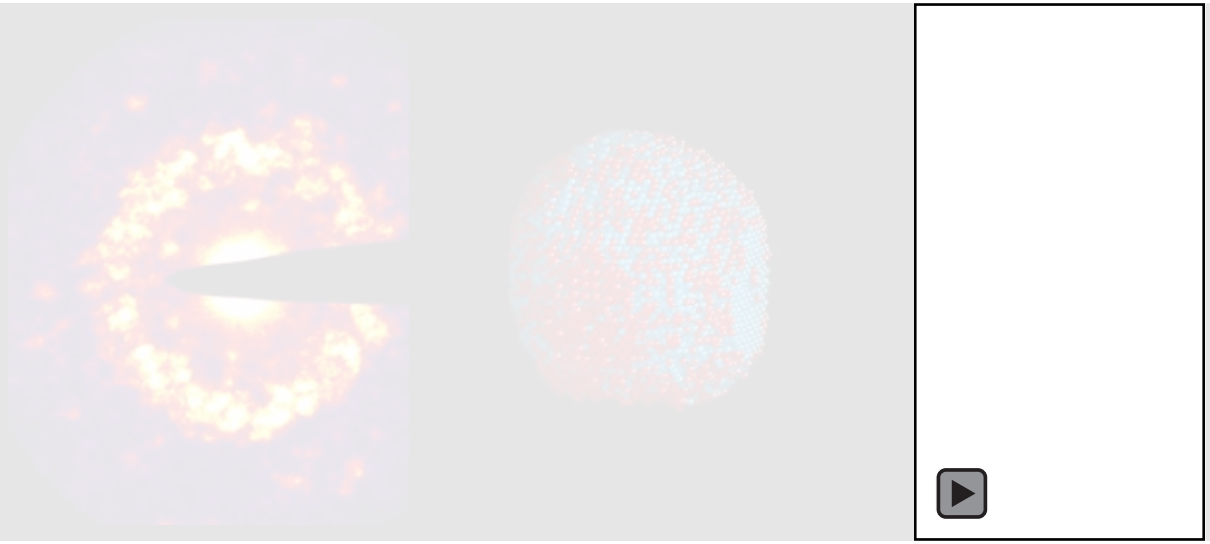
5

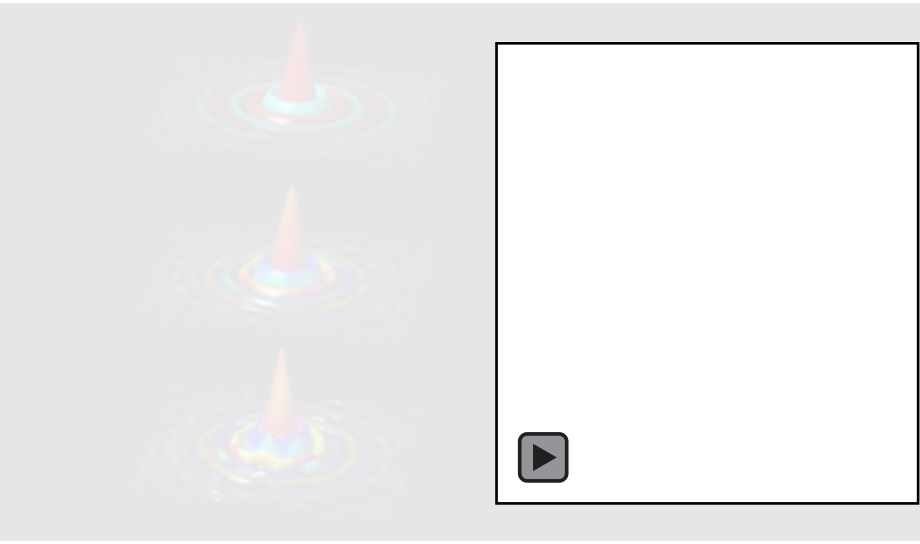
Building **physics visualization** and simulation directly into figures.

6

Making simple animations to explain **concepts in physics**.

Outline





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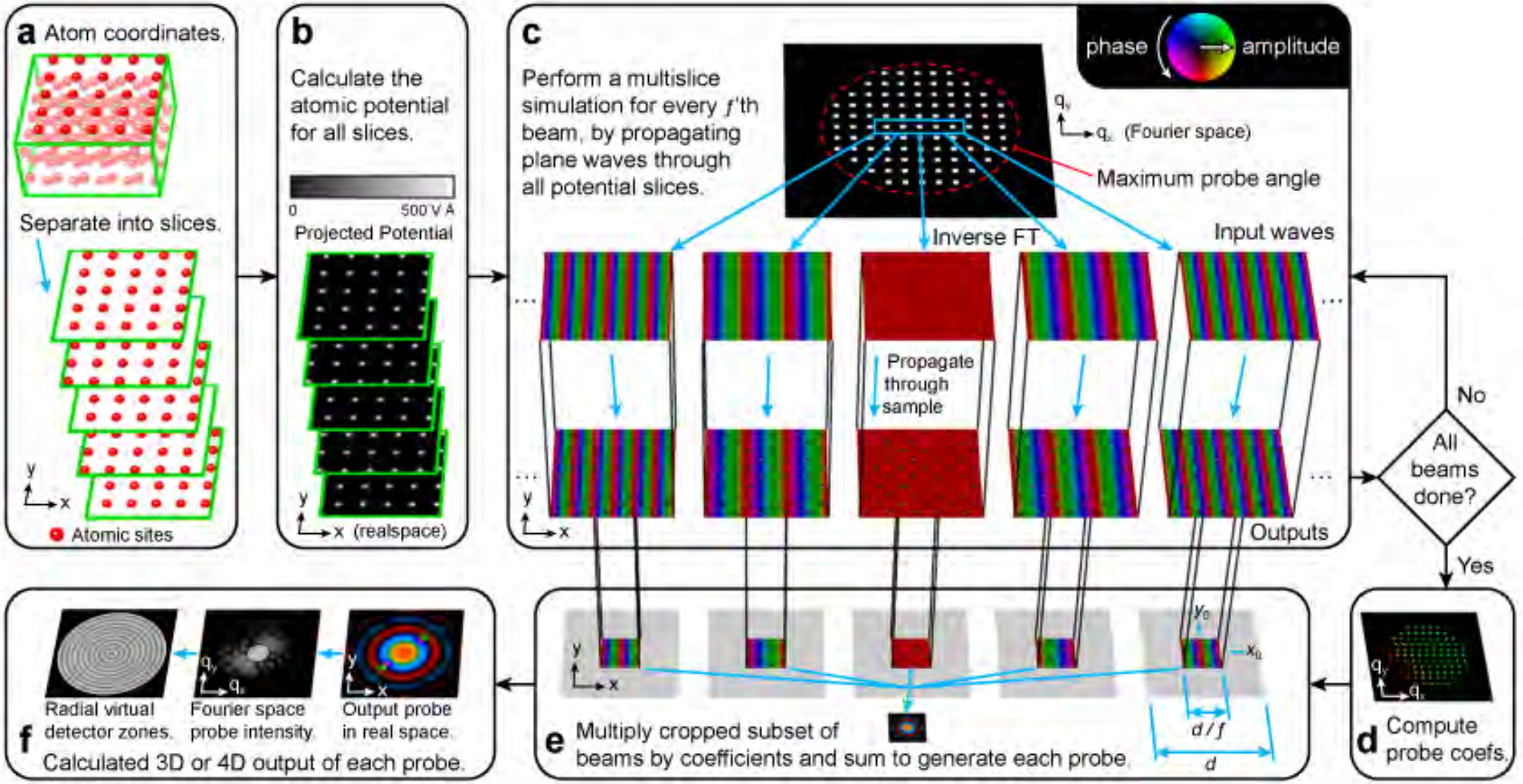
Basics – Vector Versus Raster (Bitmap)



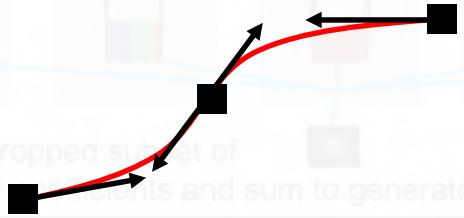
C Ophus, Advanced Structural and Chemical Imaging 3, 13 (2017).

Basics – Vector Versus Raster (Bitmap)

Vector formats can easily be “rendered” into raster.

The reverse direction is not possible however!

Vector format – objects stored as vertices, curves, faces, patches …



Raster format – RGB values stored in a grid.

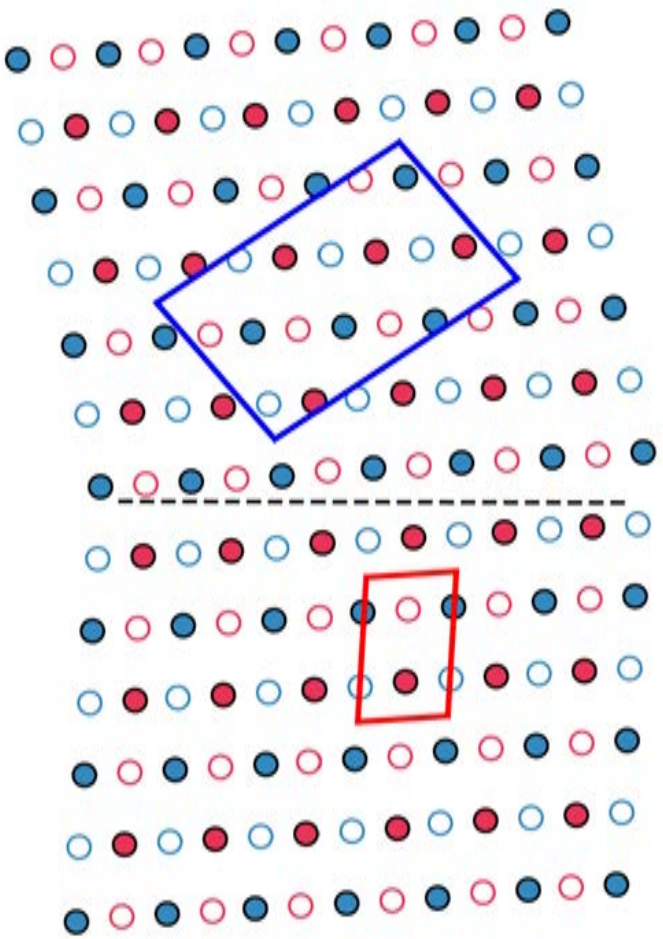
Basics – Vector and Raster File Formats

	Vector	Raster
ideal format	PDF (portable document format)	PNG (for lossless images) JPG (for lossy images)
runner up formats	SVG (scalable vector graphics) EPS (encapsulated post script)	TIFF (can contain metadata) MPG, MP4, AVI, WEBM
don't use formats	AI (adobe illustrator) CD (CorelDraw) EMF / WMF (Windows vectors) DOC, PPTX, Keynote DXF (or any other drafting format)	BMP, PSD, TGA, … GIF (Maybe the worst format ever? Terrible for animations too! Does support transparency …)

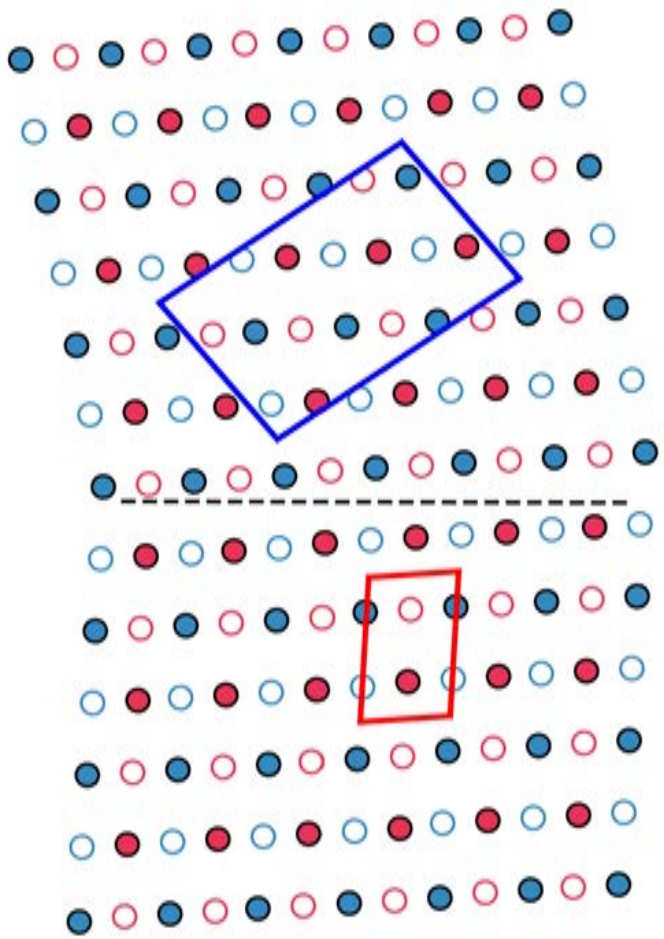
Basics – Vector and Raster Editing Software

	Vector		Raster	
Free programs	Inkscape	powerful, some quirks, SVG files	Gimp	powerful, duplicates most photoshop features
			www.photopea.com	
Good programs	Illustrator	high learning curve	Photoshop	powerful, easy to use
	CorelDraw	easy to learn		
Bad programs (for editing figures)	Microsoft Office Suite (Powerpoint)	low quality output, inconsistent support, missing most advanced tools, cannot control resolution		
	OfficeLibre (Open Office)	low quality output, inconsistent support, missing most advanced tools, cannot control resolution		

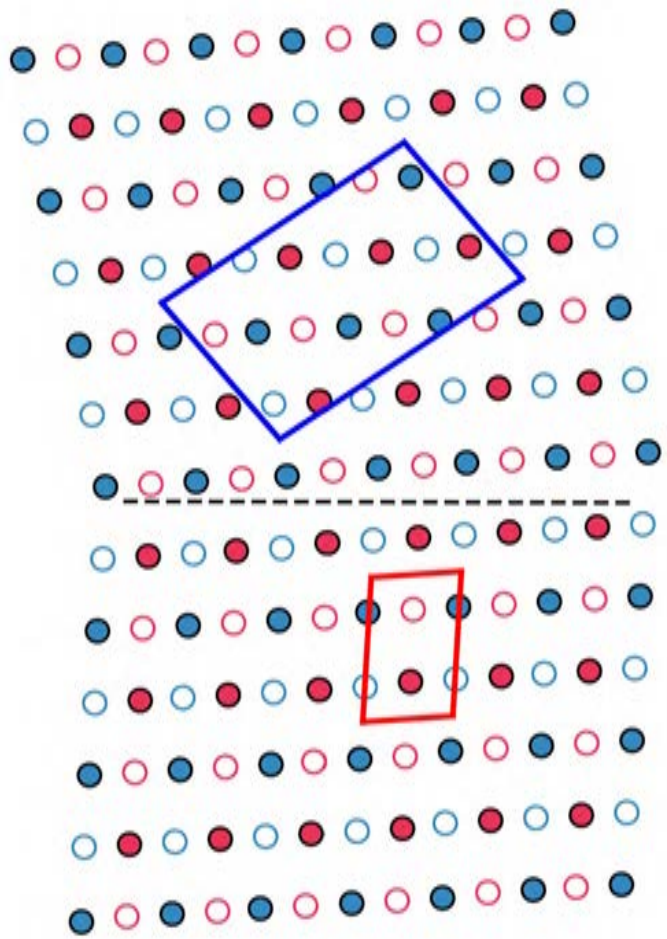
Basics – Vector and Raster File Sizes



PDF – 21 kilobytes



PNG – 187 kilobytes

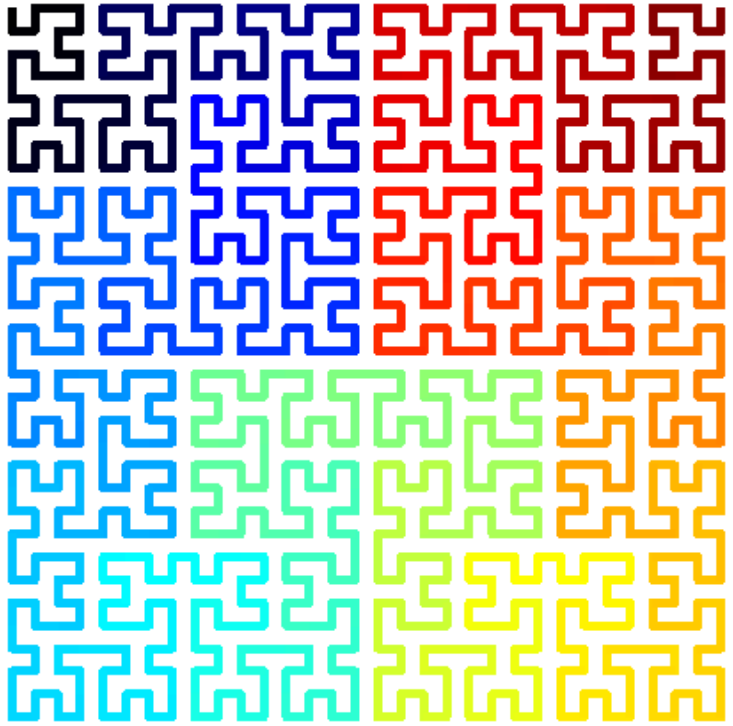


JPG – 352 kilobytes

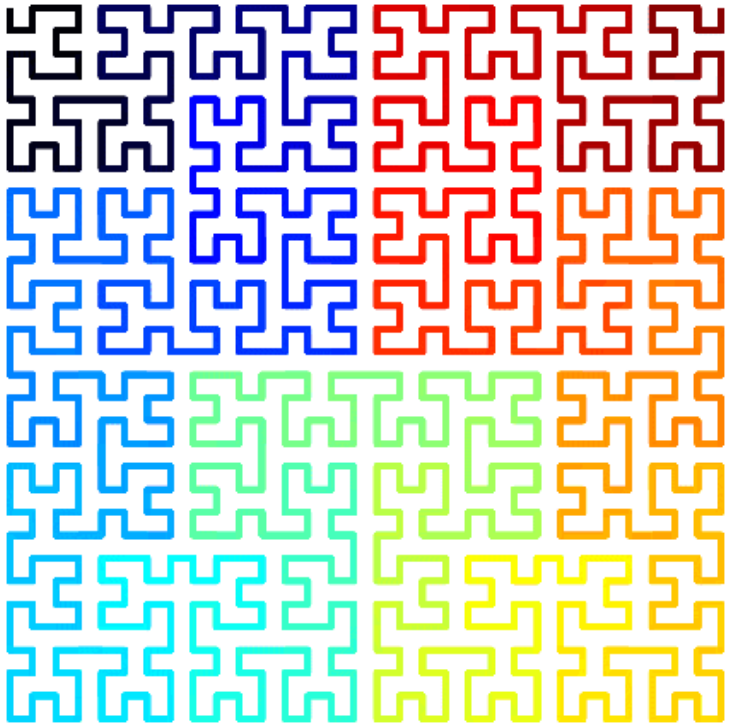
For relatively simple vector objects, PDF is the best (in general vector is also better than raster!)

X Chen et al., Physical Review Materials 4, 103611 (2020).

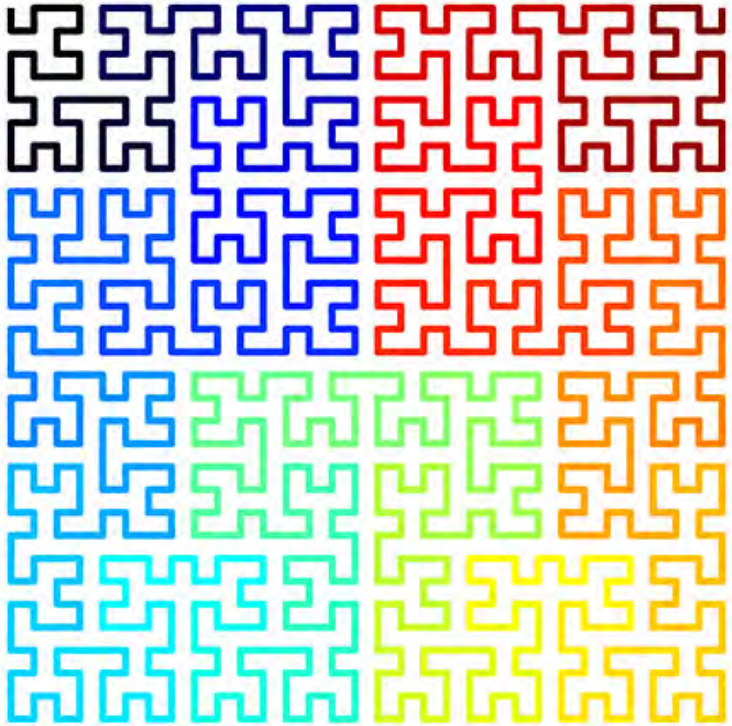
Basics – Vector and Raster File Sizes



PDF – 117 kilobytes



PNG – 15 kilobytes



JPG – 123 kilobytes

For images with few colors (<256), flat square regions, PNG compression is very good.

Hilbert patterns from – A Velazco et al., Ultrmiacroscopy 215, 113021 (2020).

Basics – Vector and Raster File Sizes

PDF – 10 851 kilobytes

PNG – 1 710 kilobytes

JPG – 576 kilobytes

If the image contains many “high energy” regions, many colors, lossy compression such as JPG is best.

C Ophus*, O Panova*, et al., Nature Materials 18, 860 (2019).

Basics – Zooming into Vector and Raster

bitmap, nearest neighbor

bitmap, bilinear

vector

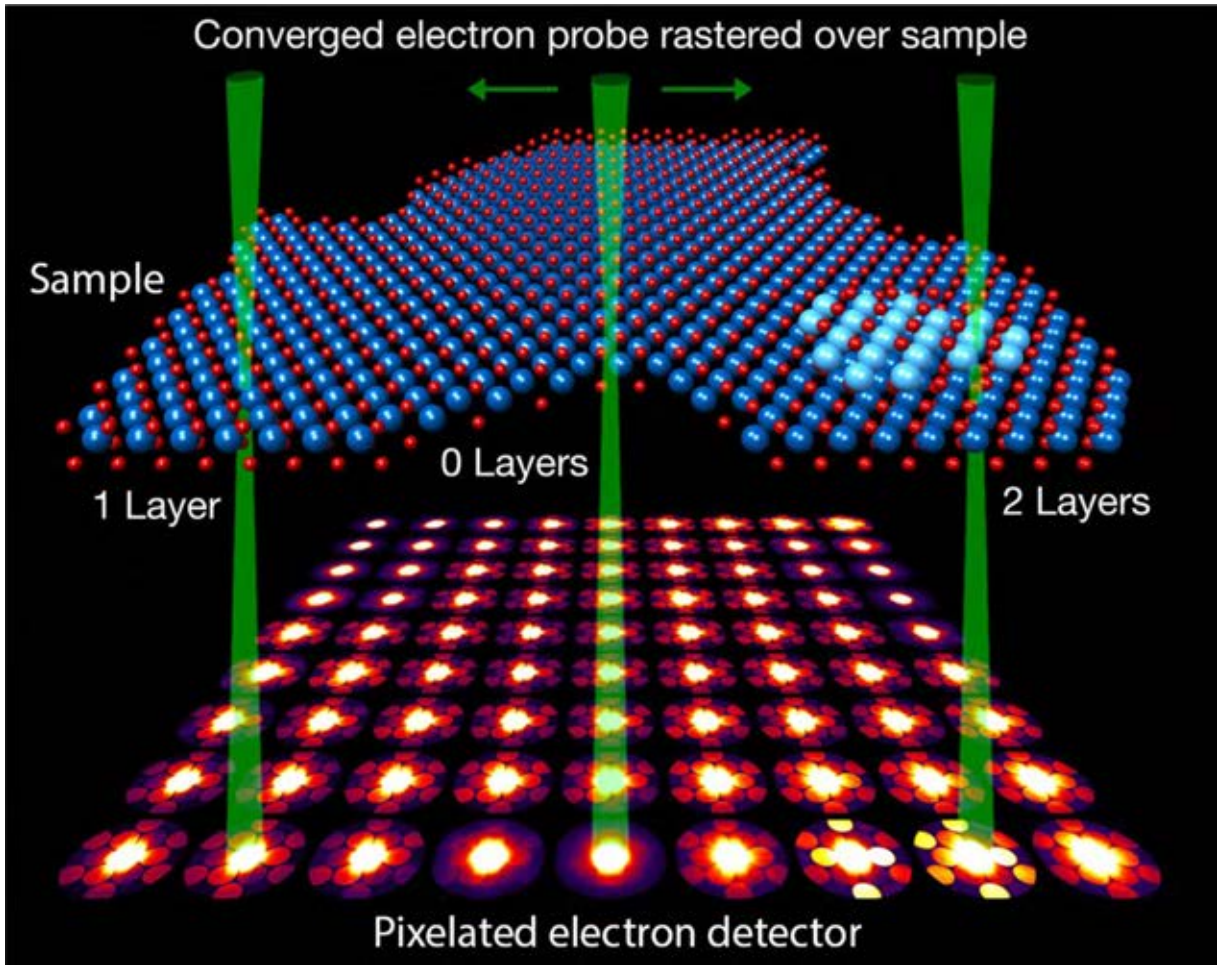
Basics – Vector and Raster Figures

Take home messages:

- Virtually every figure should be saved in **vector format** (PDF).
- **Vector** files can mix & match **images**, **text**, and **curves** such as lines & markers.
- **DO NOT** burn labels such as (a)/(b)/…, scale markers, overlays into images.
- Much easier to “remix” figures later if you cleanly **separate all objects**.
- Sometimes a PDF file size is just too large, in this case “**render**” a bitmap output.

(e.g. arXiv uploads must be <10 megs – 50 megs total)

Creating Visualization / Figures With Programming



What Language Should You Use For Figures?

Advantages

- Very large number of functions, libraries, toolboxes built in, even more on file exchange.
- Easy to use, quite fast (though not C speed)
- Very powerful 2D and 3D plotting tools.
- No compiler needed (interpreted).
- Widely used in scientific research.

- Very large number of functions and libraries included and available online.
- Easy to use, easy to extend, fast dev.
- Good plotting tools (e.g. Matplotlib).
- No compiler needed (interpreted).
- Widely used in scientific research.

Disadvantages

- Expensive license (cheap for academics).
- Poor support for GUIs, Java front end crashes.
- Slow development relative to open source.

- Slow (offset by Cython, Numba, PyTorch).
- Poor memory efficiency.
- Unreliable versioning ... e.g. Python 2 vs 3

What Language will this Tutorial Use?

Today's tutorial will use Matlab, but concepts apply just as easily to python or any language!

What Language will this Tutorial Use?

File Exchange

- export_fig – often better raster image export than built in Matlab "save."

  www.mathworks.com/matlabcentral/fileexchange

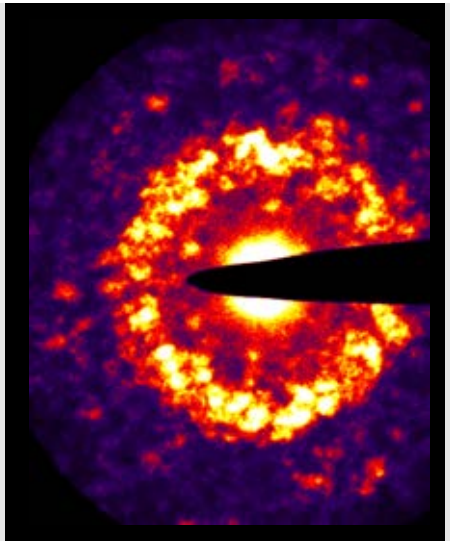
Other notes

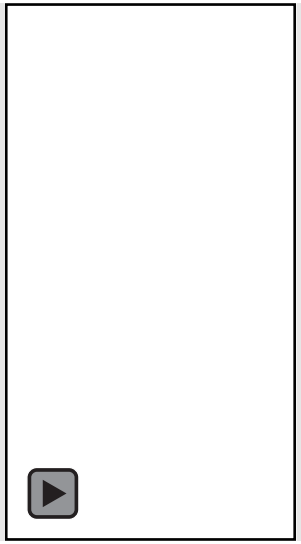
- Matlab used to have terrible PDF support – better results saving as EPS, or using export_fig. Much improved recently though! (python/matplotlib has excellent PDF support)

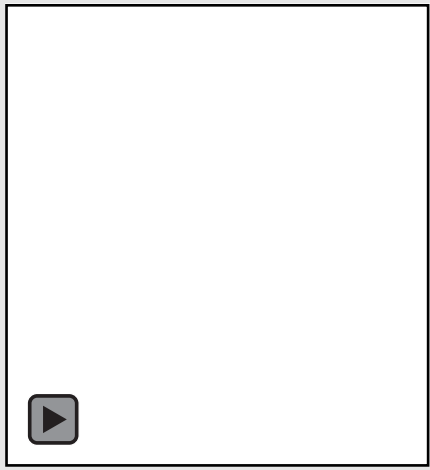
- Matlab has terrible movie support – don't even bother. Instead, export images and then use external tools to create / re-encode movies:
  - FFMPEG www.ffmpeg.org – very widespread, command line interface.
  - Handbrake handbrake.fr – Movie won't play in PPT? Easy to use, GUI.

- Always save **both the data and code** to generate plots – your future self will be grateful!

Outline







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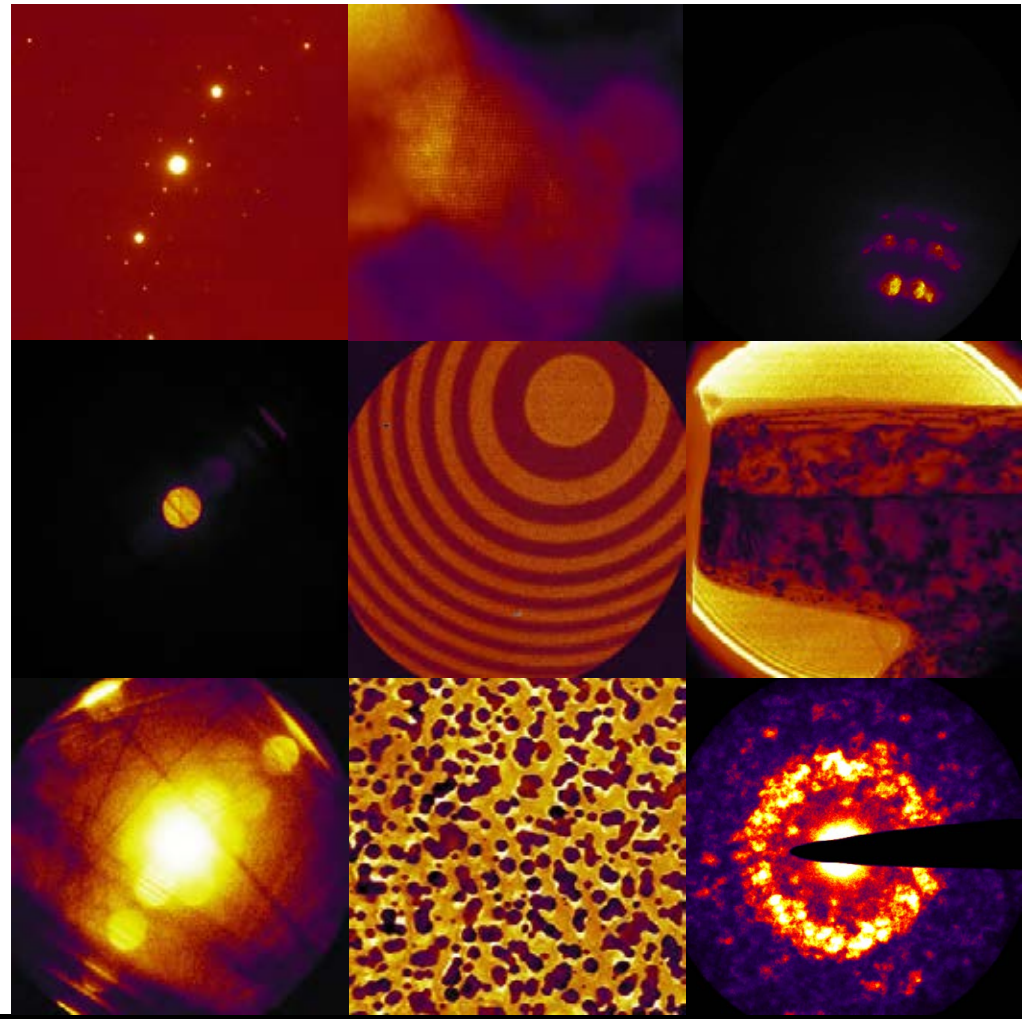
Making Image Figures from Scalar Data

Very common application – scale contrast, output imaging data in a raster file format.

Loading the data in Matlab:
>> load(**'example_02_various_images.mat'**)

Matlab has a function for saving image data:
>> imwrite(**imageArray** , **fileName**);

Let’s try it out on the sample images.

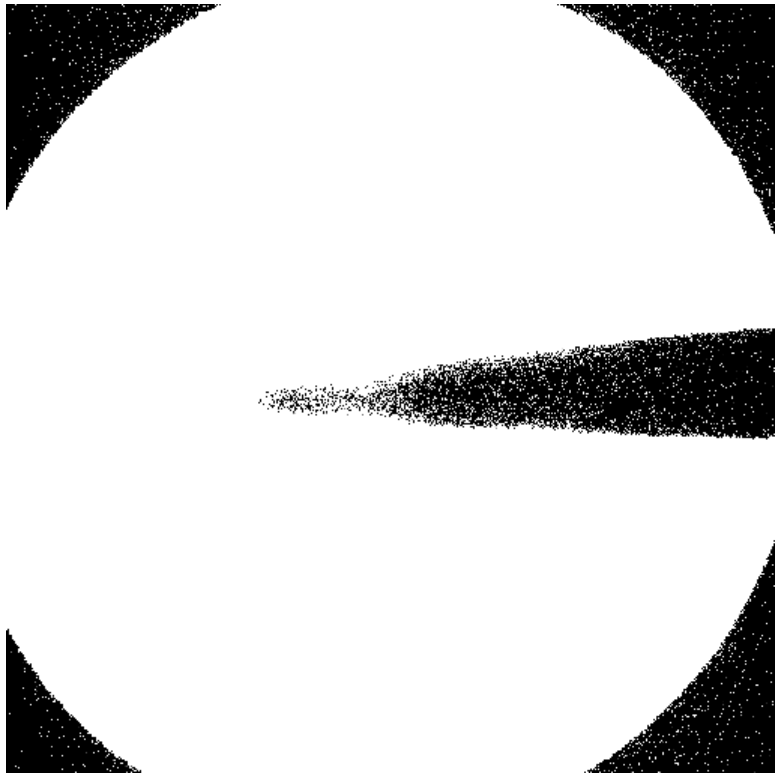


Making Image Figures from Scalar Data

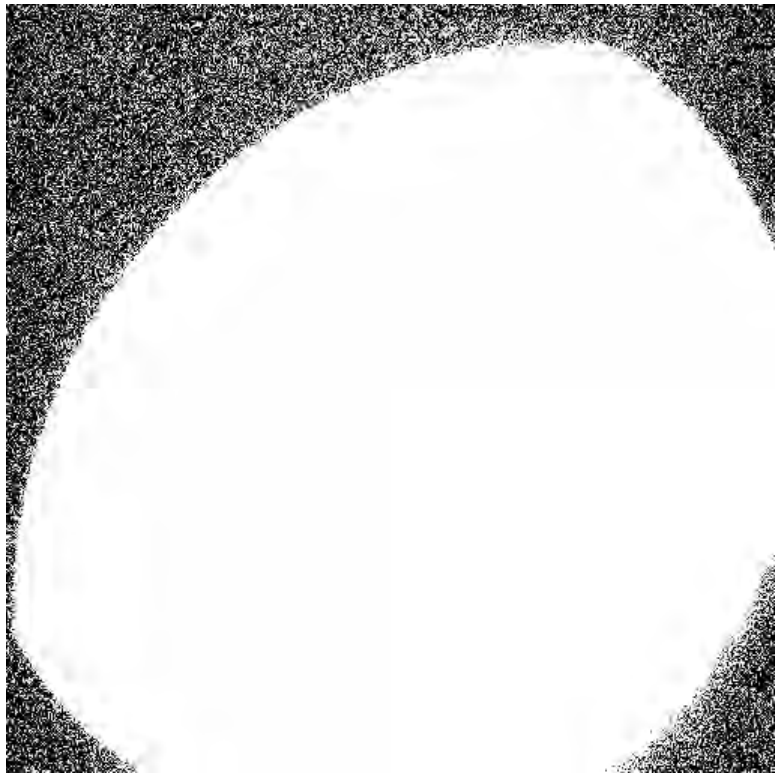
Very common application – scale contrast, output imaging data in a raster file format:

```
>> imwrite(image01_UO2_01,'image01.png');
Error using writepng>parseInputs (line 290)
Expected input to be one of these types:

double, single, logical, uint8, uint16

Instead its type was uint32.
Error in writepng (line 20)
[results, unmatched] = parseInputs(data,map
Error in imwrite (line 472)
        feval(fmt_s.write, data, map, filen
```

imwrite(image01_UO2_01,'image01.png');



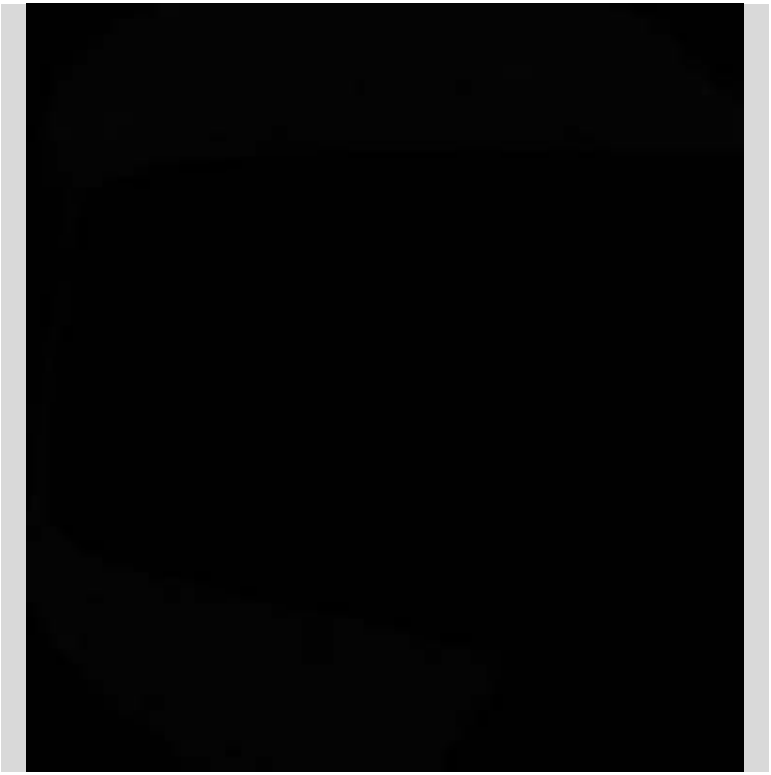
imwrite(image02_amor_diff,'image02.png');



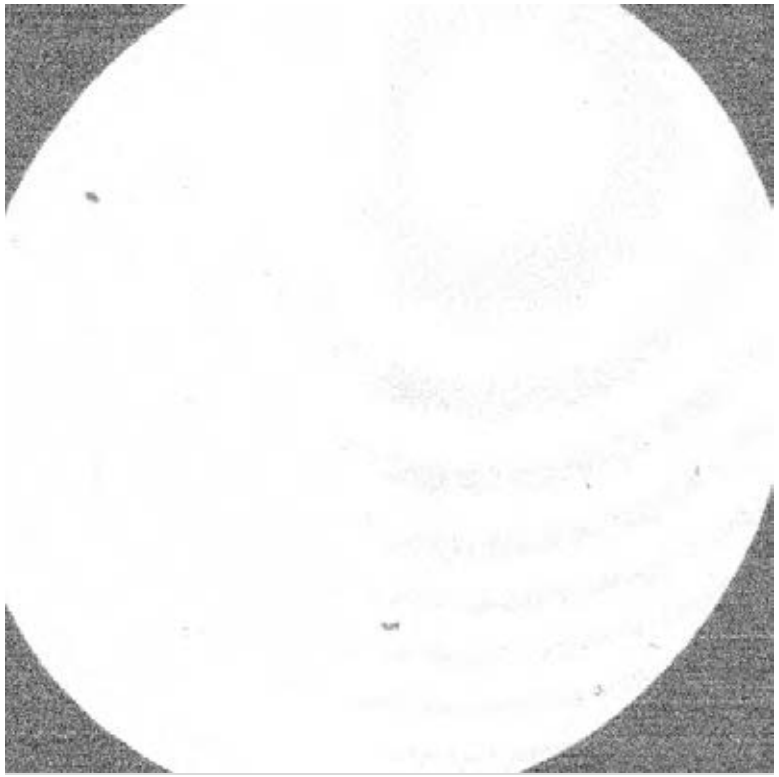
imwrite(image03_diff,'image03.png');

Making Image Figures from Scalar Data

Very common application – scale contrast, output imaging data in a raster file format:



imwrite(image04_pillar,'image04.png');



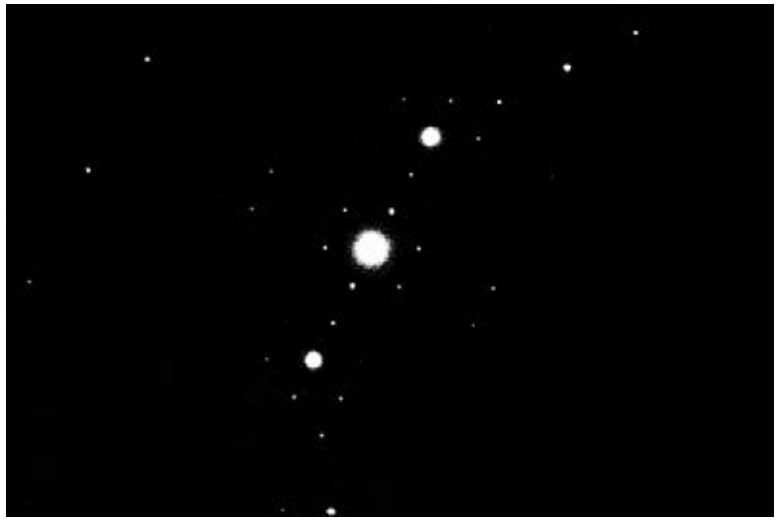
imwrite(image05_rings01,'image05.png');

```
>> imwrite(image06_gold,'image06.png');
Warning: Data loss and unexpected result
> In imwrite (line 447)
Error using writepng>parseInputs (line
Expected input to be one of these types

double, single, logical, uint8, uint16

Instead its type was int32.
Error in writepng (line 20)
[results, unmatched] = parseInputs(data,
Error in imwrite (line 472)
        feval(fmt_s.write, data, map, f
```

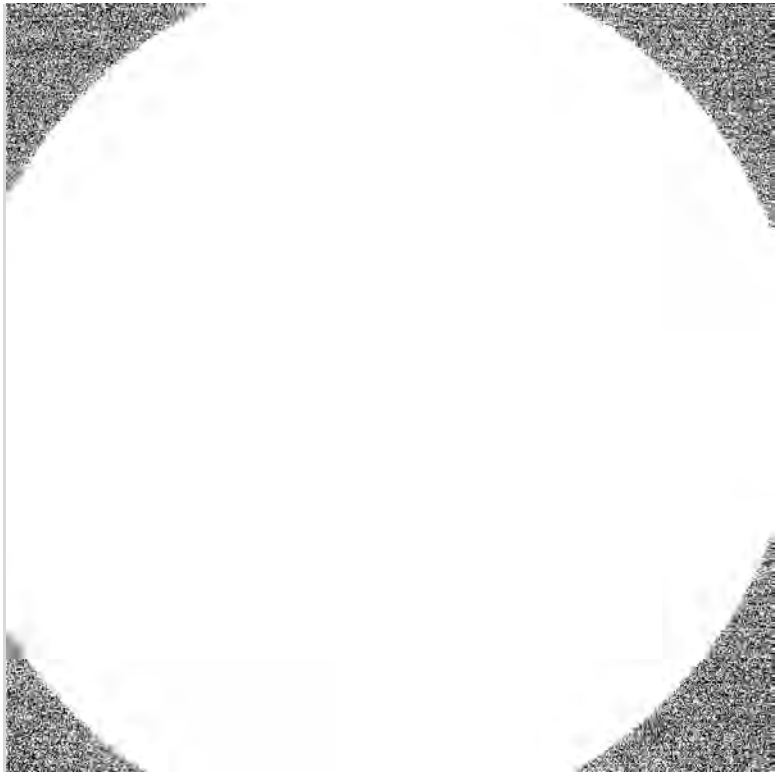
imwrite(image06_gold,'image06.png');

Making Image Figures from Scalar Data

Very common application – scale contrast, output imaging data in a raster file format:



imwrite(image07_diff01,'image07.png');



imwrite(image08_CBED01,'image08.png');

imwrite(image09_Pt,'image09.png');

Making Image Figures from Scalar Data

Convert to floating point, scale intensity from minimum to maximum value:

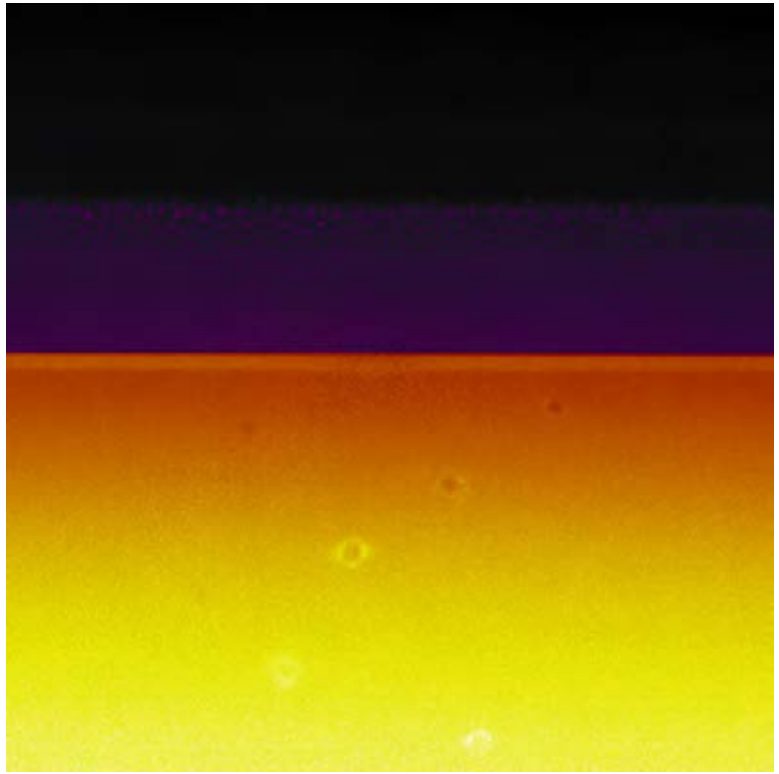

```
function [ ] = plotImageFullRange( imageInput, fileNameBase )

% convert to double floating point
imageInput = double( imageInput );

% scale image from 0 to 1
imageInput(:) = imageInput - min( imageInput(:) );
imageInput(:) = imageInput / max ( imageInput(:) );

% output file
fileName = [ fileNameBase '.png' ];
imwrite( round(imageInput*255)+1 , inferno , filename );
```

scale image intensity to be from 1 to 256

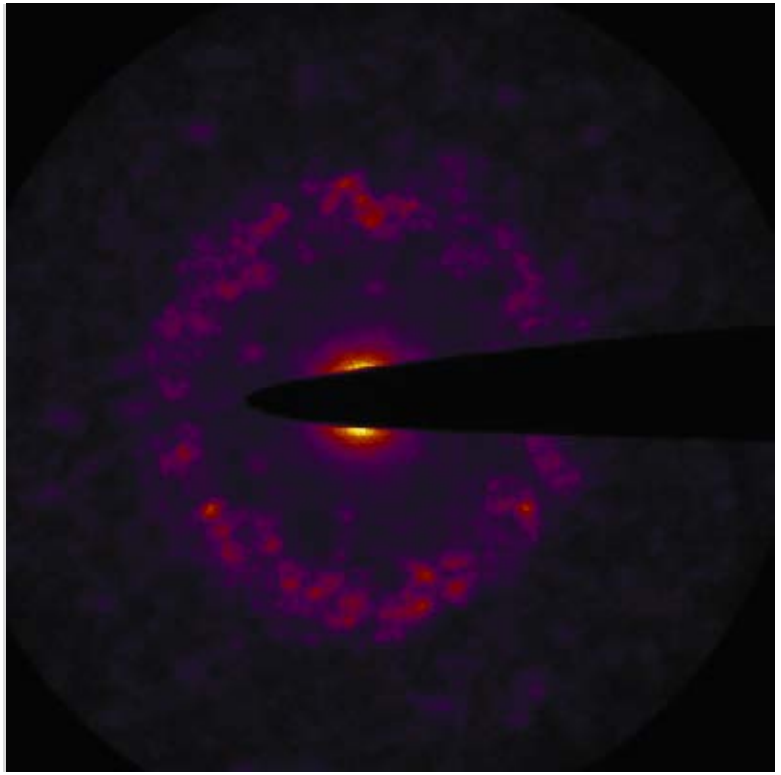
colormap: min value (1) max value (256)

Making Image Figures from Scalar Data

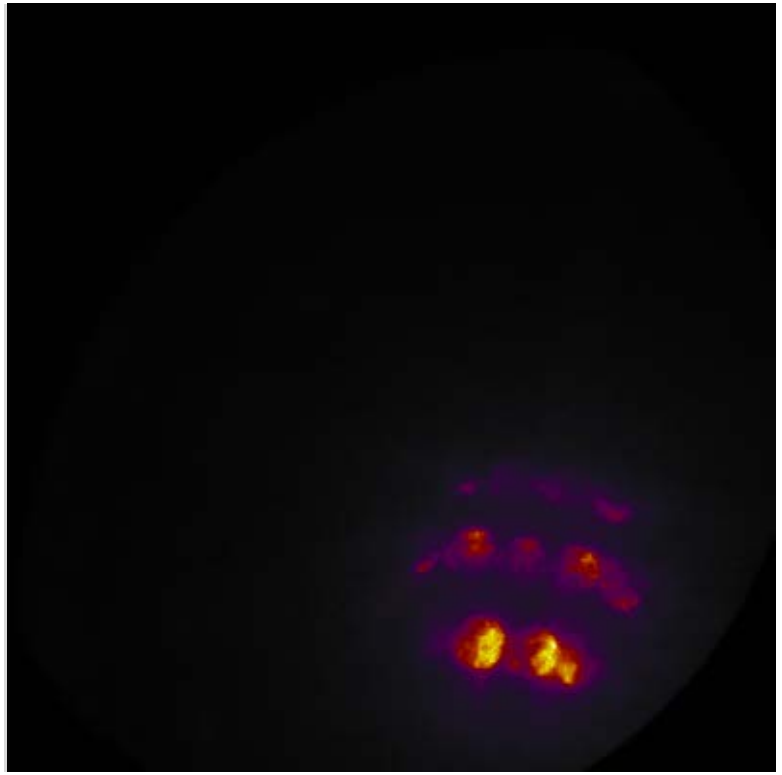
Convert to floating point, scale intensity from minimum to maximum value:



plotImageFullRange(image01_UO2_01,'image01');



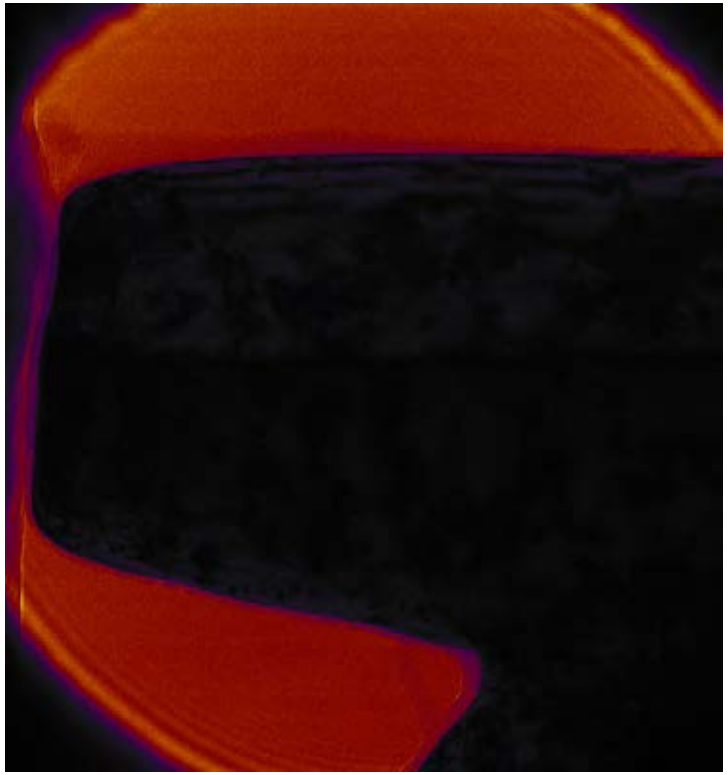
plotImageFullRange(image02_amor_diff,'image02');



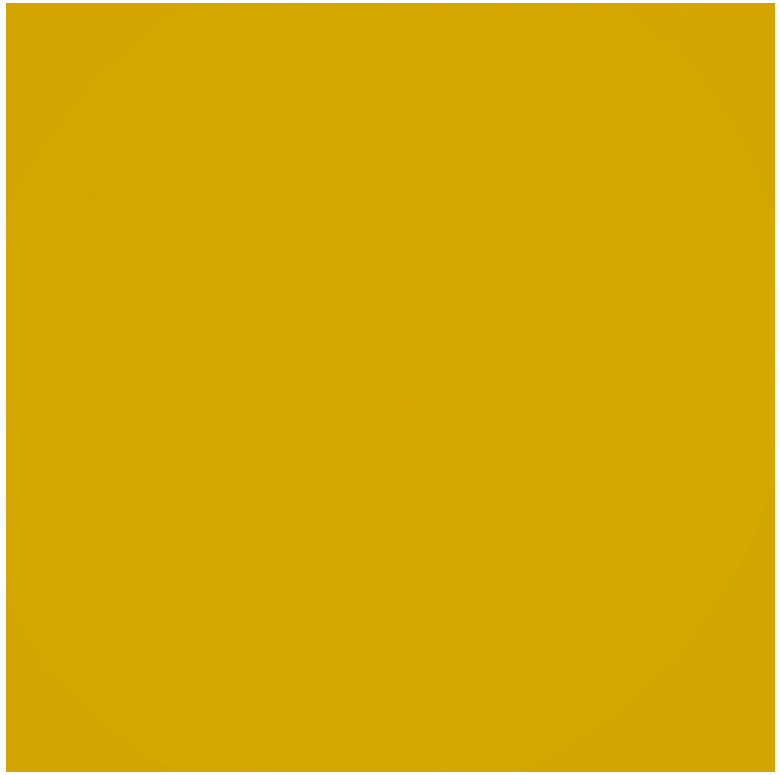
plotImageFullRange(image03_diff,'image03');

Making Image Figures from Scalar Data

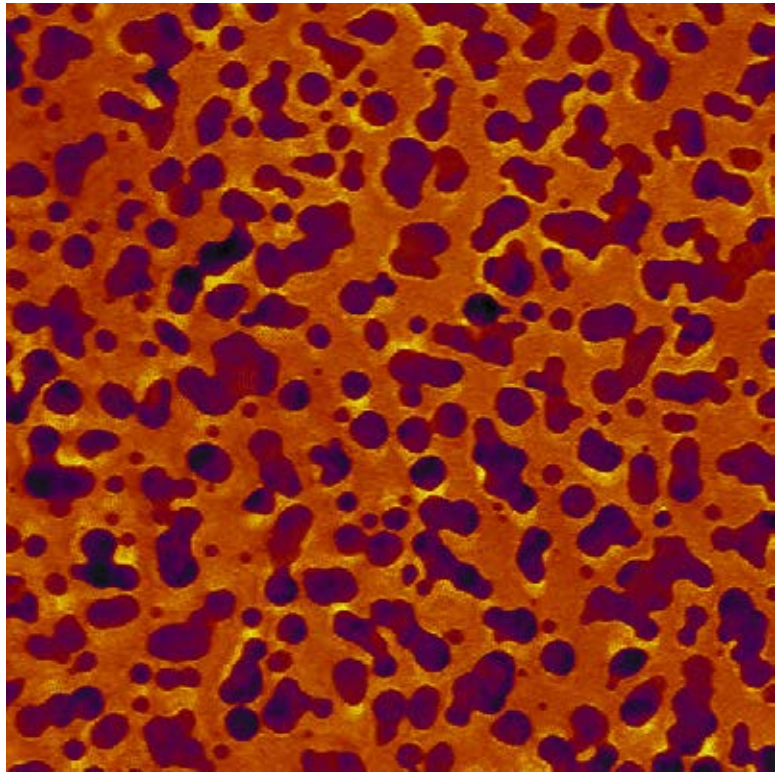
Convert to floating point, scale intensity from minimum to maximum value:



plotImageFullRange(image04_pillar,'image04');



plotImageFullRange(image05_rings01,'image05');



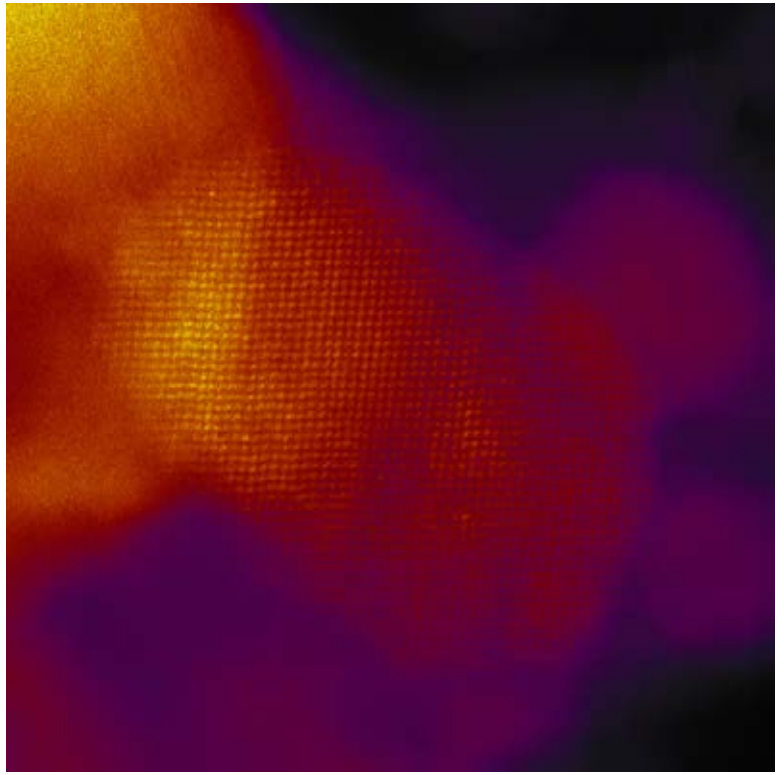
plotImageFullRange(image06_gold,'image06');

Making Image Figures from Scalar Data

Convert to floating point, scale intensity from minimum to maximum value:

plotImageFullRange(image07_diff01,'image07');

plotImageFullRange(image08_CBED01,'image08');



plotImageFullRange(image09_Pt,'image09');

Making Image Figures from Scalar Data

Scale intensity automatically, using statistics:

Mean and std. dev. work for most images

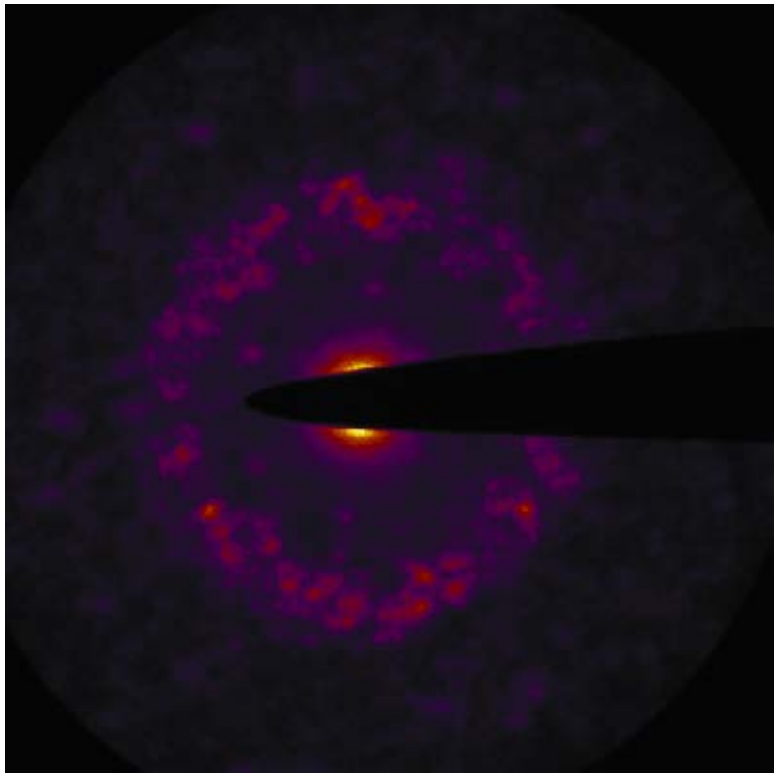
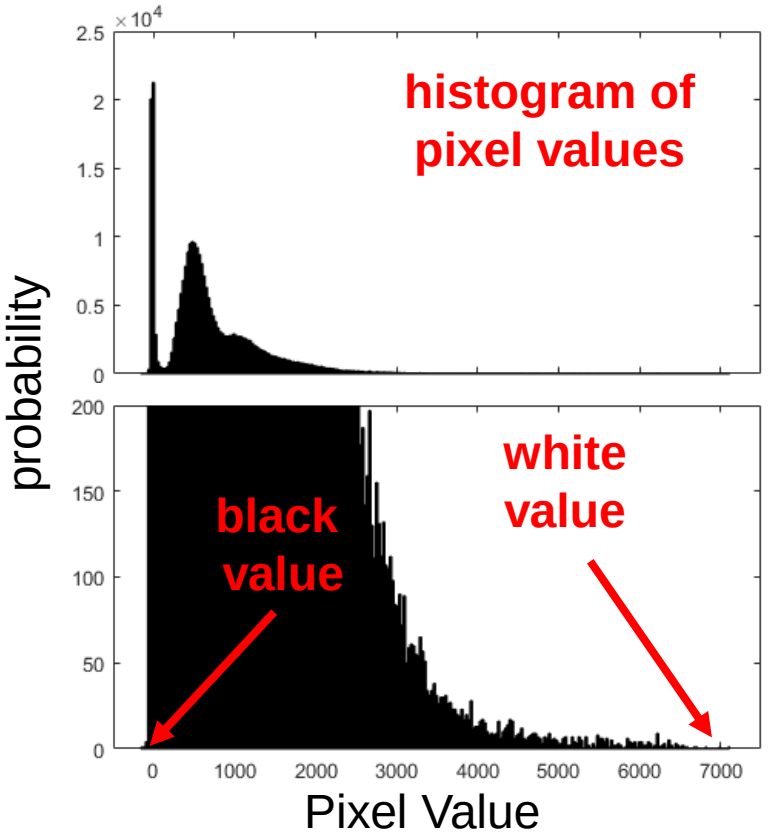
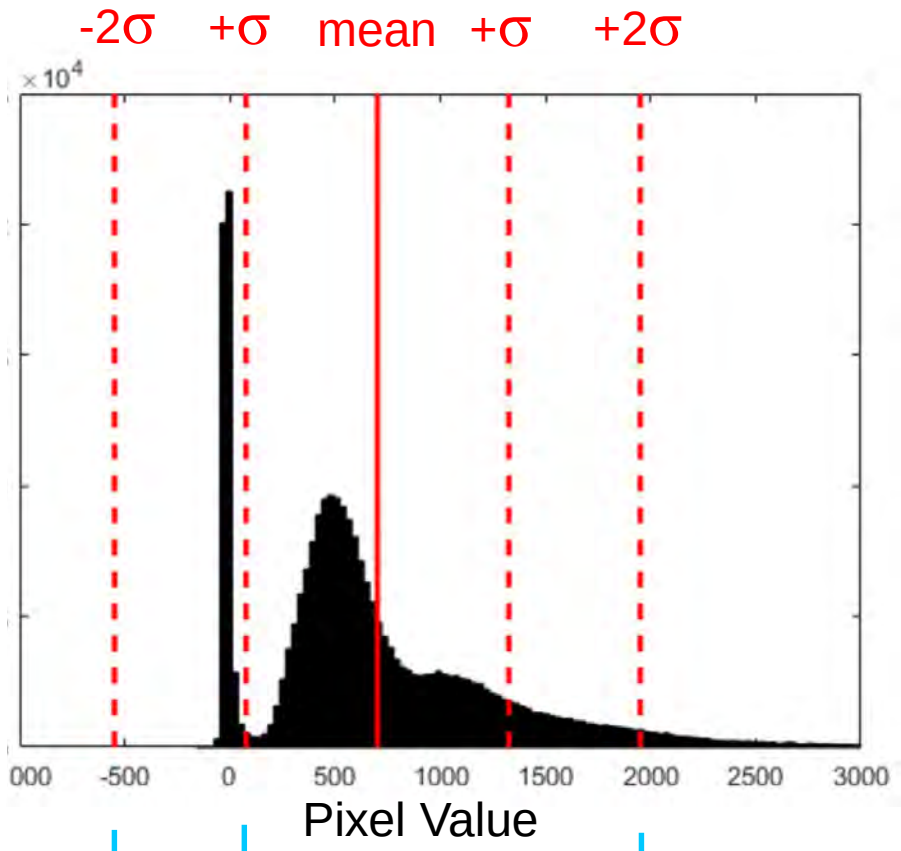


image02_amor_diff

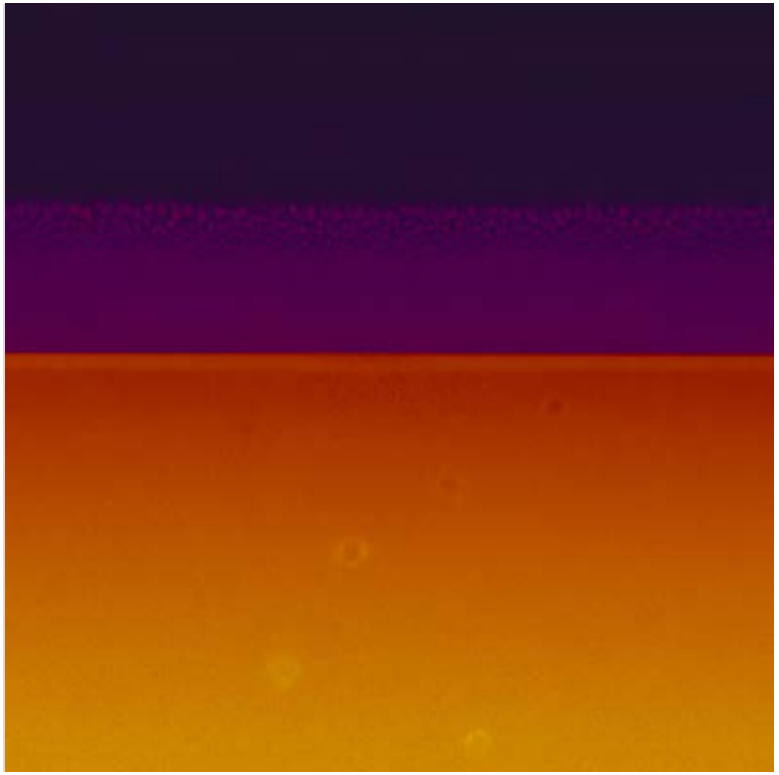




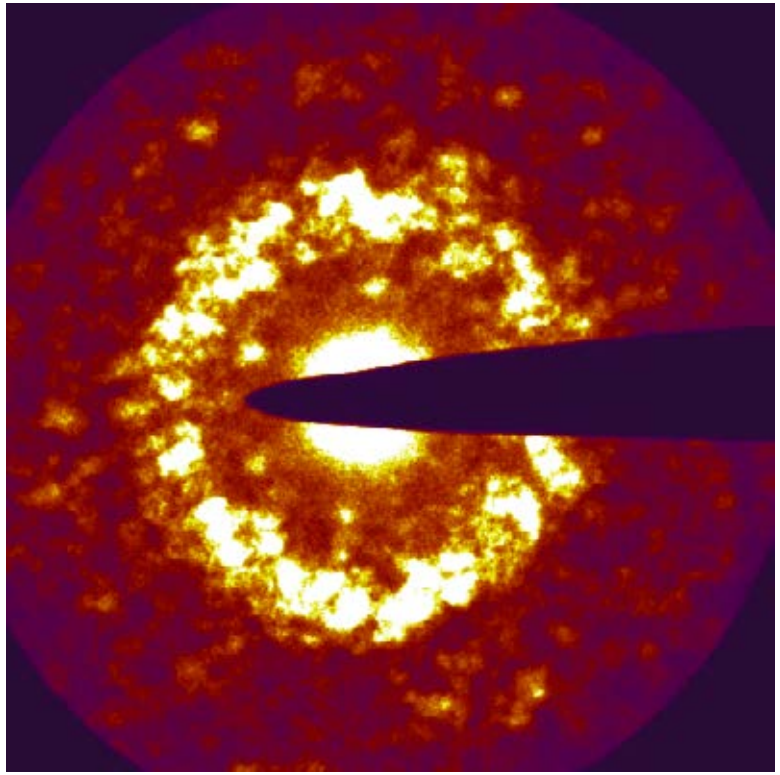
Colormap – this is a mapping from pixel values to RGB triplet

Making Image Figures from Scalar Data

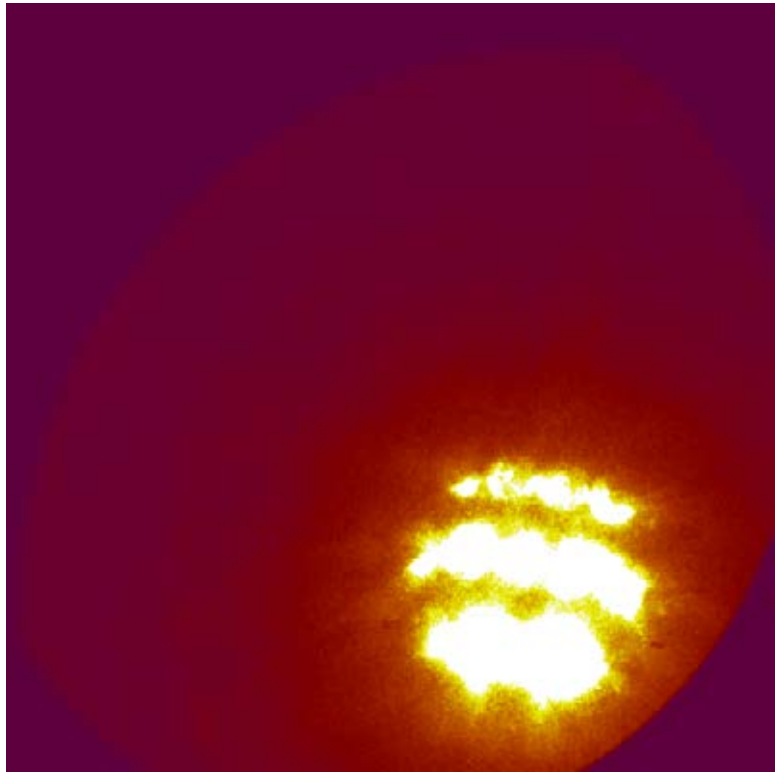
Scale intensity automatically from -2 to +2 standard deviations of intensity:



imwrite(image01_UO2_01,'image01.png');



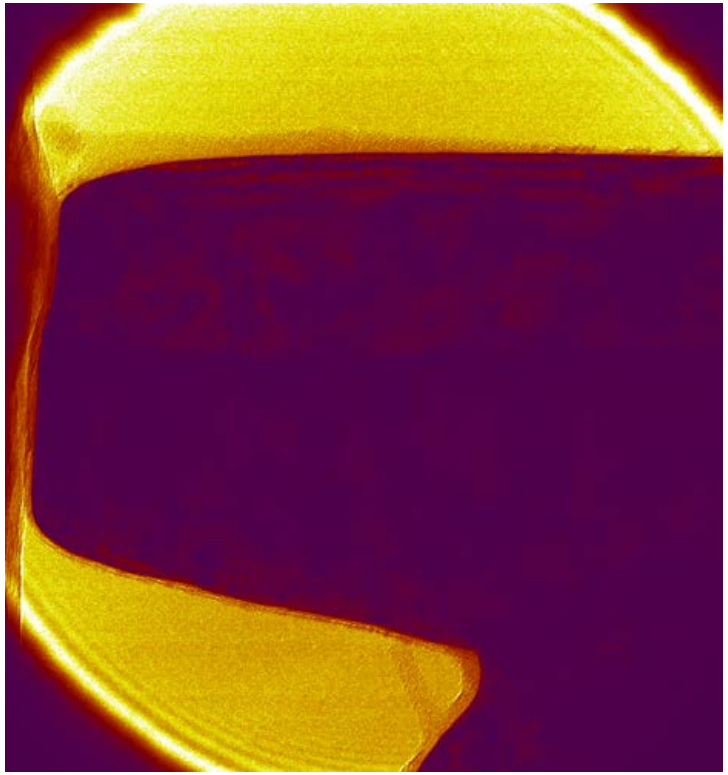
imwrite(image02_amor_diff,'image02.png');



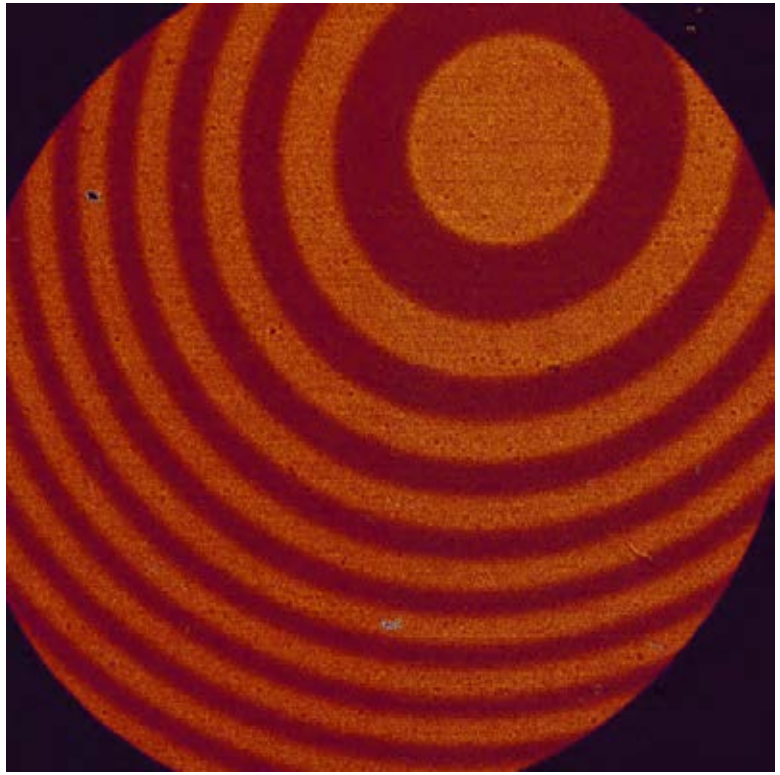
imwrite(image03_diff,'image03.png');

Making Image Figures from Scalar Data

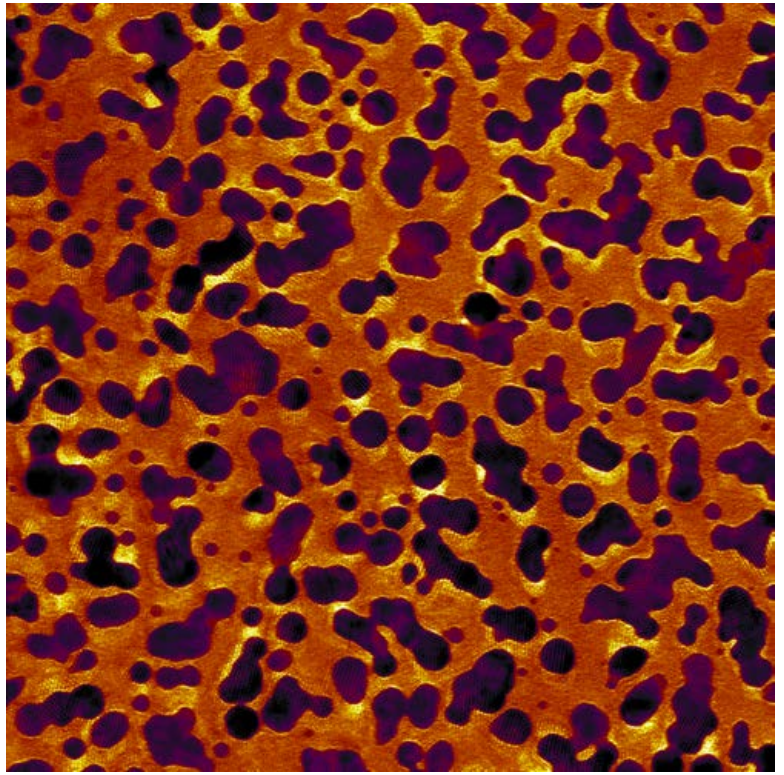
Scale intensity automatically from -2 to +2 standard deviations of intensity:



imwrite(image01_UO2_01,'image01.png');



imwrite(image02_amor_diff,'image02.png');

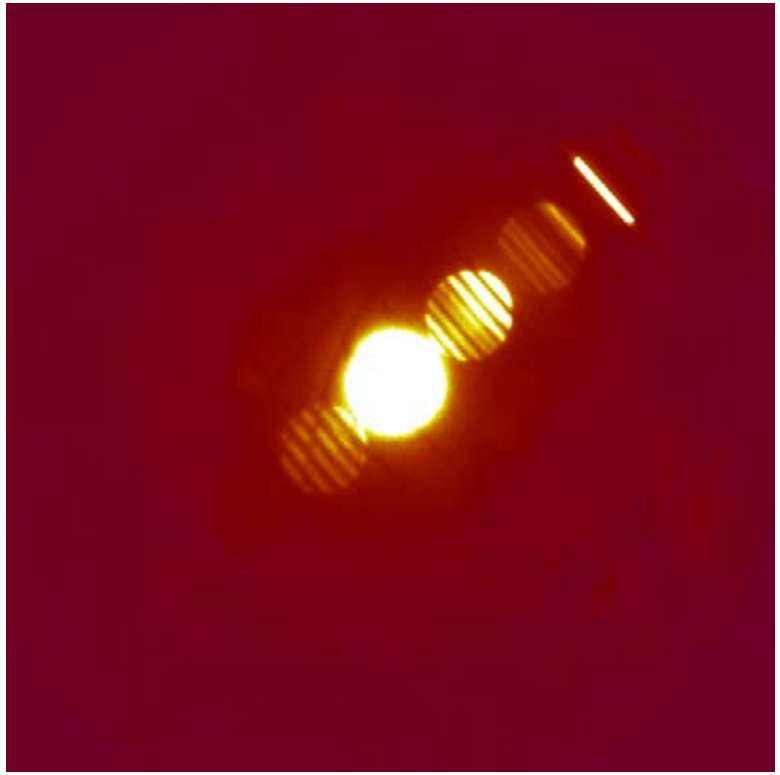


imwrite(image03_diff,'image03.png');

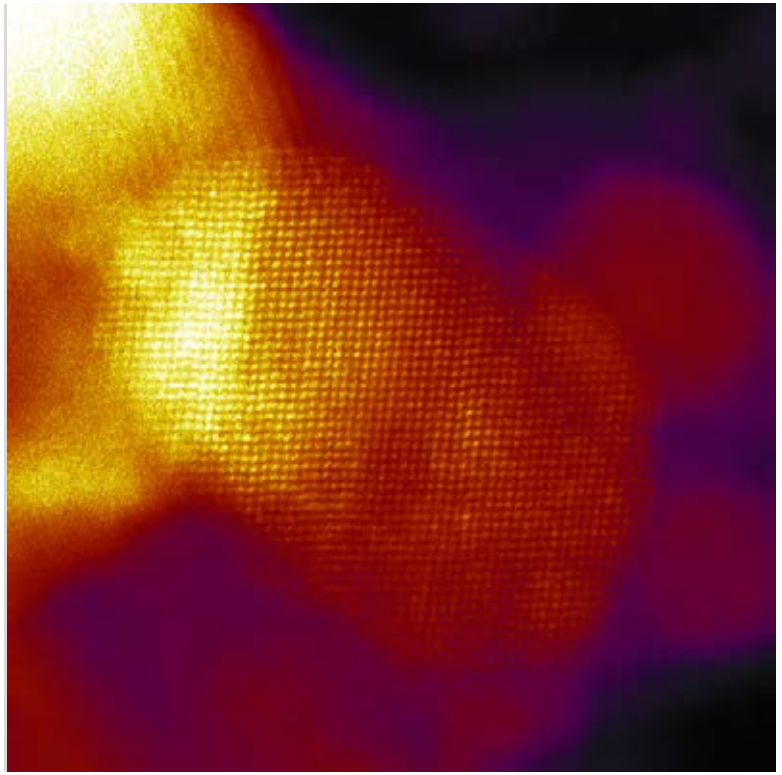
Making Image Figures from Scalar Data

Scale intensity automatically from -2 to +2 standard deviations of intensity:

imwrite(image01_UO2_01,'image01.png');



imwrite(image02_amor_diff,'image02.png');



imwrite(image03_diff,'image03.png');

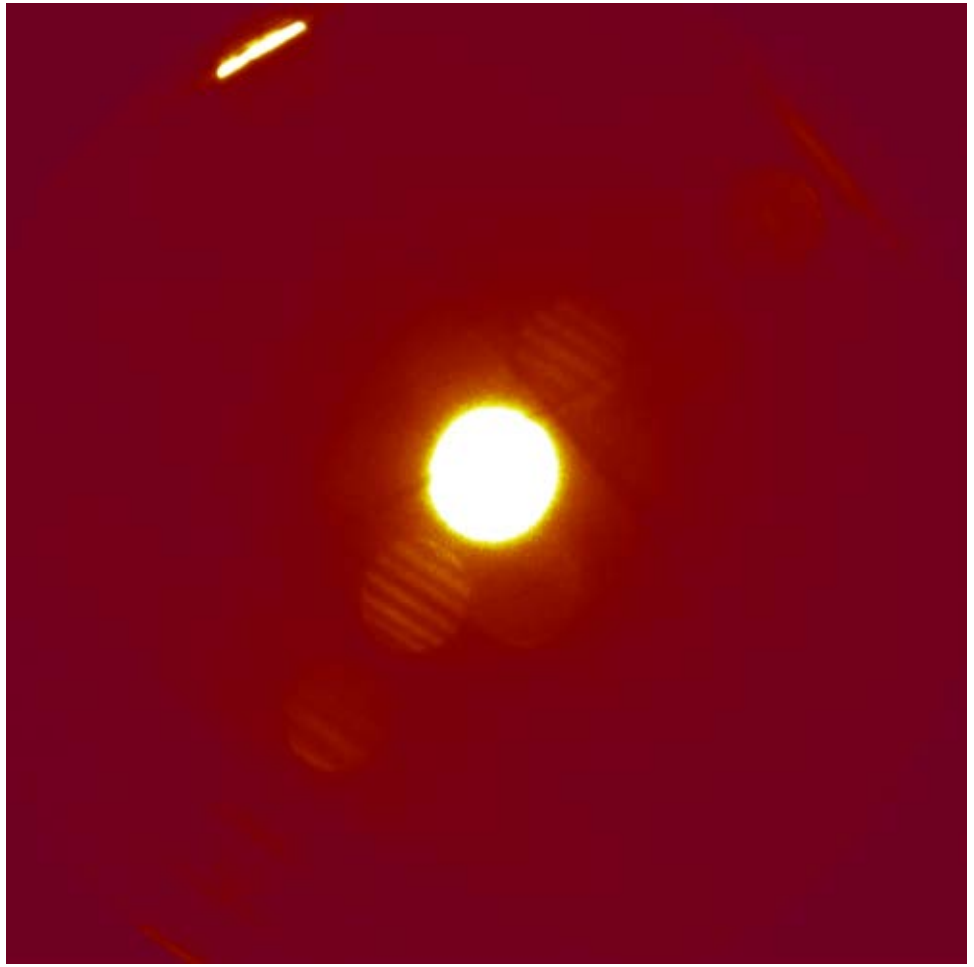
Making Image Figures from Scalar Data

The rest of the examples have been put into a single general purpose script:

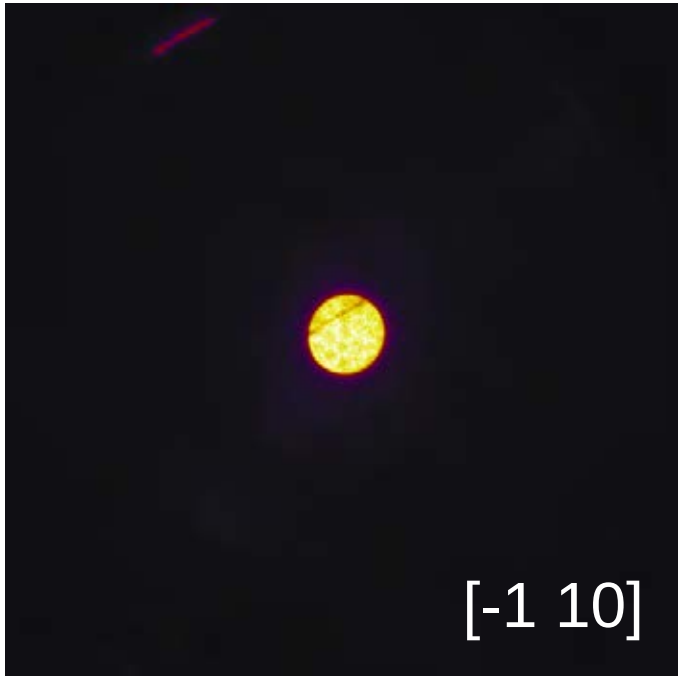
plotImage(…)

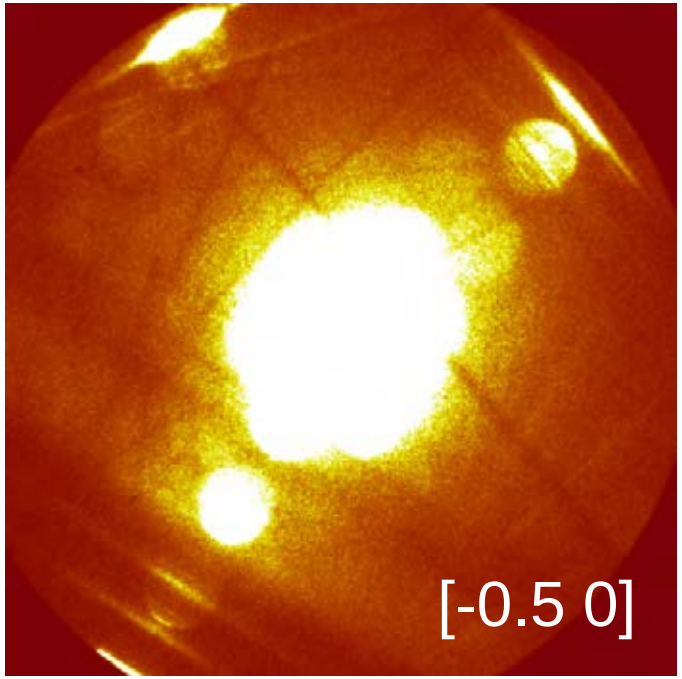
Making Image Figures from Scalar Data

Many other automatic scaling schemes are possible, for example:



plotImage(image08_CBED03,'image08');



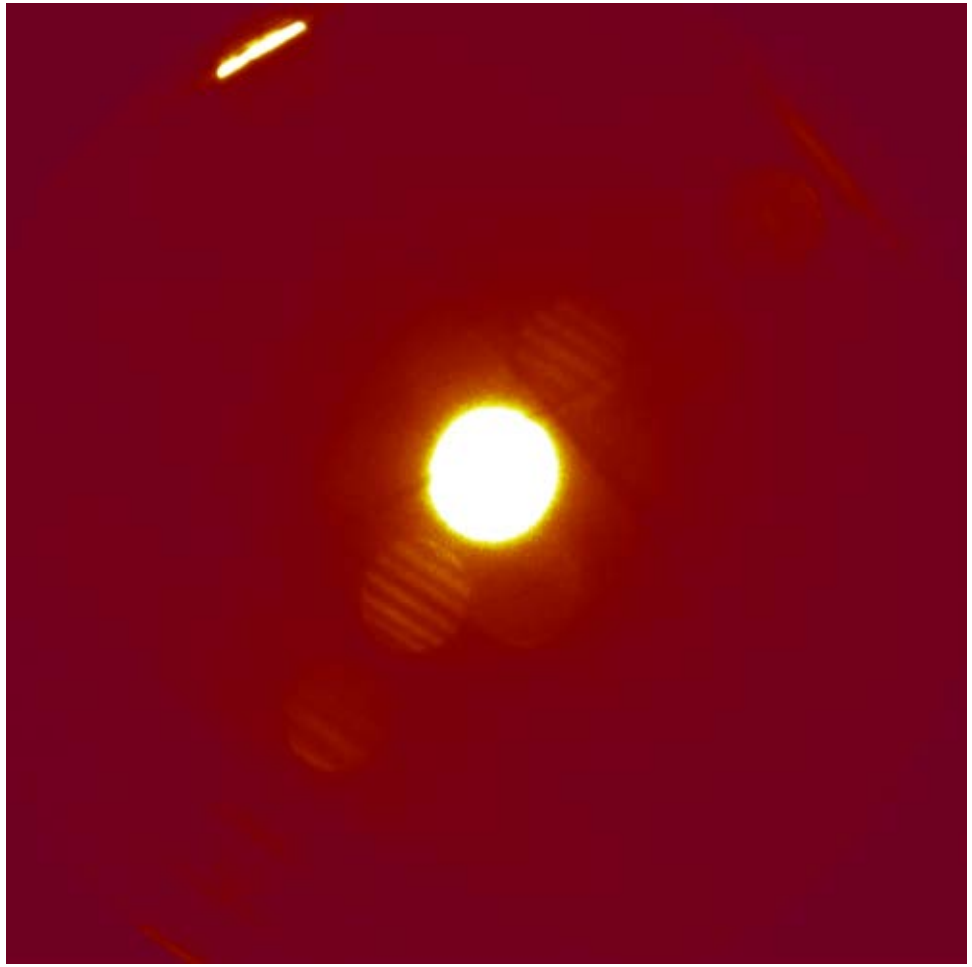


plotImage(image08_CBED03,'image08‘, [minVal maxVal]);

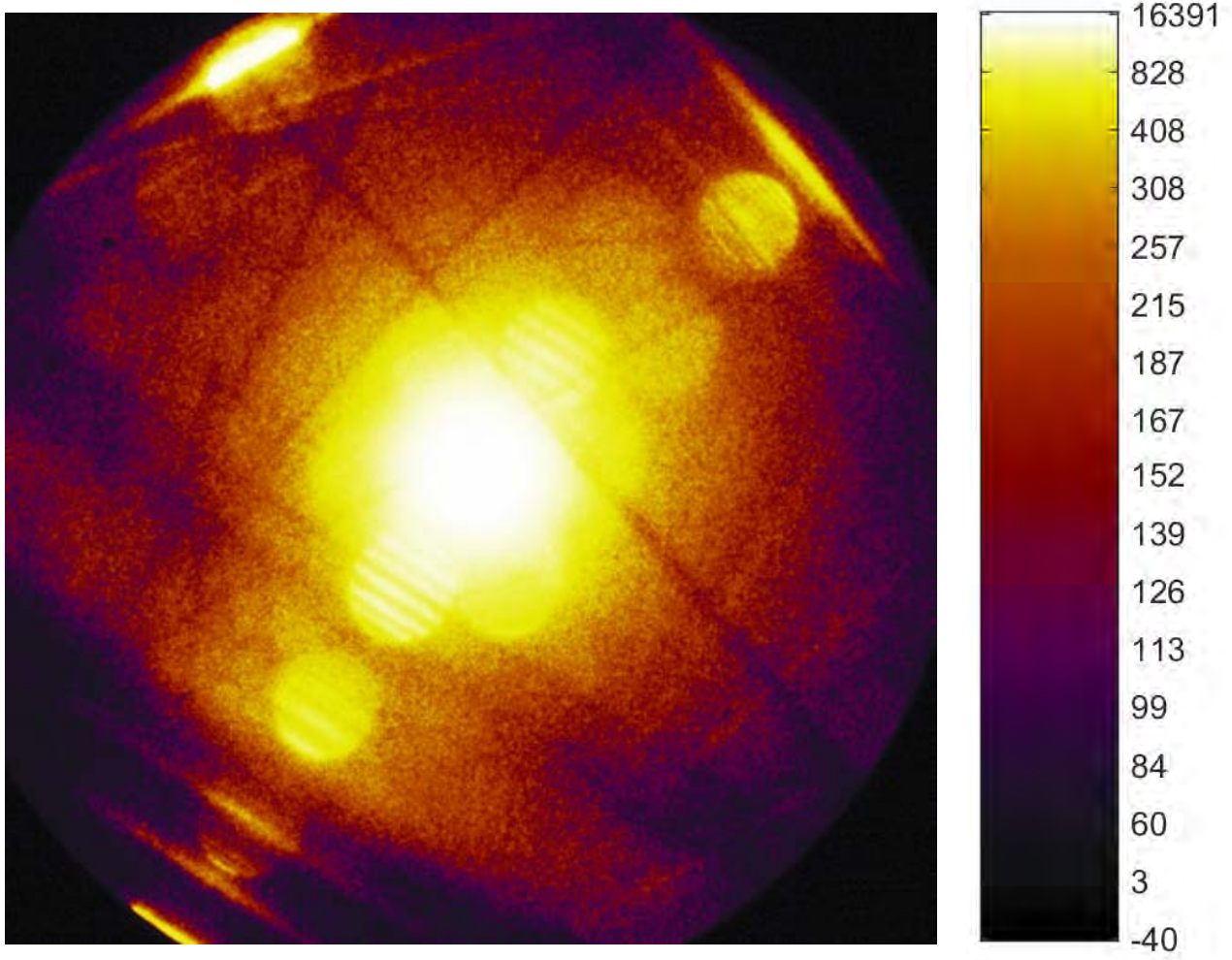
Is it impossible to linearly visualize all image regions?

Making Image Figures from Scalar Data

Many other automatic scaling schemes are possible, for example:



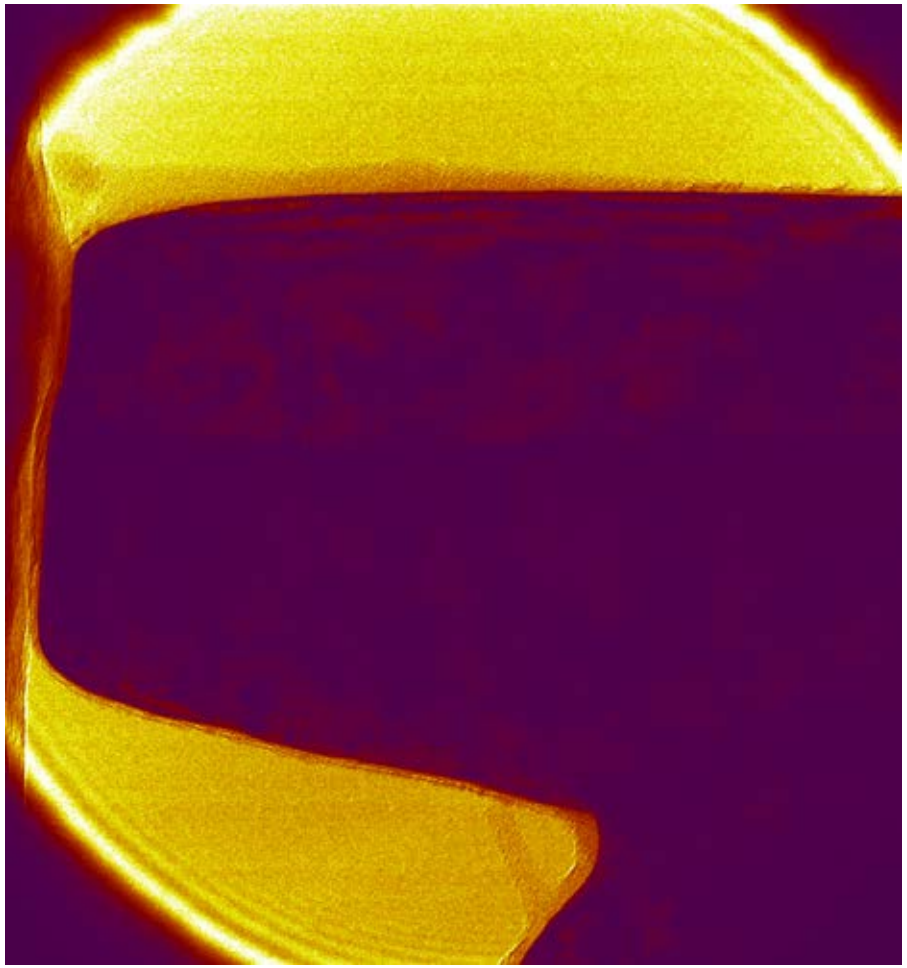
plotImage(image08_CBED03,'image08');



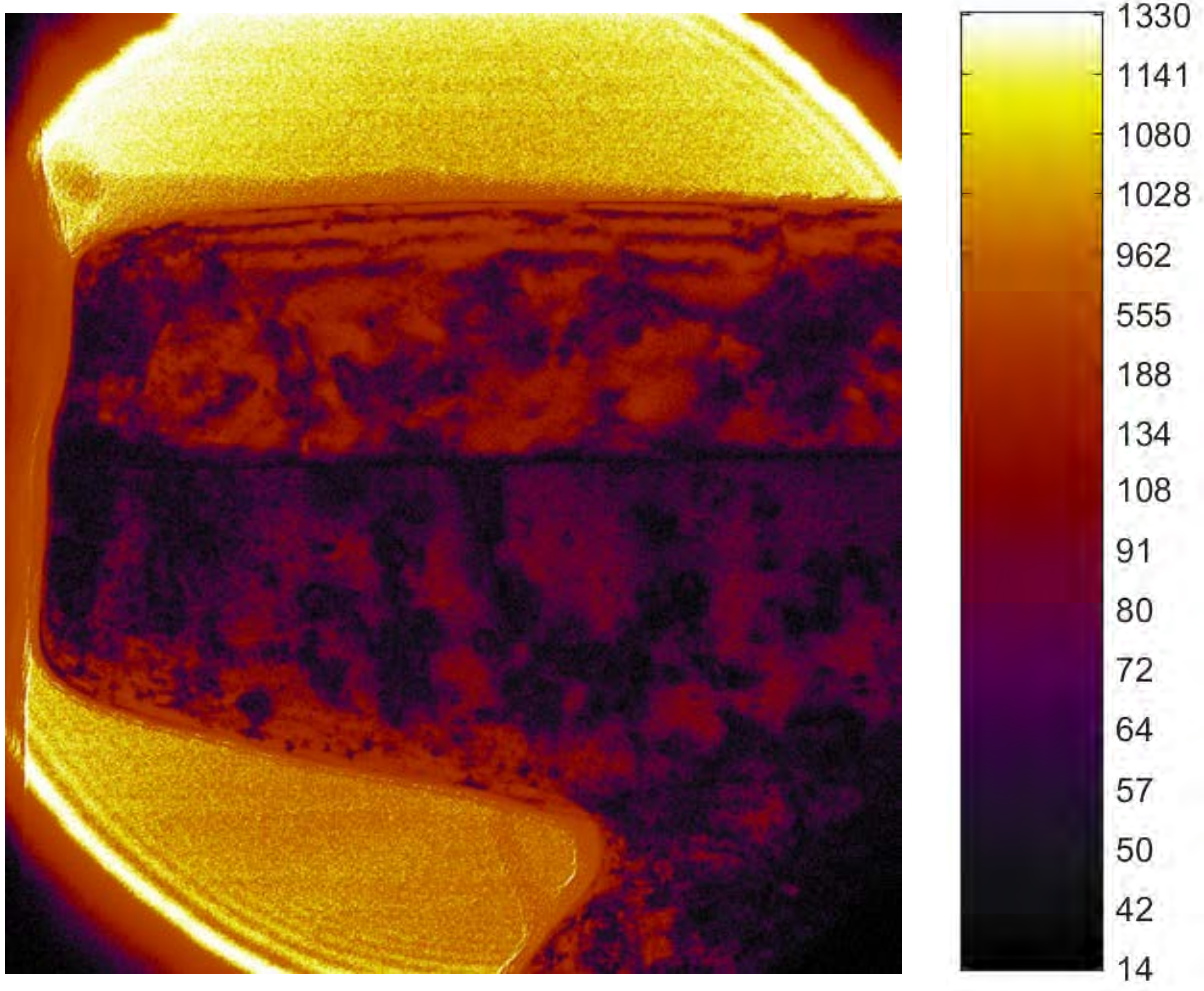
plotImage(image08_CBED03,'image08‘,’ordered’);

Making Image Figures from Scalar Data

Many other automatic scaling schemes are possible, for example:



plotImage(image04_pillar, 'image04');



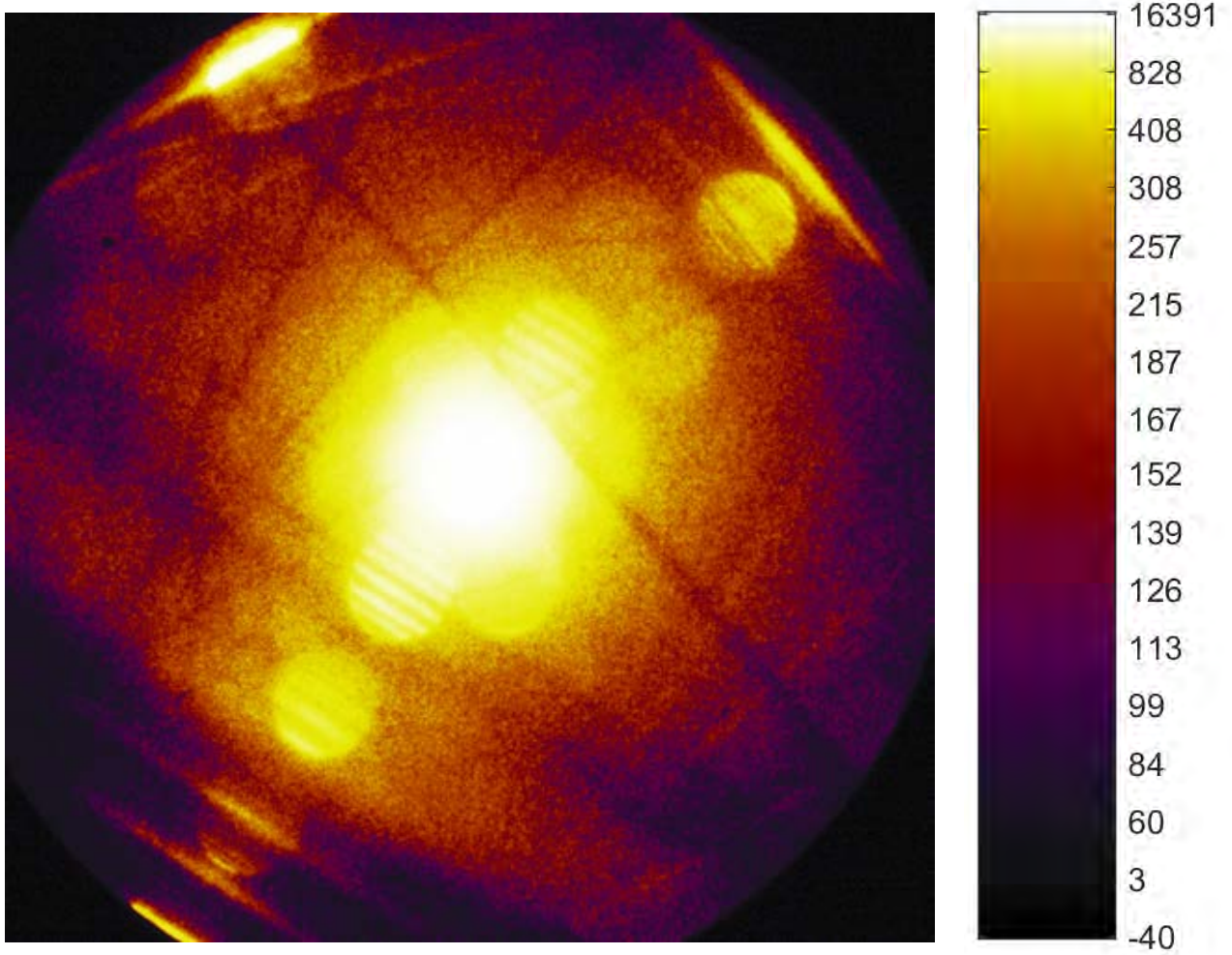
plotImage(image04_pillar, 'image04‘,’ordered’);

Making Image Figures from Scalar Data

Many other automatic scaling schemes are possible, for example:

Ordered Method

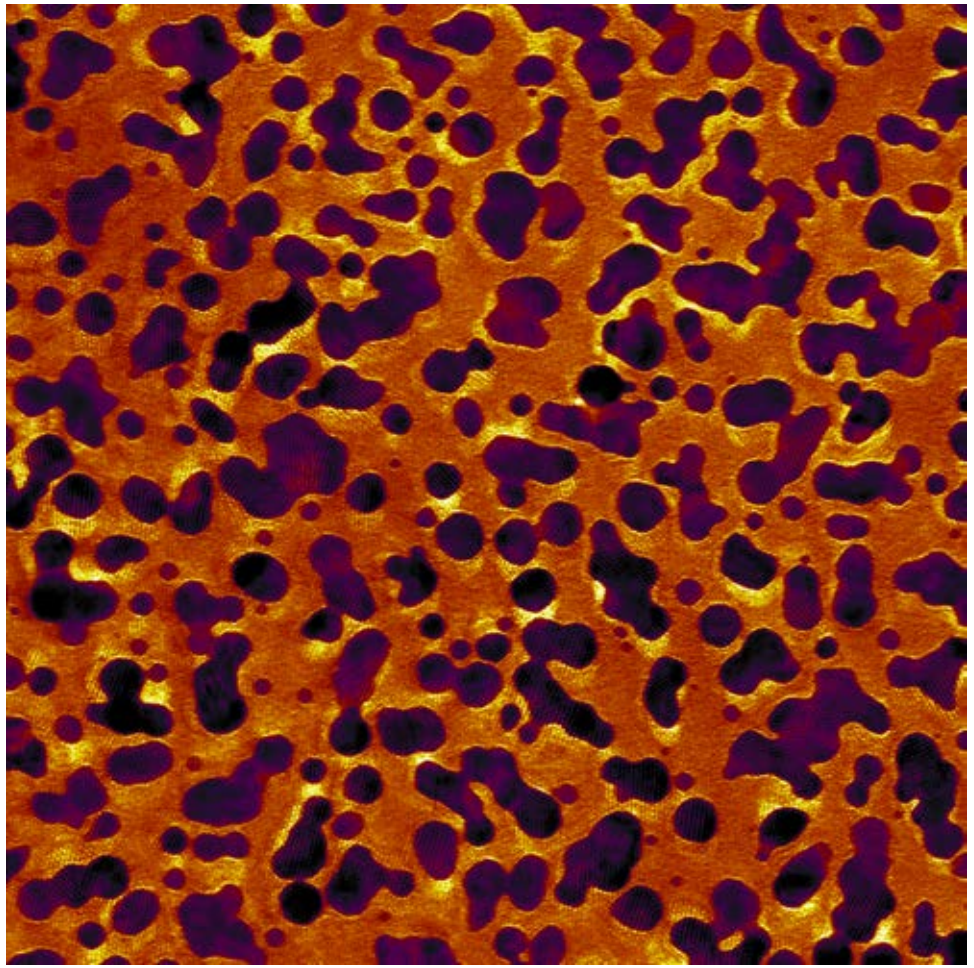
- All pixels of image are sorted from lowest to highest values.
- For a colormap with 100 colors specified, we assign falling in the range 0.00-0.01 to the first color, from 0.01-0.02 to the second color and so on.
- Note that this means the color legend will in general NOT be linear, logarithmic, or any simple relationship.



plotImage(image08_CBED03,'image08‘,’ordered’);

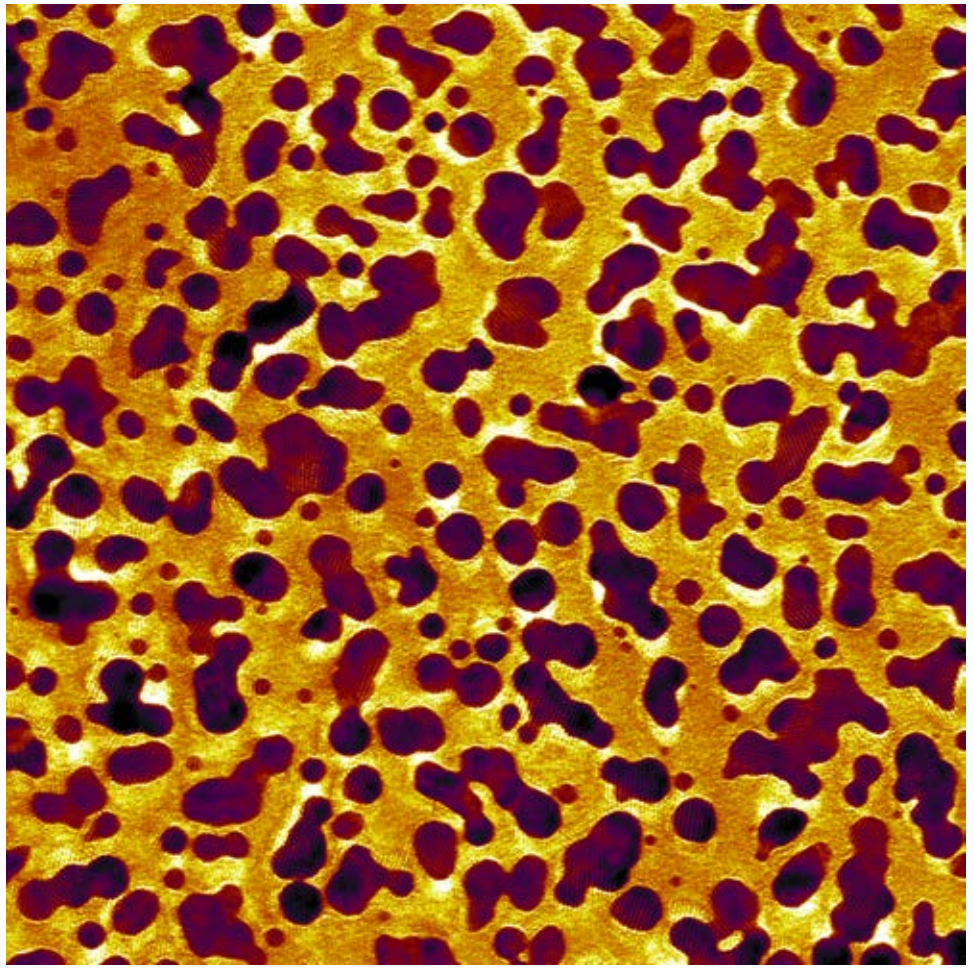
Making Image Figures from Scalar Data

Many other automatic scaling schemes are possible, for example:



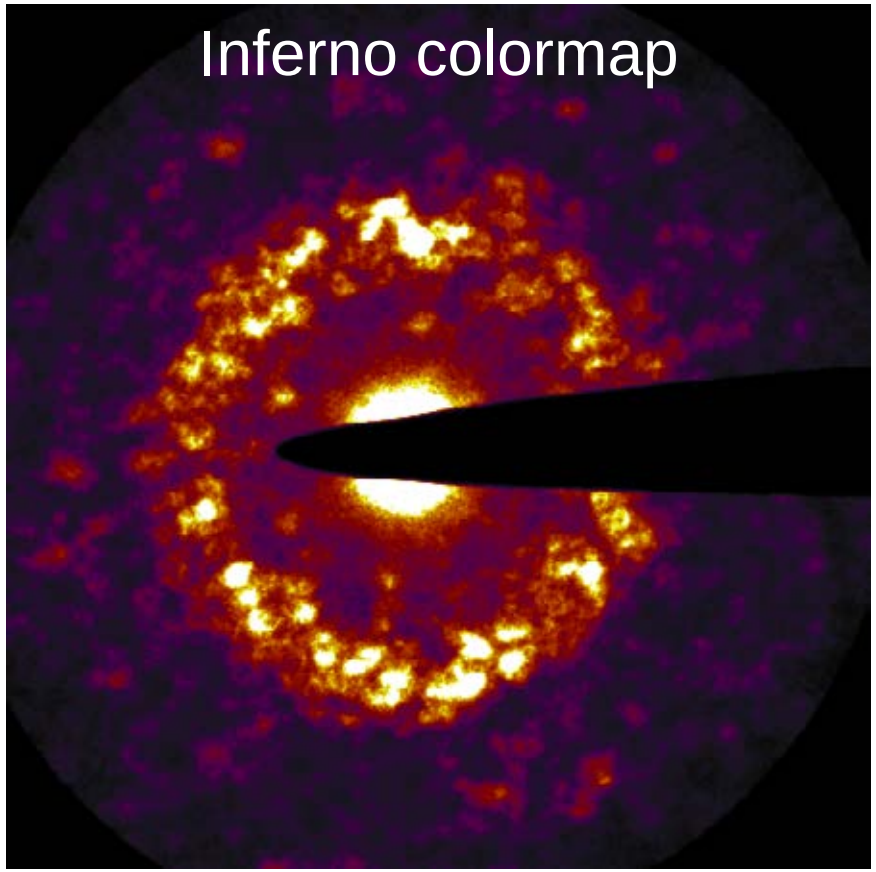
plotImage(image06_gold, 'image06');

Asymmetric uses a different std. dev. in the positive and negative direction.

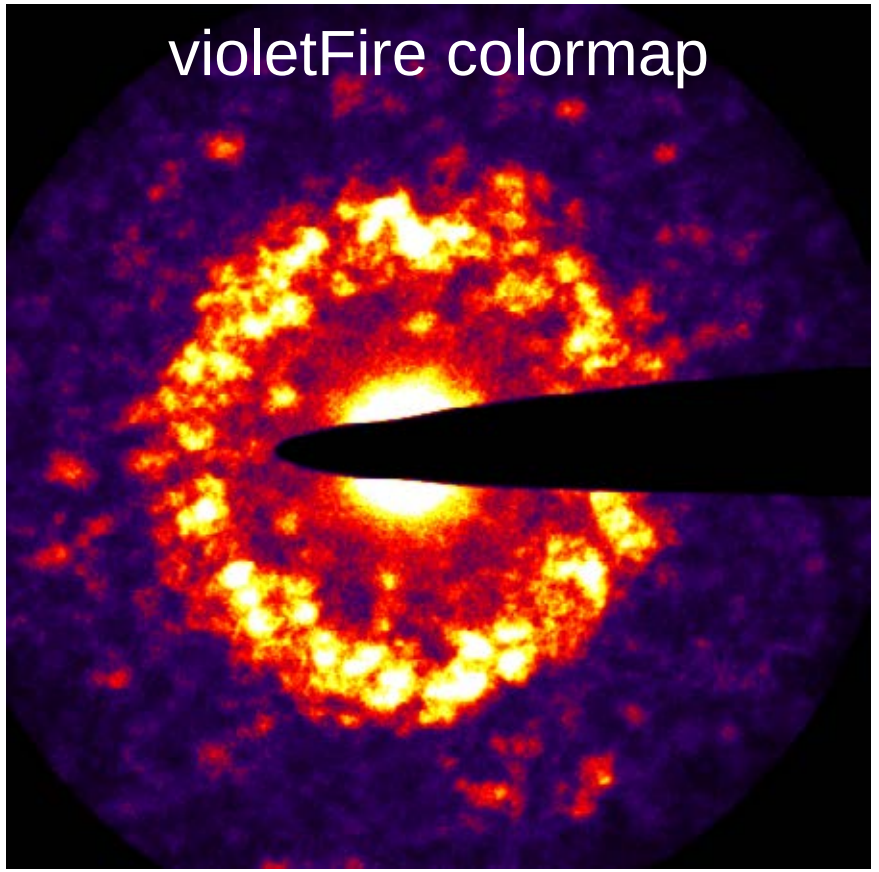


plotImage(image06_gold, 'image06', 'asymmetric');

A Note on Colormaps



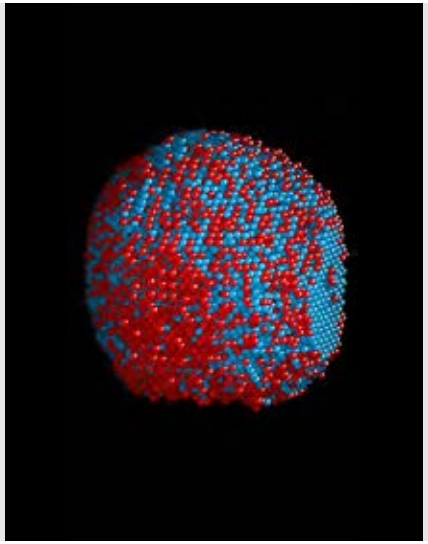
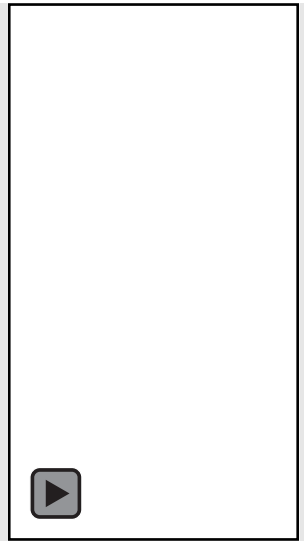
plotImage(image02_amor_diff,[-1 3],'image02_inferno');

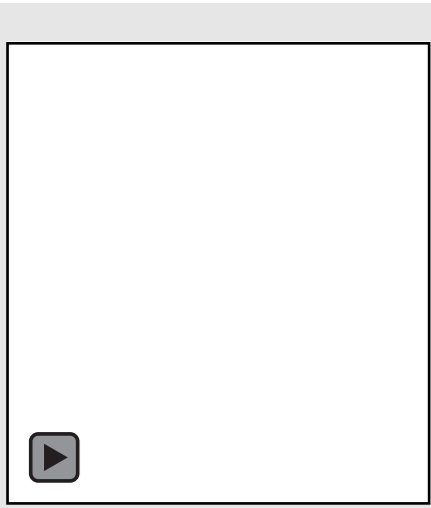


plotImage(image02_amor_diff,violetFire,[-1 3],'image02_violetFire');

“Eye-balled” the inferno colormap - my own similar map “violetFire” from several years back is brighter, but doesn’t have the same perceptual uniformity.

Outline



1

Basic concepts when making figures and movies – raster vs vector.

2

Scaling, coloring and saving scalar and vector **imaging data**.

3

Plotting **points in 3D**, highlight internal features – e.g. atomic coordinates.

4

Animating 3D points, making **movies** – e.g. atomic coordinates.

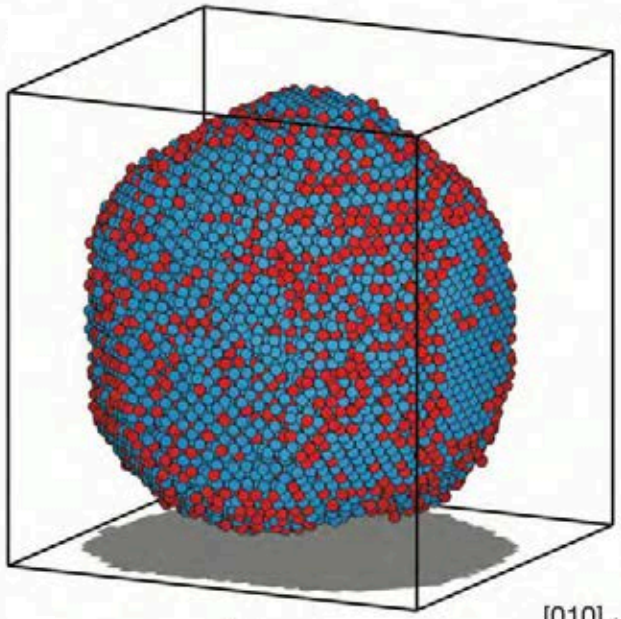
5

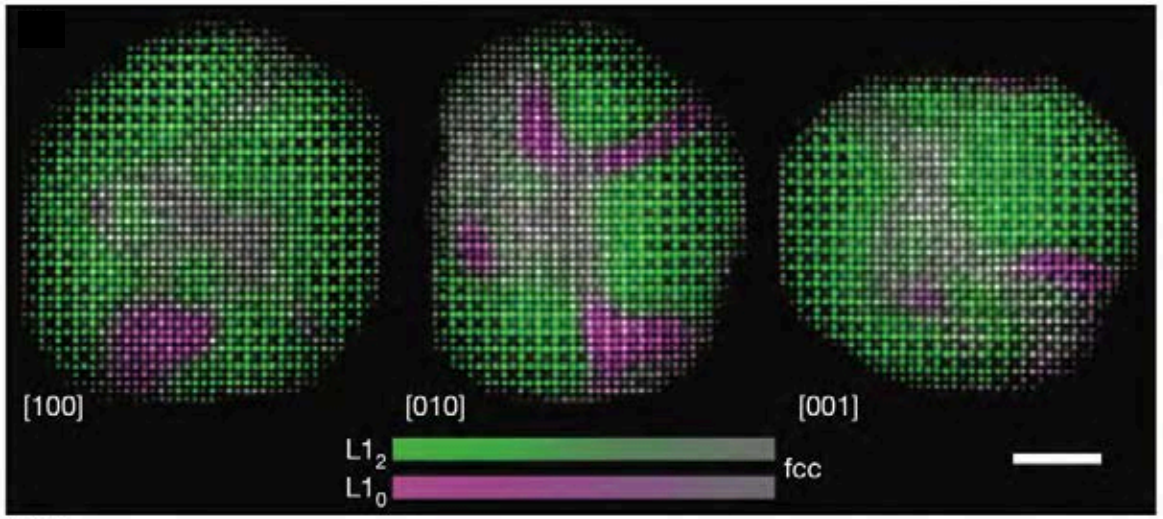
Building **physics visualization** and simulation directly into figures.

6

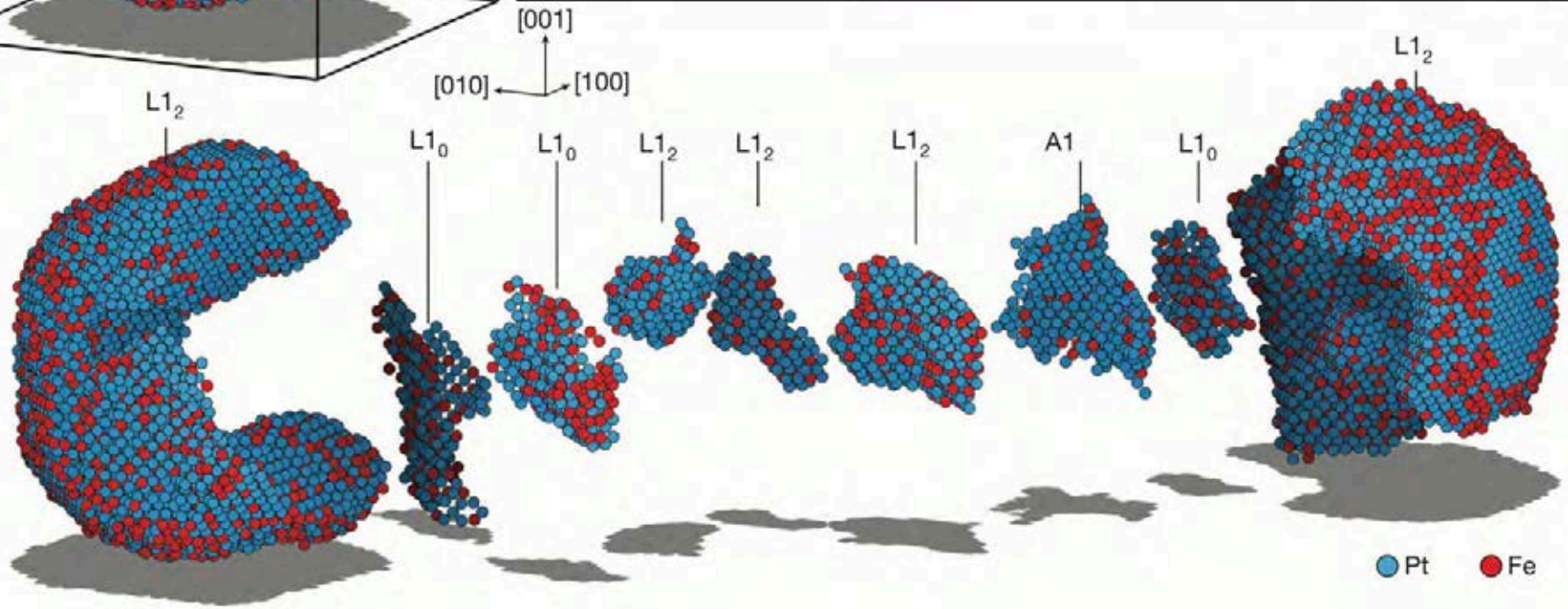
Making simple animations to explain **concepts in physics**.

Common Vis Task – Plotting 3D Atoms





atomic electron tomography: position and species



- Fe
- Pt

GBs: $L1_2$ and $L1_0$ grains

Tutorial on how I drew this panel:

Y Yang*, CC Chen*, MC Scott*, C Ophus*, et al., Nature 542, 74 (2017)

Common Visualization Task – 3D Atoms

For generating plots from code, you should “plot as you code.”

By monitoring your vis progress, you can catch mistakes early!
As your visualization codes become more advanced, you will perform less checks.

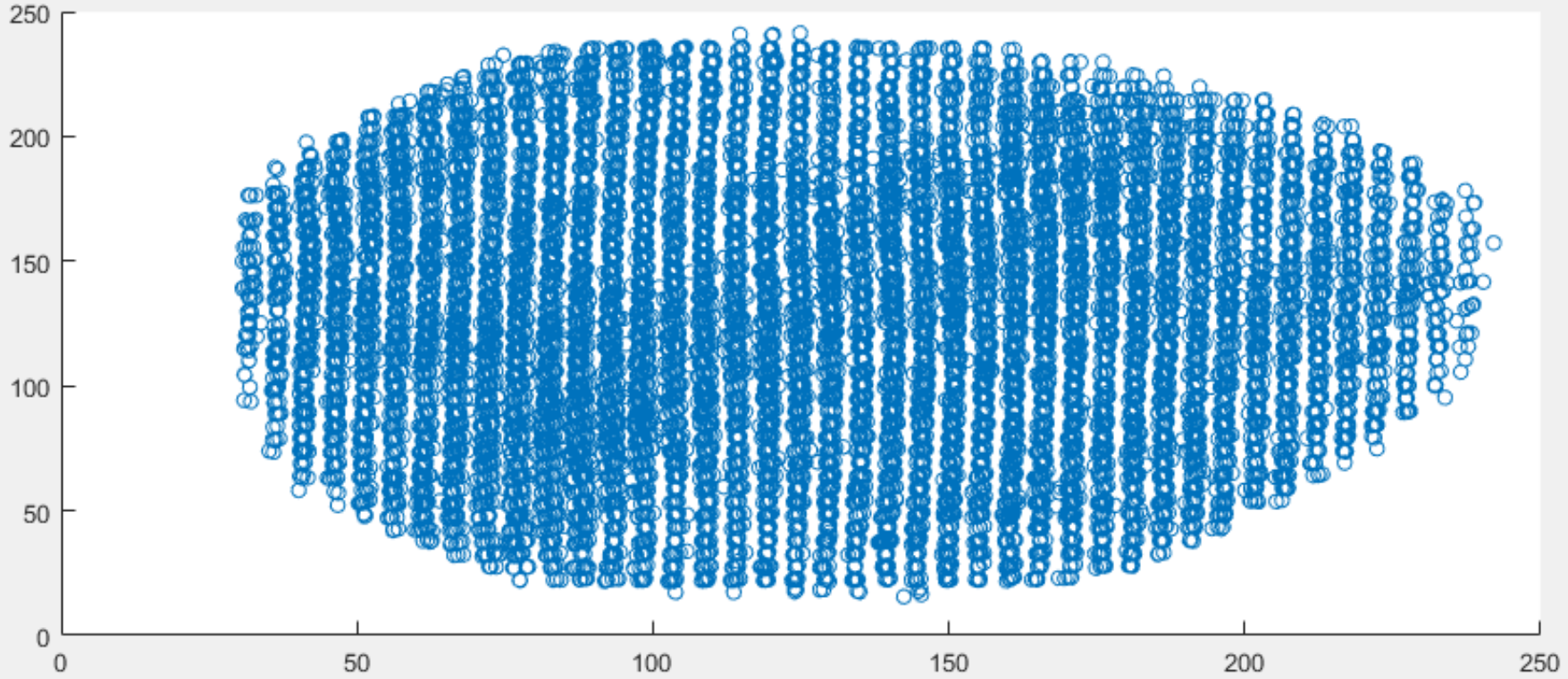
Load the atomic coordinate data:
>> load('atomData02.mat’)

Running the plotting scripts:
>> plotAtoms00(**atomData**, **atomLattice**);
>> plotAtoms01(**atomData**, **atomLattice**);

Our goal is to understand all of the plotting elements in plotAtoms01(…)

Various plotting commands are commented out, we will take a visual tour through these commands. To try it yourself, just uncomment / comment the appropriate lines of code!

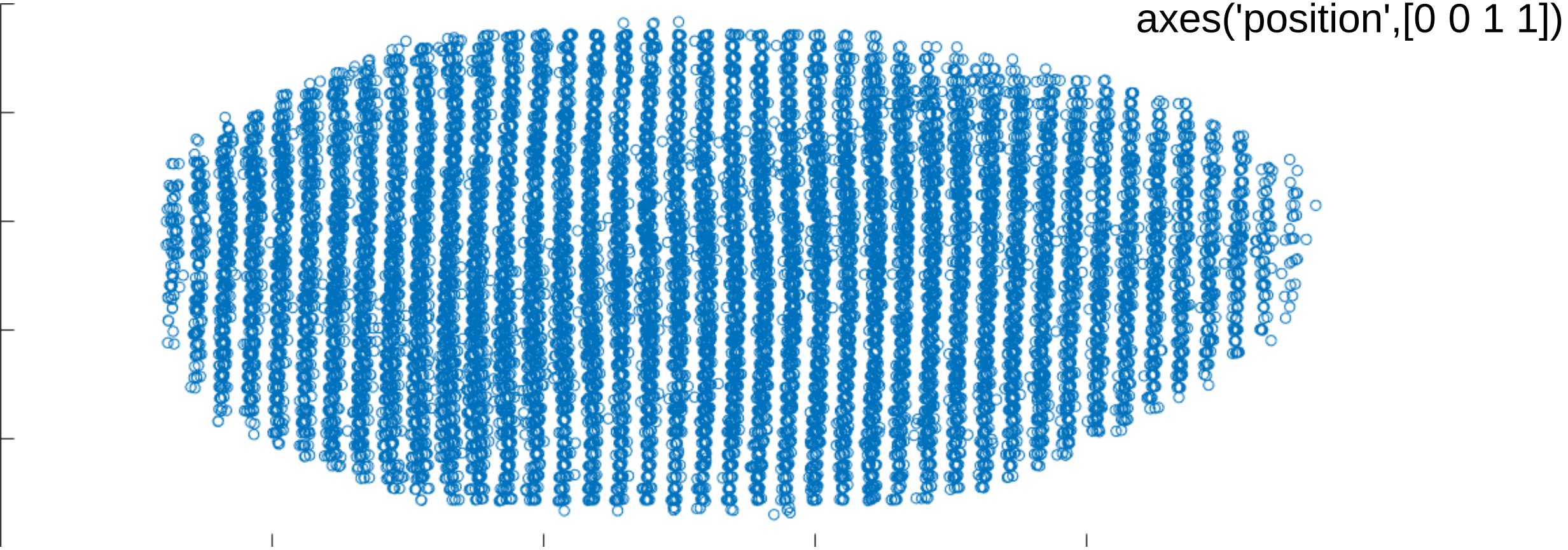
Common Visualization Task – 3D Atoms




```
scatter3( ...
    atomPos(:,1),...
    atomPos(:,2),...
    atomPos(:,3));
```

A 3D scatter plot of the coordinates, default appearance – pretty ugly!

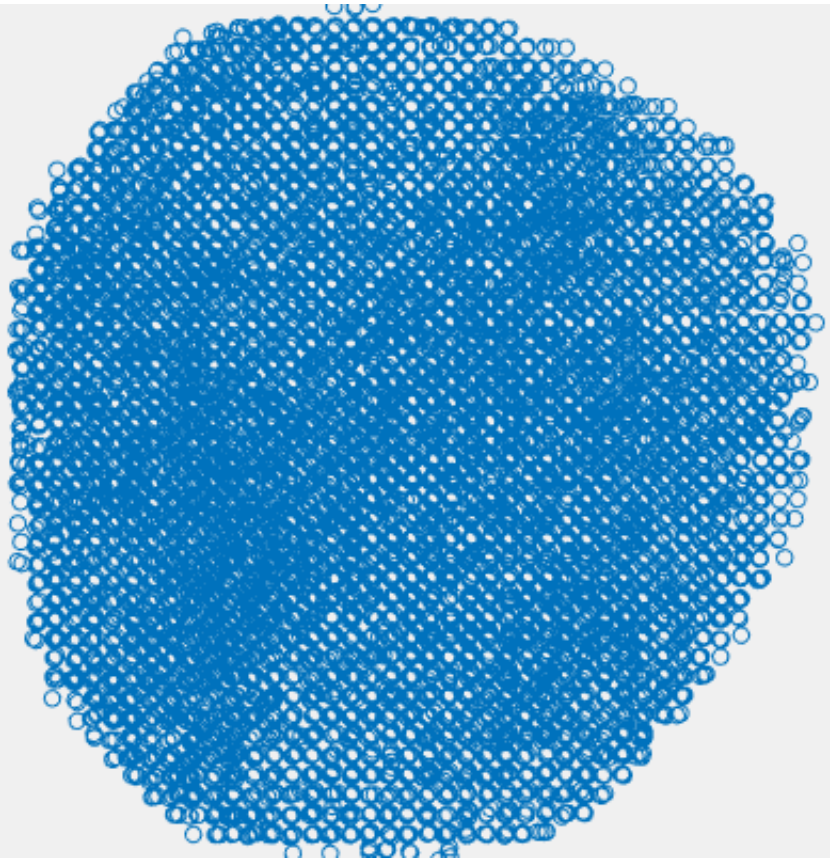
Common Visualization Task – 3D Atoms



This “axes” command will stretch the axes to fill the field of view.

[x_origin y_origin x_width y_width] – all values normalized from 0 to 1.

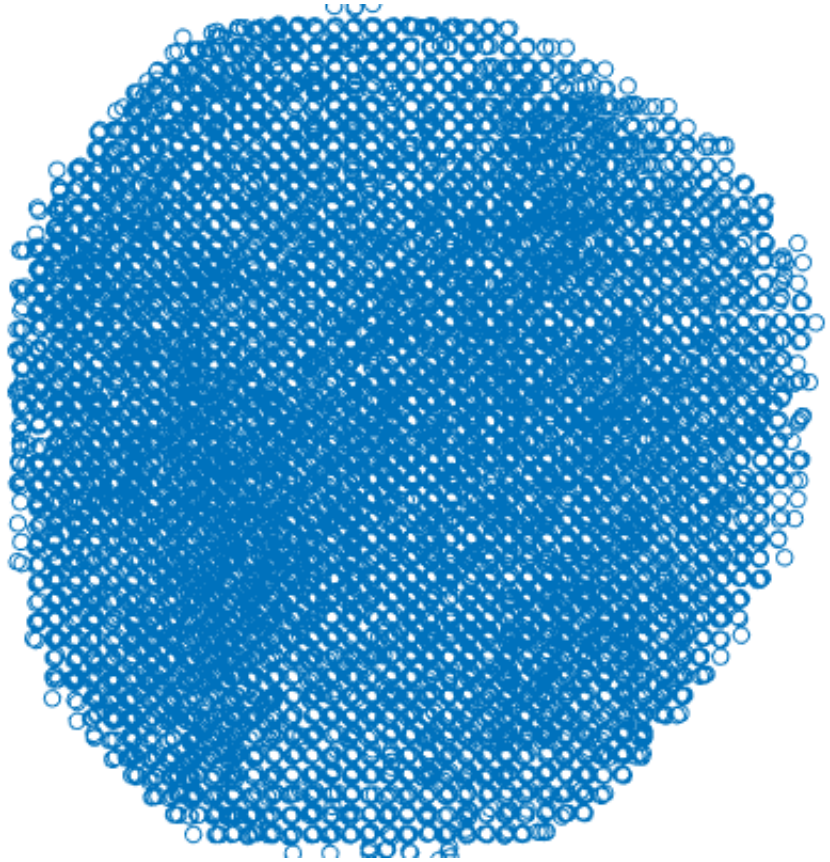
Common Visualization Task – 3D Atoms



axis equal off

Set the aspect ratio of the 3 directions to be equivalent, hide the axes objects.

Common Visualization Task – 3D Atoms



```
set(gcf,'color','w');
```

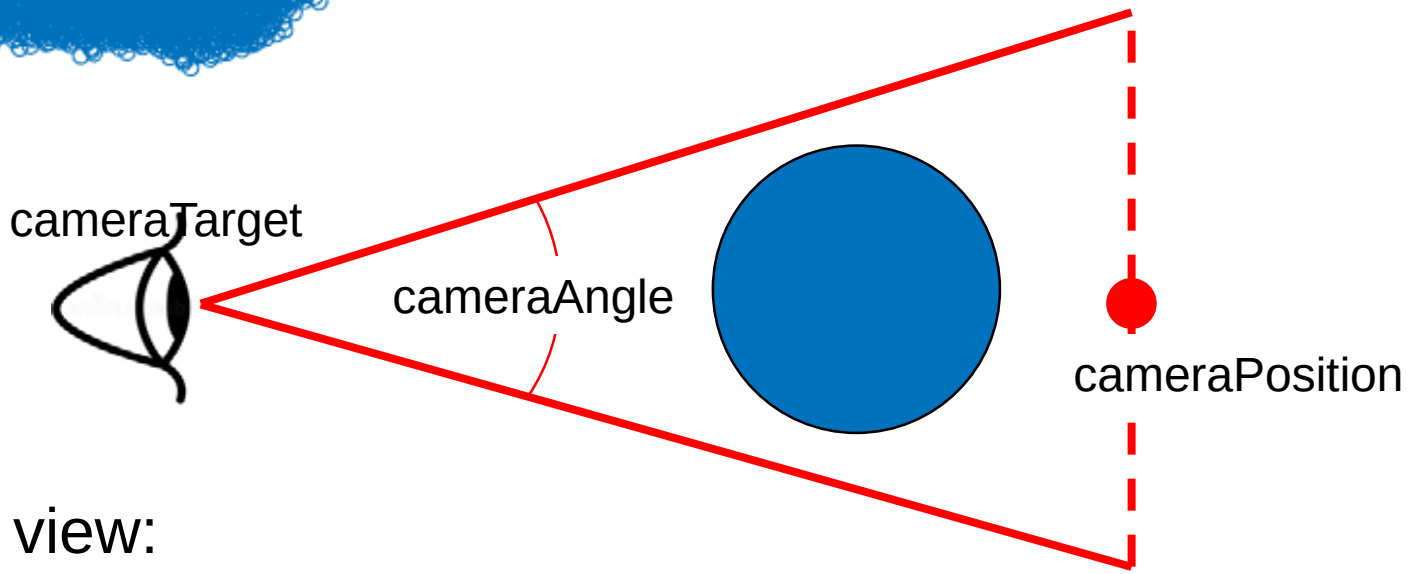
or equivalently

```
set(gcf,'color’,[1 1 1]);
```

“gcf” = get current figure handle, set its color to white (red = 1, green = 1, blue = 1)

Common Visualization Task – 3D Atoms

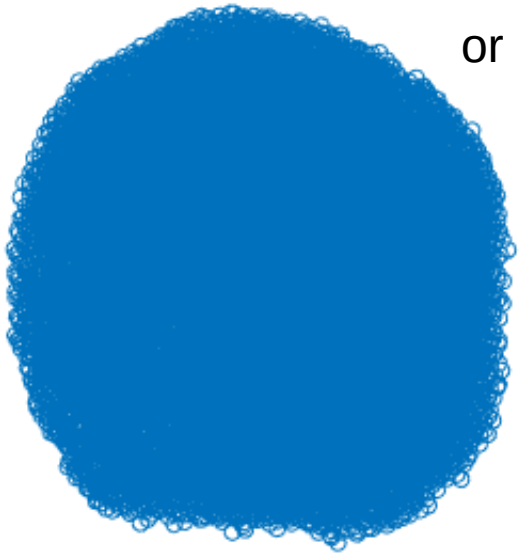
```
camtarget(cameraTarget)
campos(cameraTarget …
                + cameraPosition);
camva(cameraAngle)
camproj('perspective')
```



Set up a rendering camera for a 3D view:

Common Visualization Task – 3D Atoms

```
for a0 = 1:3
        atomPos(:,a0) = atomPos(:,a0) - mean(atomPos(:,a0));
end

or              atomPos = atomPos - mean(atomPos, 1);
```

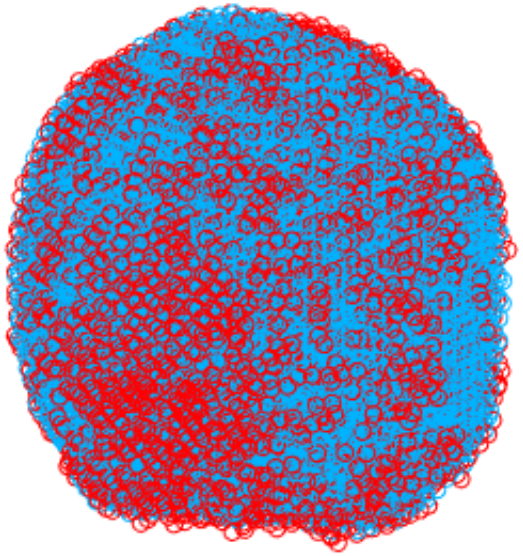


Center the group of atoms on (x,y,z) = (0,0,0) by subtracting the mean position.

Common Visualization Task – 3D Atoms

Pt

Fe



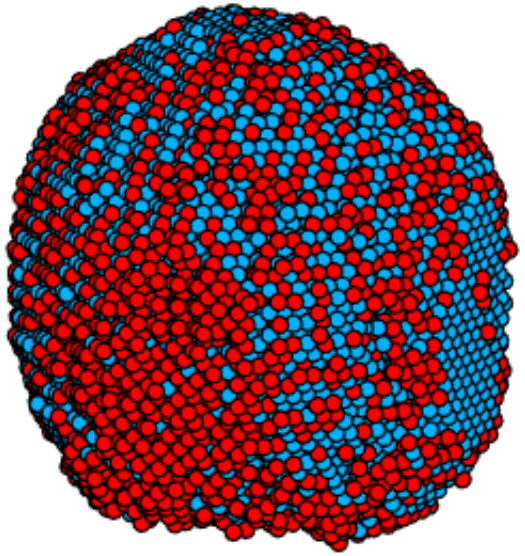
```
scatter3( ...
    atomPos(:,1),...
    atomPos(:,2),...
    atomPos(:,3),...
    ones(numberAtoms,1)*atomSize,...
    atomRGB);
```

Give a unique color (and marker size) to each atom, in order to identify Fe and Pt sites.

Common Visualization Task – 3D Atoms

Pt

Fe

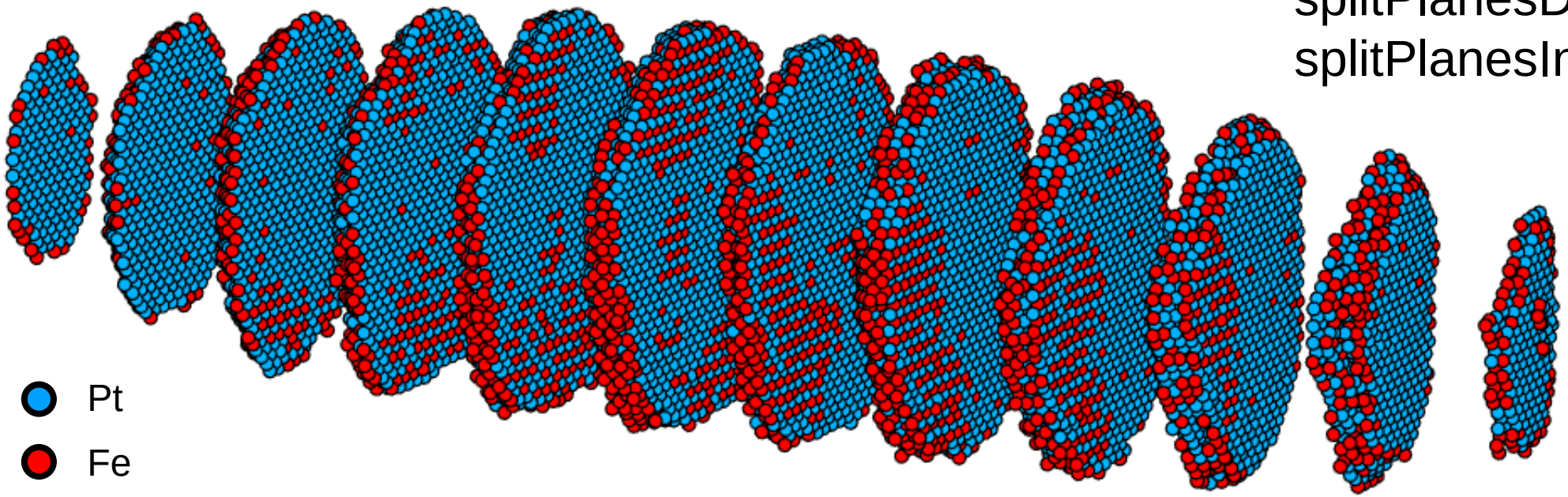


```
scatter3( ...
    atomPos(:,1),...
    atomPos(:,2),...
    atomPos(:,3),...
    ones(numberAtoms,1)*atomSize,...
    atomRGB,...
    'filled','marker',’o’,…
'linewidth',atomLinewidth,...
    'markeredgecolor',atomColorEdges);
```

Update the marker appearance, filled circles, black edges, etc.

Common Visualization Task – 3D Atoms

splitPlanesBunch = 2;
splitPlanesDistance = 70;
splitPlanesIndex = 2;

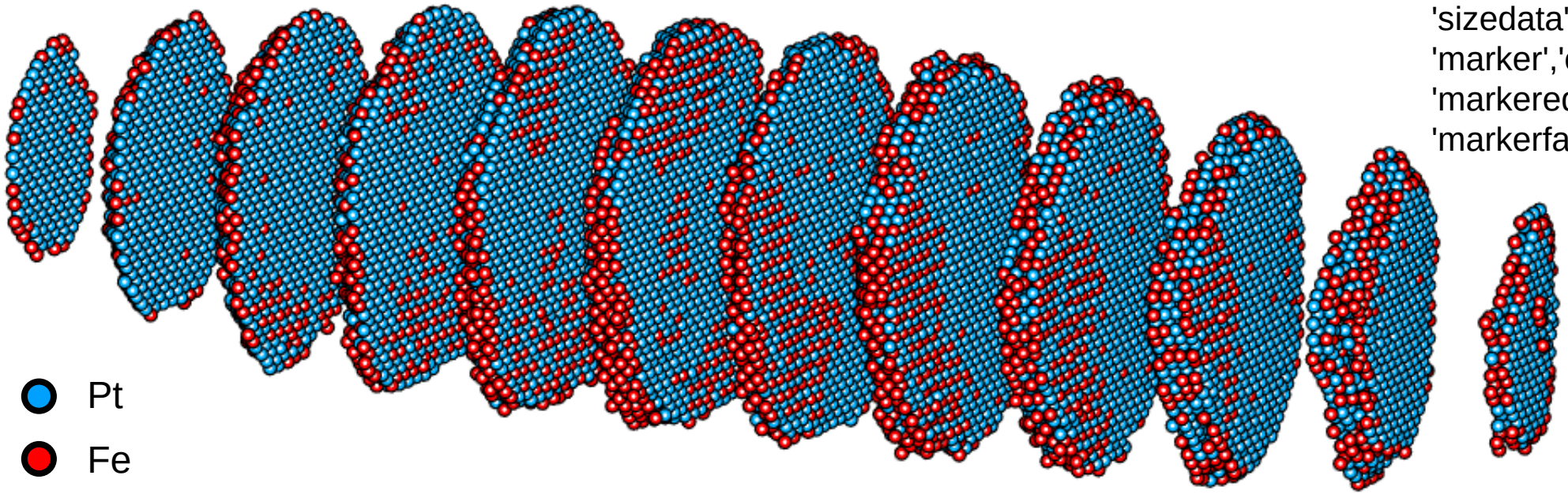


Now we're moving beyond simple scatter plots – atoms are "bunched" up into sets of 4 atomic planes, and then each plane is moved 70 plotting units apart from the neighboring planes. This operation performed along dimension 2 (y axis).

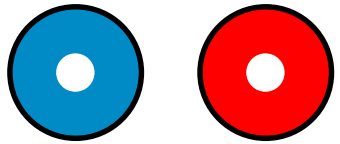
This plotting allows us to see the rich internal structure of this experiment – note the alternating Fe-Pt atomic planes.

Common Visualization Task – 3D Atoms

```
scatter3( ...
        atomPos(:,1),...
        atomPos(:,2),...
        atomPos(:,3),...
        'sizedata',atomSizeTint,...
        'marker','o',...
        'markeredgecolor','none',...
        'markerfacecolor',atomColorTint);
```

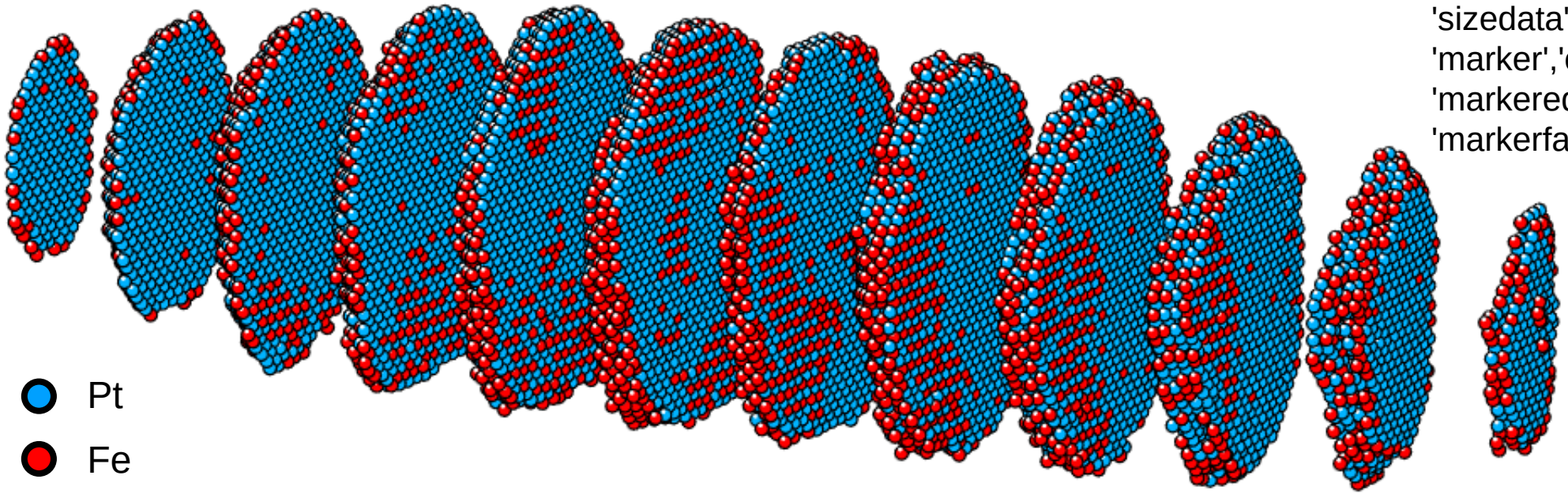


Let’s make a fake specular reflection spot:

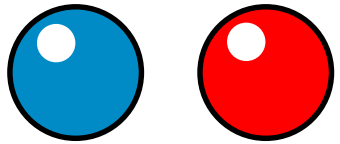


Common Visualization Task – 3D Atoms

```
scatter3( ...
        atomPos(:,1) + shiftTint(1),...
        atomPos(:,2) + shiftTint(2),...
        atomPos(:,3) + shiftTint(3),...
        'sizedata',atomSizeTint,...
        'marker','o',...
        'markeredgecolor','none',...
        'markerfacecolor',atomColorTint);
```

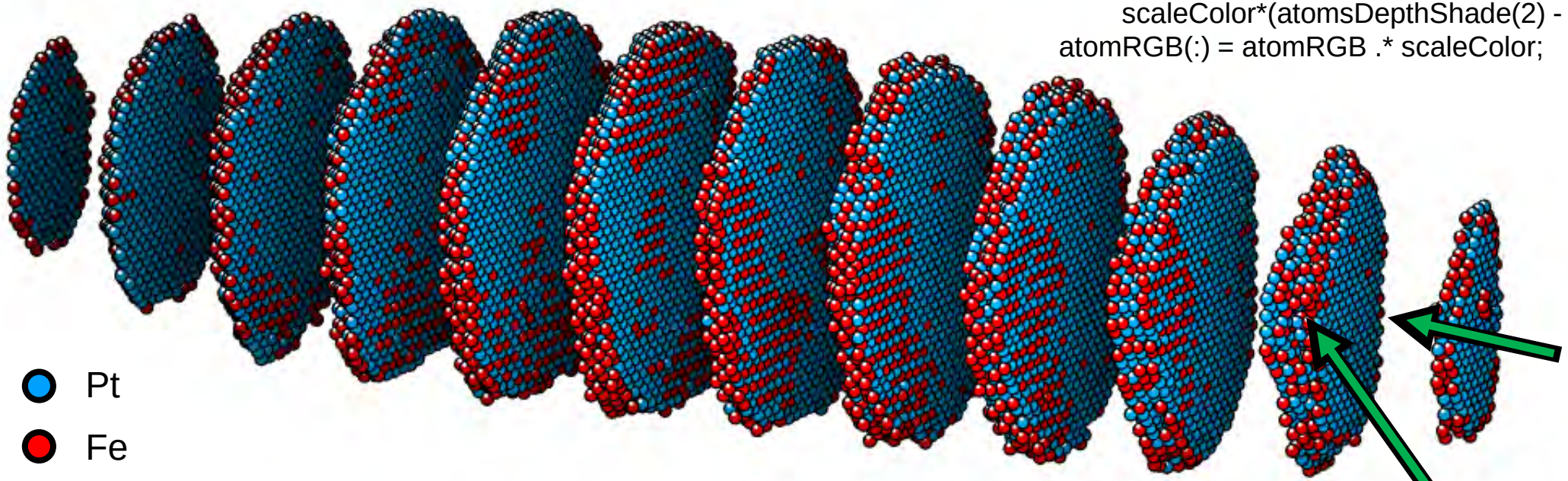


Let’s make a fake specular reflection spot:



Common Visualization Task – 3D Atoms

```
scaleColor = distCamera - min(distCamera);
scaleColor(:) = scaleColor / max(scaleColor);
scaleColor(:) = 3*scaleColor(:).^2 - 2*scaleColor(:).^3;
scaleColor(:) = scaleColor.^atomsDepthPower;
scaleColor = atomsDepthShade(1) + ...
      scaleColor*(atomsDepthShade(2) - atomsDepthShade(1));
atomRGB(:) = atomRGB .* scaleColor;
```



Pt

Fe

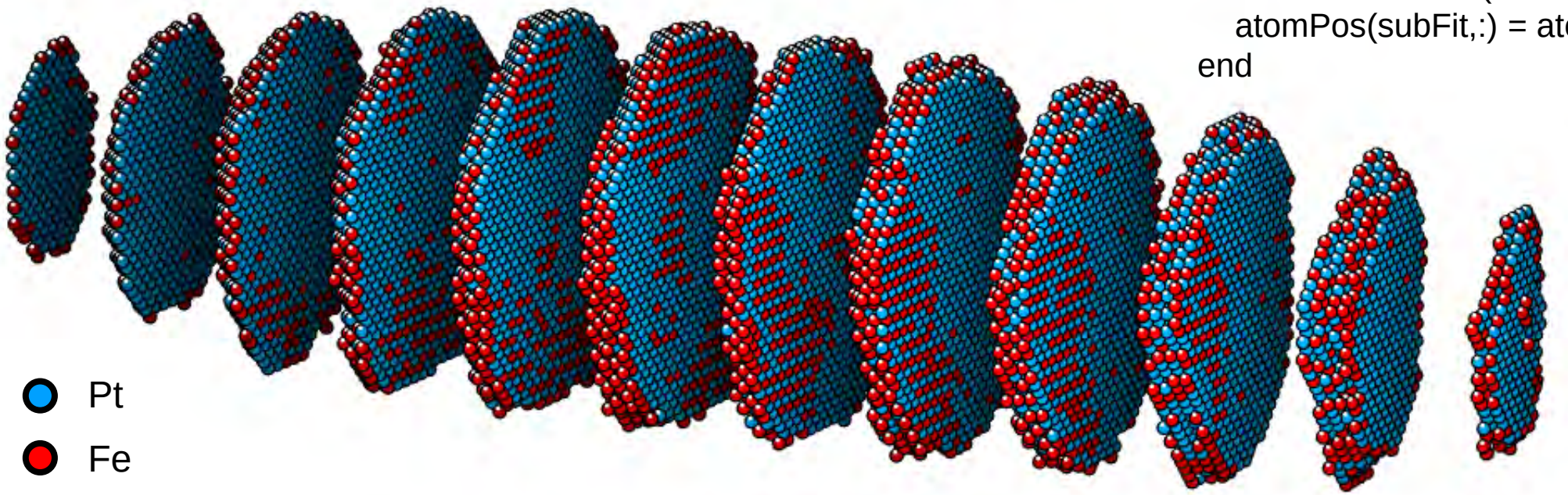
Sites far from the camera are shaded to a darker color.

Sites closest to the camera are left alone.

This is a subtle effect to create a 3D view – “depth cueing”

Common Visualization Task – 3D Atoms

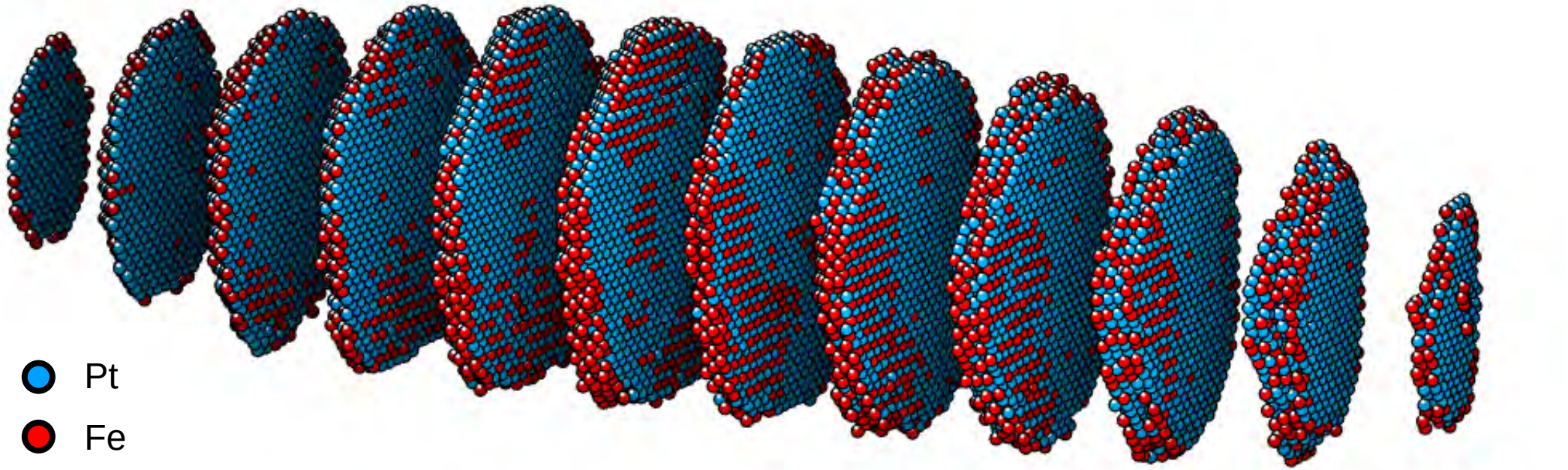
```
if flagMoveAtomsToLattice == true
    subFit = ~isinf(sum(atomLattice,2)) ...
        & ~isnan(sum(atomLattice,2));
    lat = atomLattice(subFit,:) \ atomPos(subFit,:);
    atomPos(subFit,:) = atomLattice(subFit,:) * lat;
end
```



This line is complex – moving the atoms from their measured sites to best fit lattice.

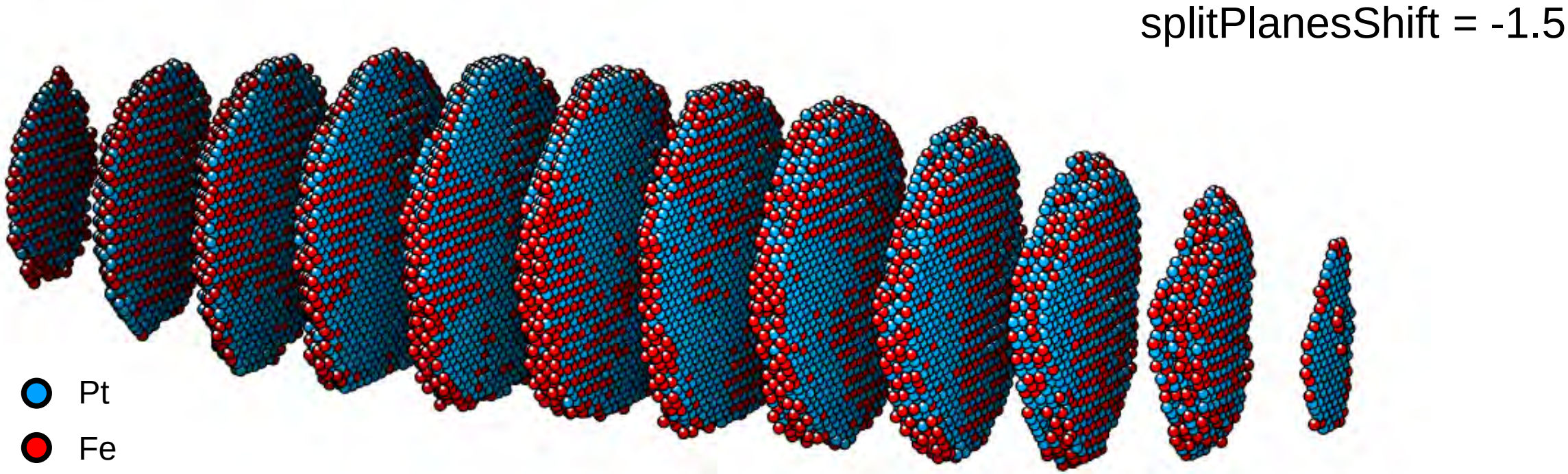
Common Visualization Task – 3D Atoms

flagMoveAtomsToLattice = false



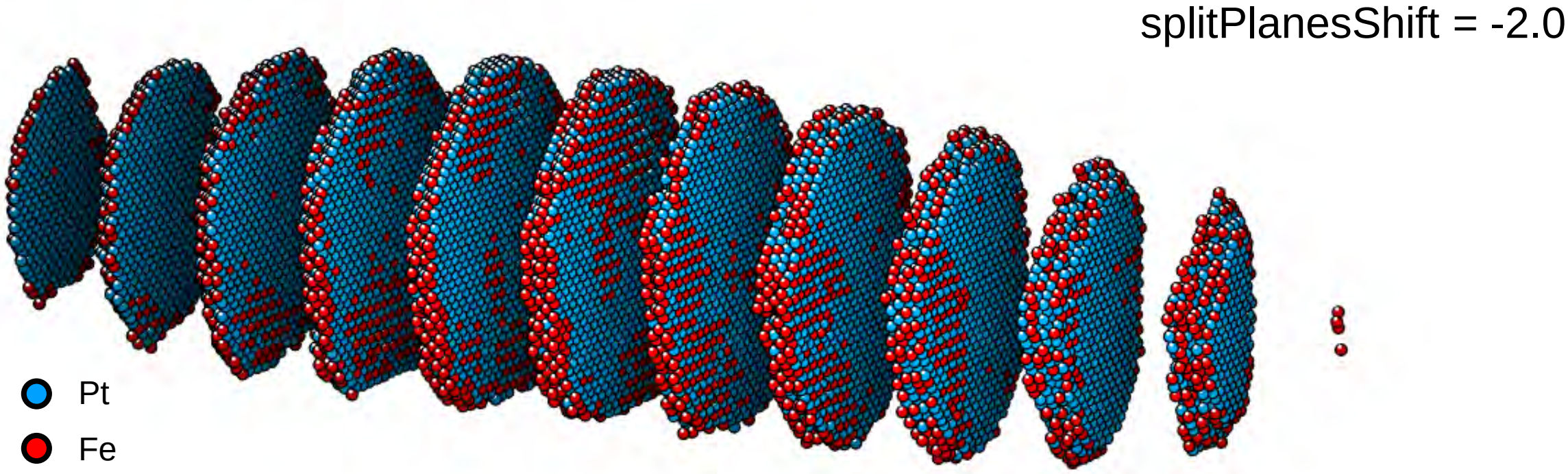
Turning that flag back off – flags are useful to plot multiple conditions / parameters.

Common Visualization Task – 3D Atoms



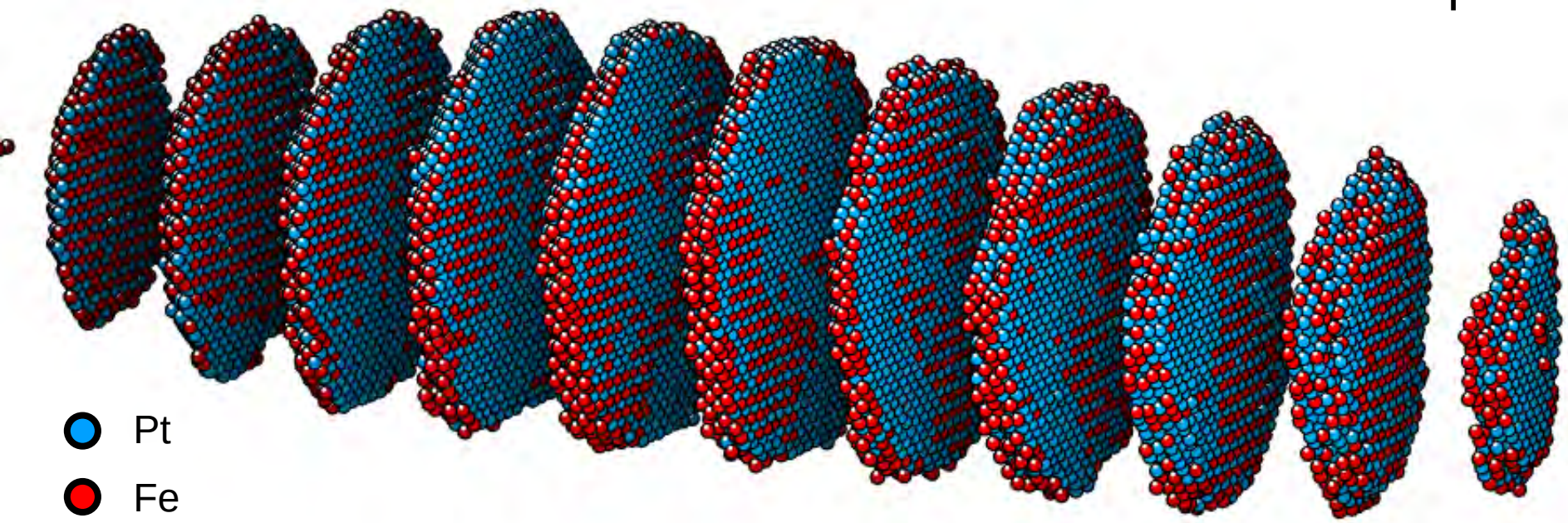
Shifting the planes we are cutting at.

Common Visualization Task – 3D Atoms



Shifting the planes we are cutting at.

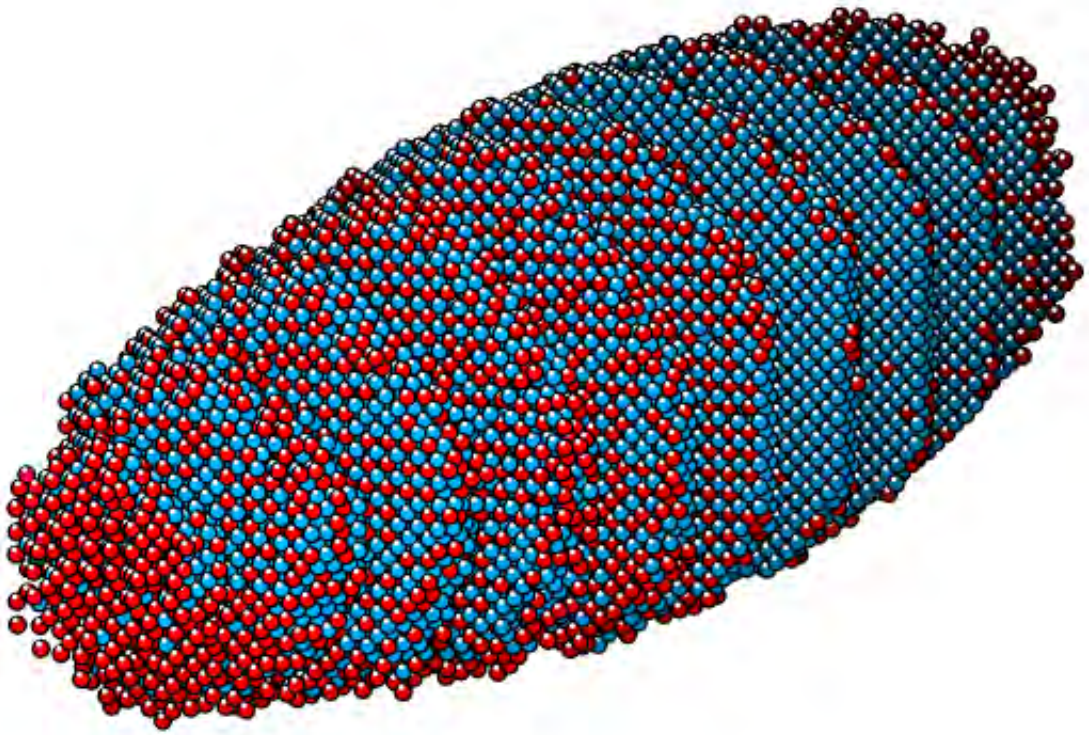
Common Visualization Task – 3D Atoms



Shifting the planes we are cutting at.

Common Visualization Task – 3D Atoms

splitPlanesIndex = 1

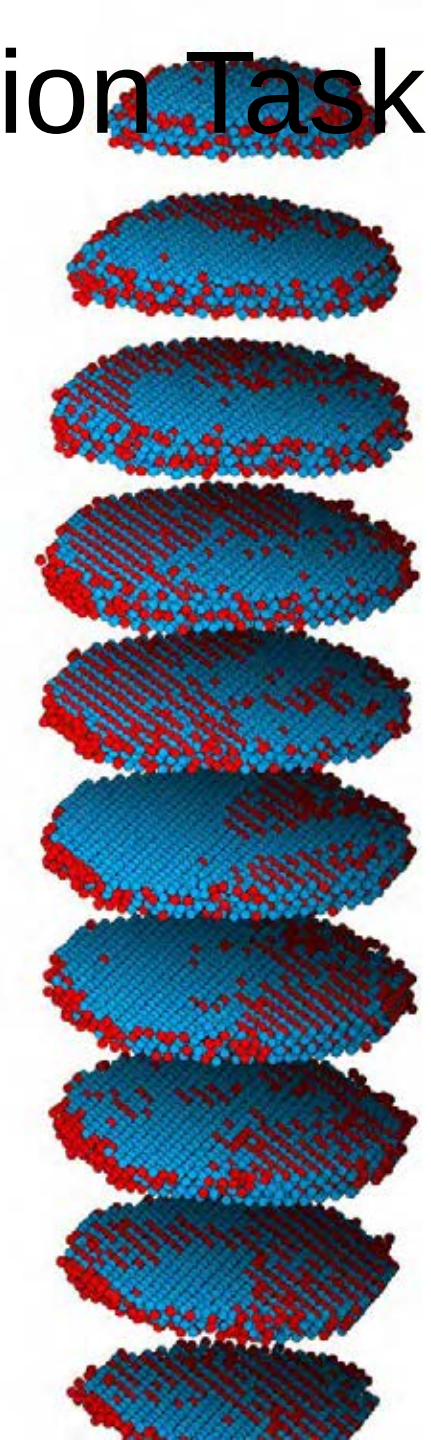


Pt

Fe

Splitting apart the particle along the 1st dimension.

Common Visualization Task – 3D Atoms

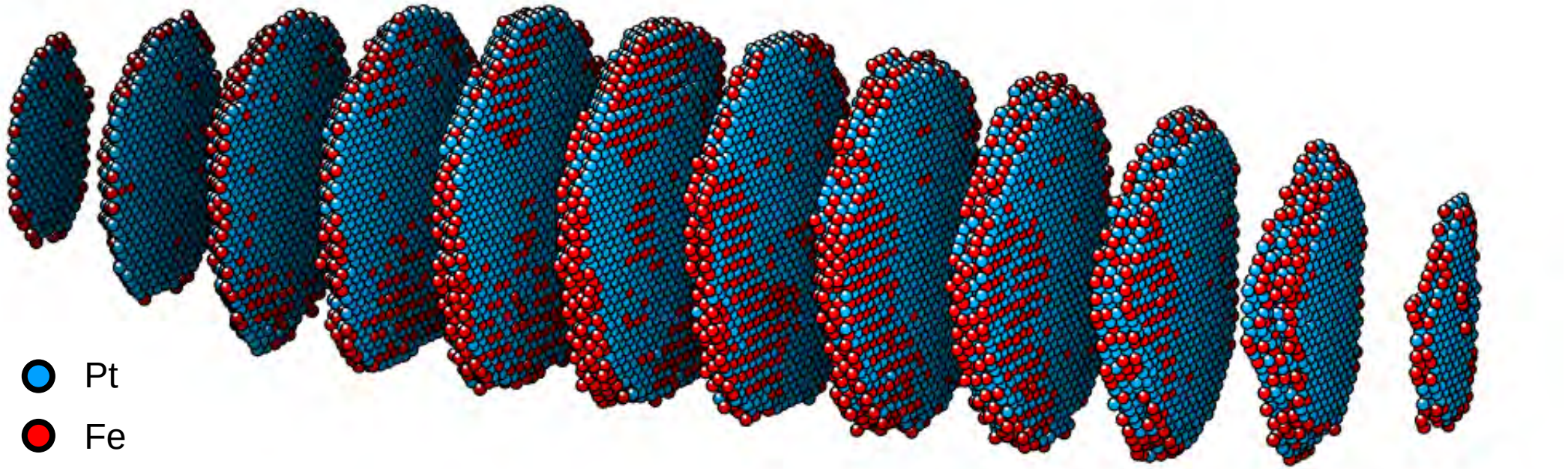


splitPlanesIndex = 3

- Pt
- Fe

Splitting apart the particle along the 3rd dimension.

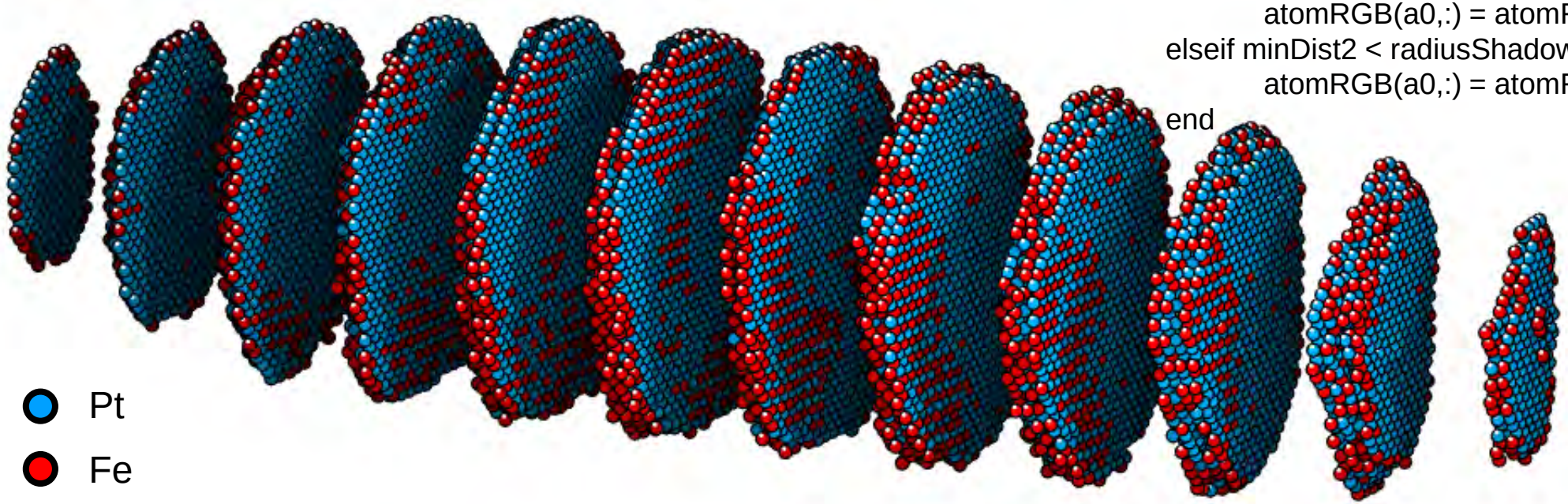
Common Visualization Task – 3D Atoms



So far we are just manipulating parameters and positions – can we do more?

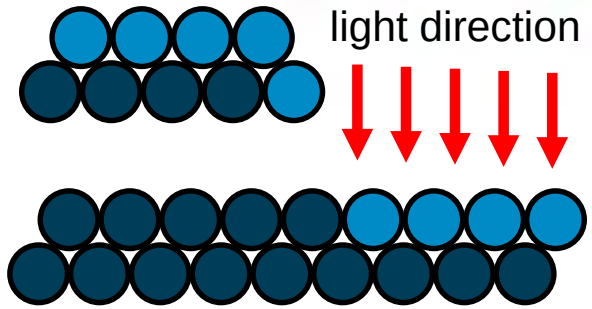
Common Visualization Task – 3D Atoms

```
distProj2(:) = sum(cross(atomPos - xyz0, vecRep).^2,2);
sub(:) = sum((atomPos - xyz0).*vecShadow,2) > 0;
        minDist2 = min(distProj2(sub));

if minDist2 < radiusShadow2(1)
            atomRGB(a0,:) = atomRGB(a0,:) * shadingShadow(1);
elseif minDist2 < radiusShadow2(2)
            atomRGB(a0,:) = atomRGB(a0,:) * shadingShadow(2);
end
```



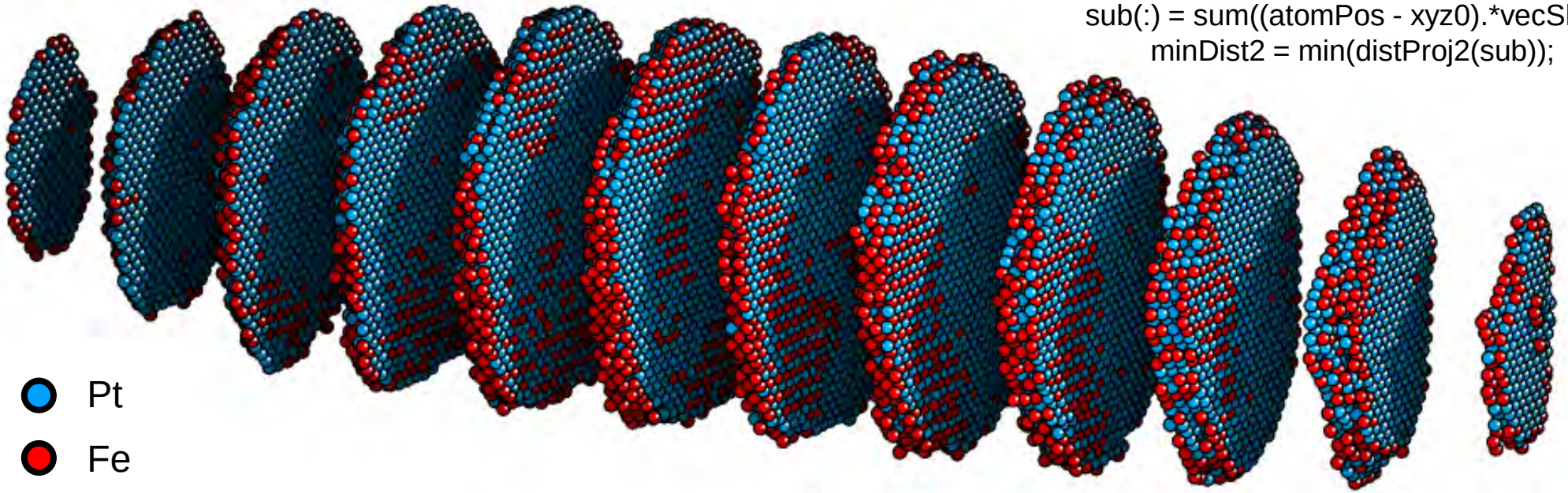
Pt

Fe



Ray traced shadows!

Common Visualization Task – 3D Atoms

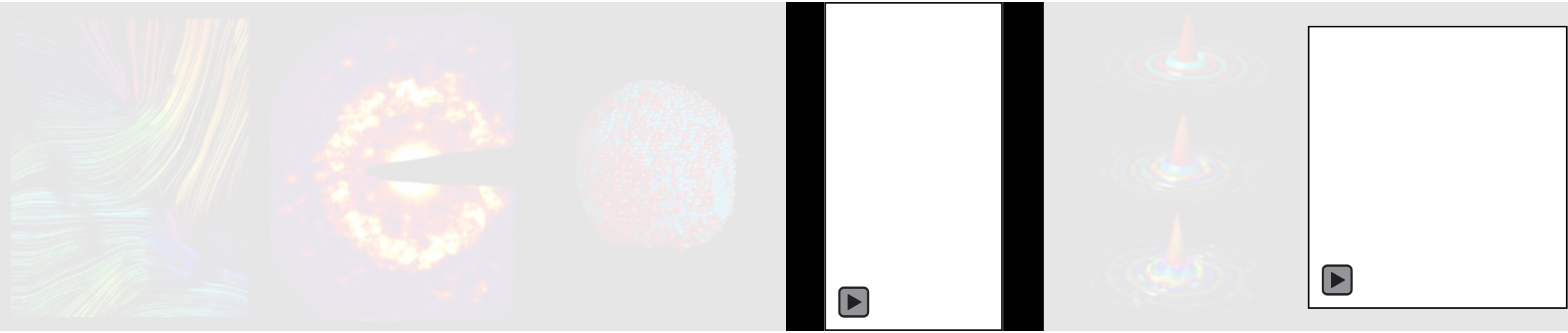



```
distProj2(:) = sum(cross(atomPos - xyz0, vecRep).^2,2);
sub(:) = sum((atomPos - xyz0).*vecShadow,2) > 0;
        minDist2 = min(distProj2(sub));
```

```
if minDist2 < radiusShadow2(1)
            atomRGB(a0,:) = atomRGB(a0,:) * shadingShadow(1);
            subShadowed(a0) = true;
        elseif minDist2 < radiusShadow2(2)
            atomRGB(a0,:) = atomRGB(a0,:) * shadingShadow(2);
            subShadowed(a0) = true;
end
```

description

Outline



1 **Basic concepts** when making figures and movies – raster vs vector.

2 Scaling, coloring and saving scalar and vector **imaging data**.

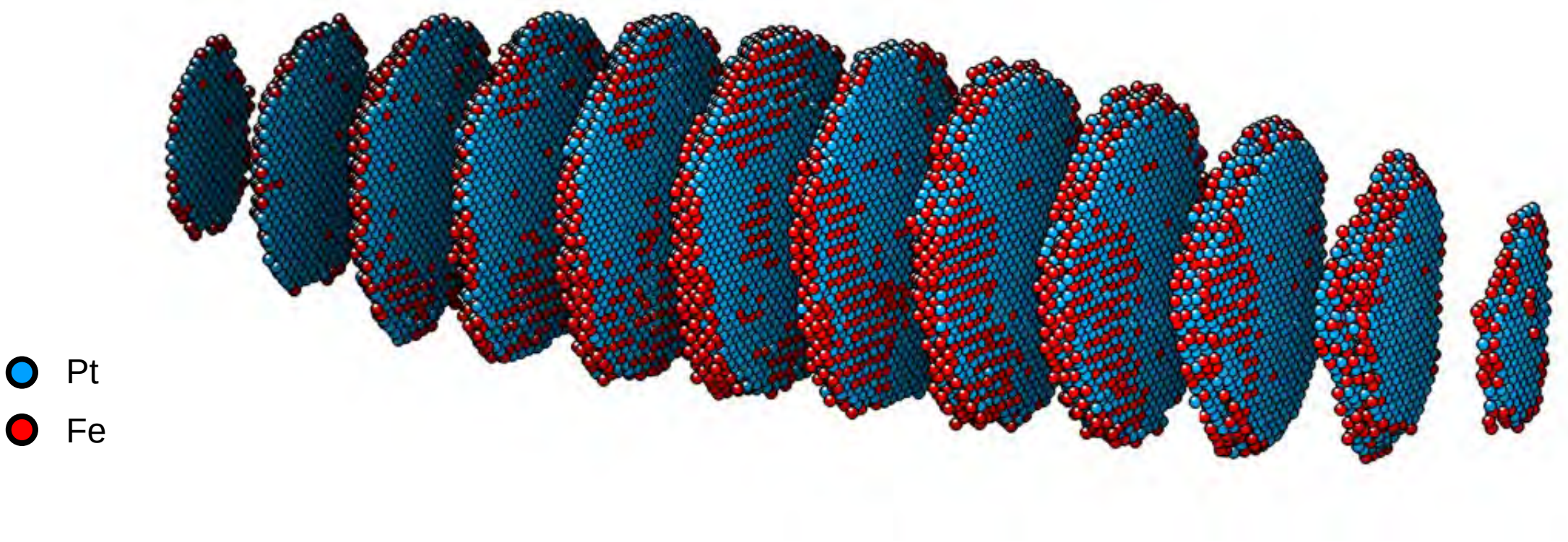
3 Plotting **points in 3D**, highlight internal features – e.g. atomic coordinates.

4 **Animating 3D** points, making **movies** – e.g. atomic coordinates.

5 Building **physics visualization** and simulation directly into figures.

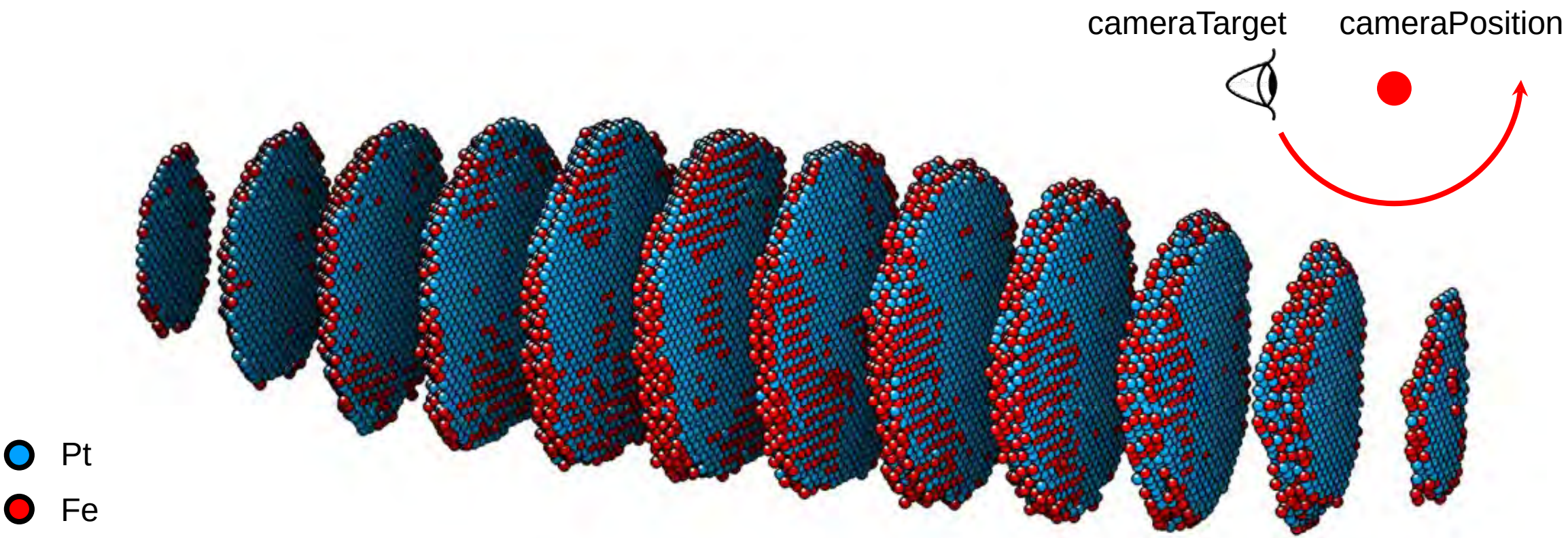
6 Making simple animations to explain **concepts in physics**.

Making Movies from Images Using FFMPEG



Each time plotting script is called, move camera, save image.

Making Movies from Images Using FFMPEG



Each time plotting script is called, move camera, save image.

Making Movies from Images Using Code

Step 1 – Modify drawing script to have input variables.

Step 2 – Write a second script to repeatedly call the first script, changing the inputs.

Step 3 – Each time the drawing script is called, render an image, output to file.

Step 4 – Use FFMPEG to stitch / encode images into a movie. Handbrake edit if needed.

Tutorial example, animated 3D atoms plot with animAtoms01a(), animAtoms01b()

Making Movies from Images Using FFMPEG

FFMPEG command line example for low frame rate movies:

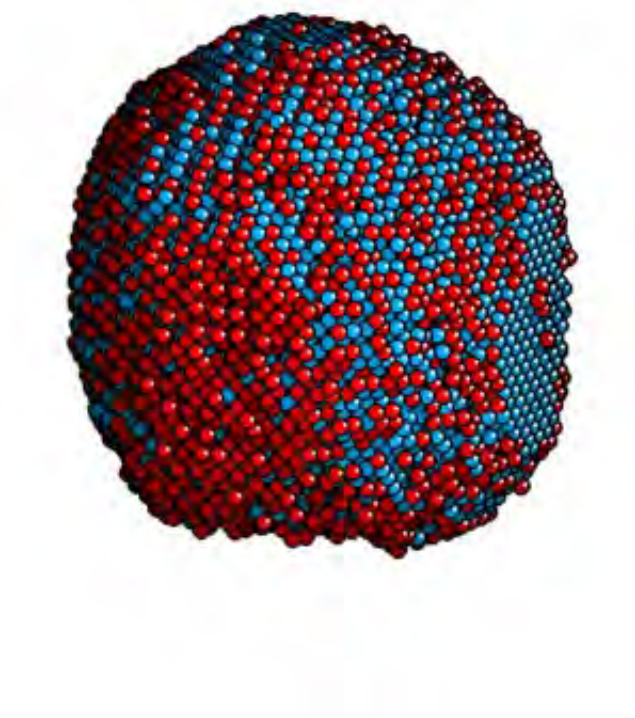
```
ffmpeg
-f image2
-i image%04d.png
-vcodec mpeg4
-qmax 4
-vf setpts=4.0*PTS
movieFileName.mp4
```

FFMPEG command line example for high frame rate movies:

```
ffmpeg
-f image2 -r 60 -i image%04d.png
-c:v libx264 -preset slow
-profile:v high -level:v 4.0
-pix_fmt yuv420p -filter:v fps=fps=60
movieFileName.mp4
```

These are just examples – lots of settings to tweak in FFMPEG!

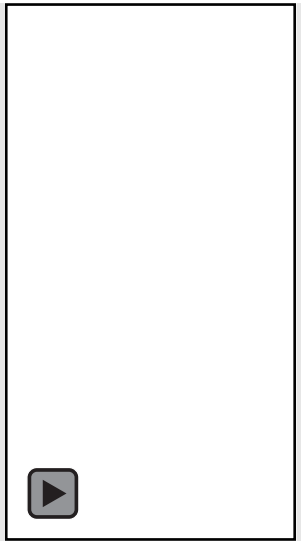
Making Movies from Images Using FFMPEG

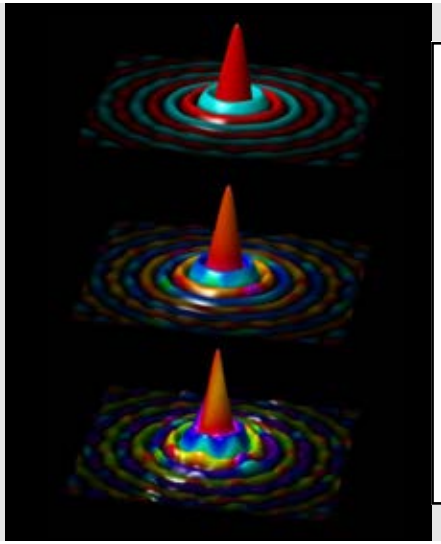


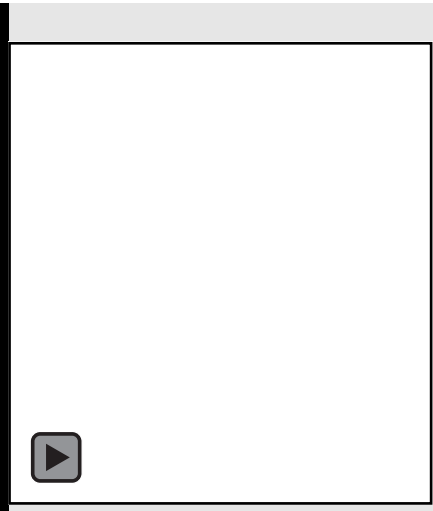
- Pt
- Fe

Each time plotting script is called, change splitPlanes from 0 to 70, save image.

Outline







1

Basic concepts when making figures and movies – raster vs vector.

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5

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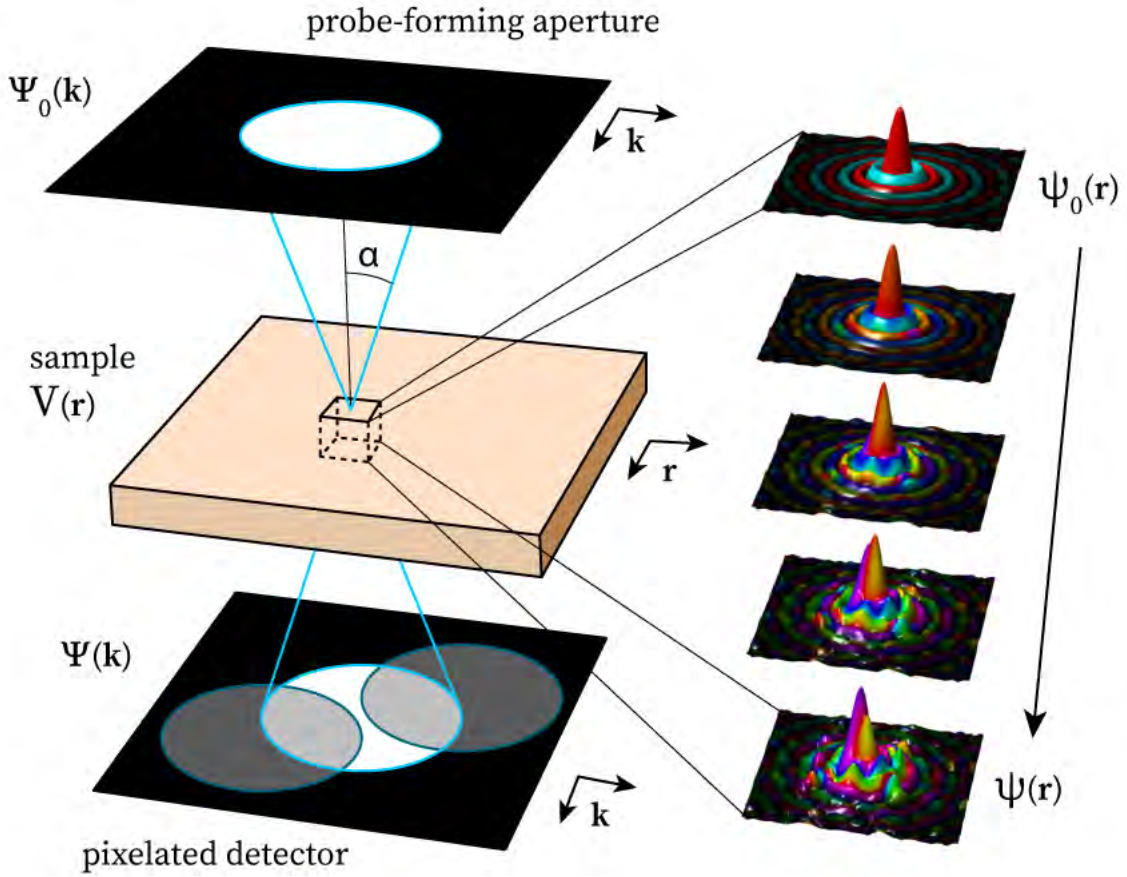
6

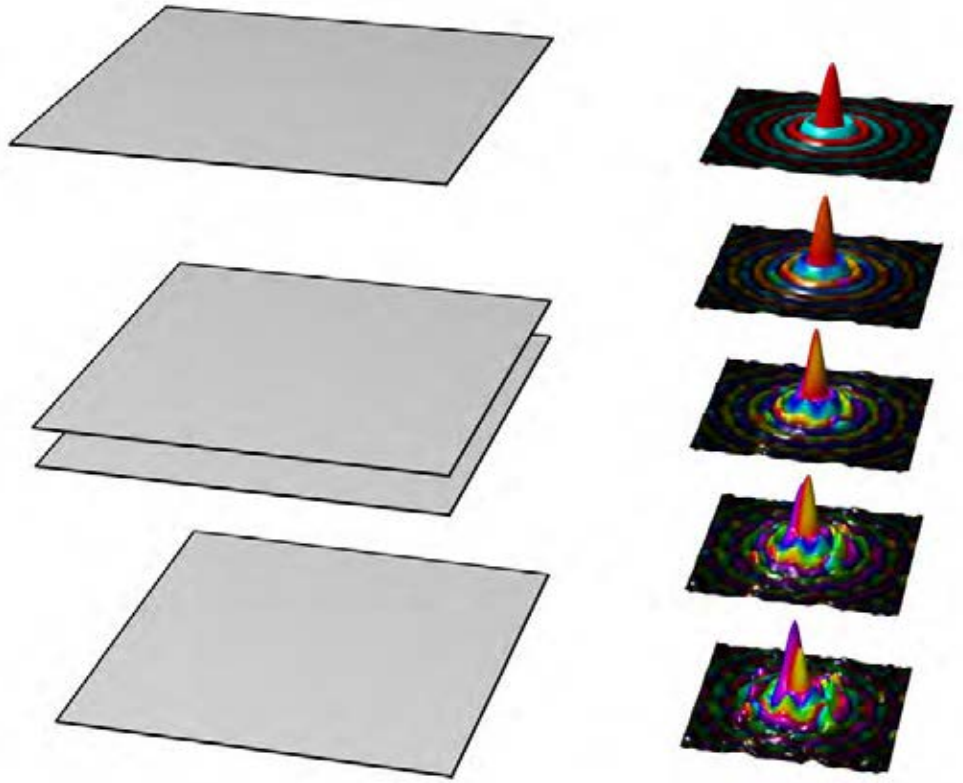
Making simple animations to explain **concepts in physics**.

Building Physics into Figure Generation

Final figure – STEM probe wavefunction



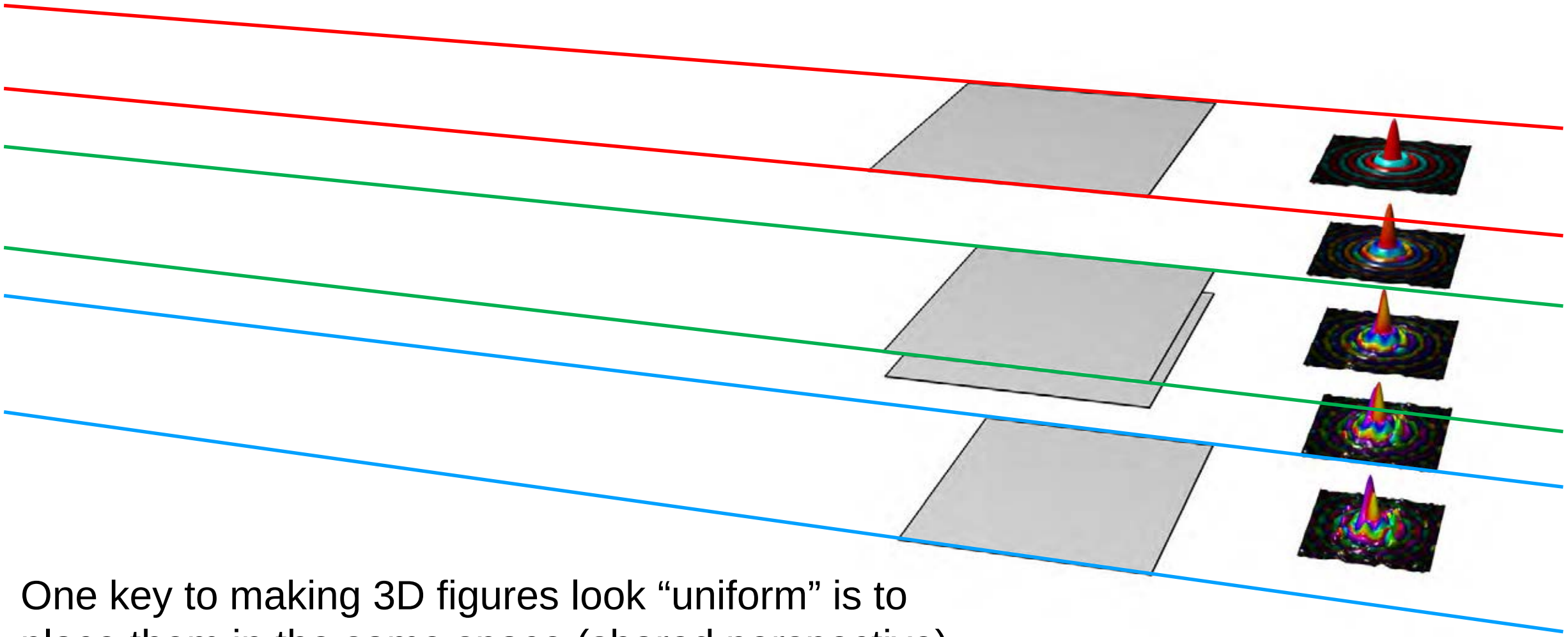
Original figure generated in Matlab



To modify: play with settings, run schematic01();

B Savizky et al., arXiv:2003.09523 (2020).

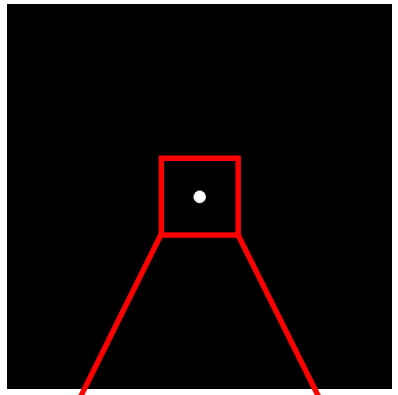
Building Physics into Figure Generation

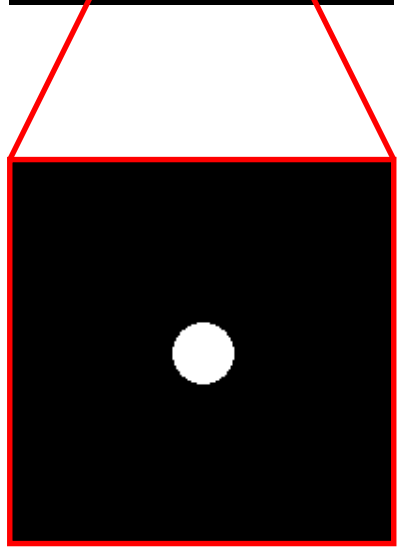


One key to making 3D figures look “uniform” is to place them in the same space (shared perspective).

Building Physics into Figure Generation

Initial probe

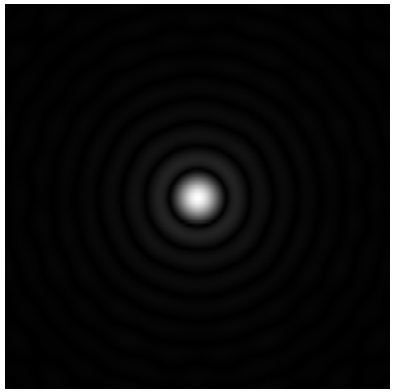




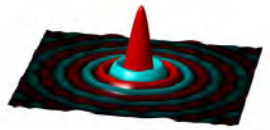
Fourier

Transform

absolute



phase



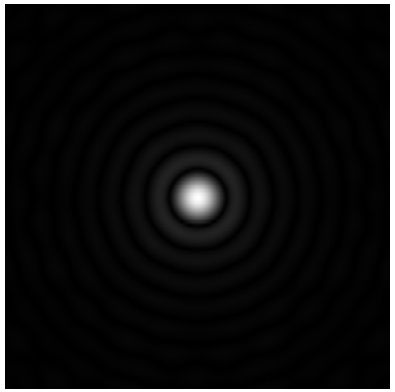
$$\Psi = \begin{cases} 1 & q < q_{Probe} \\ 0 & q > q_{Probe} \end{cases}$$

Building Physics into Figure Generation

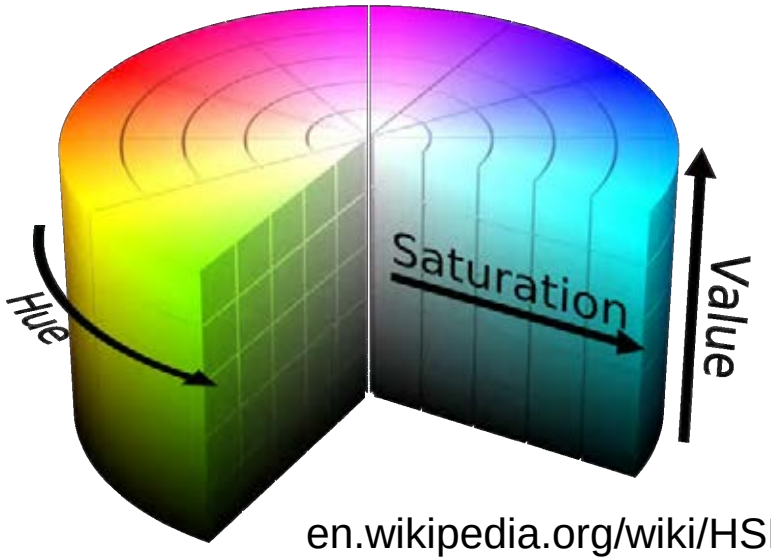
How can we represent complex numbers?

Two values per pixel requires a vector representation with at least 2 coordinates:

absolute



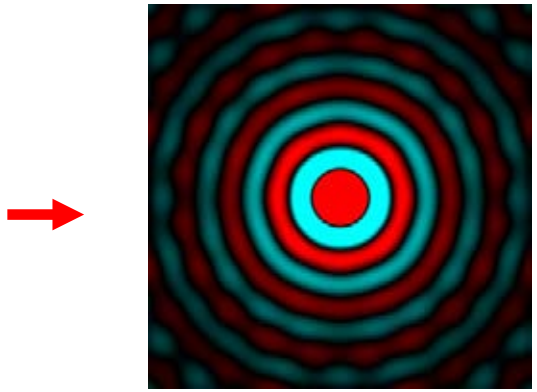
phase



en.wikipedia.org/wiki/HSL_and_HSV

We can map the amplitude to value (or saturation), and phase to the hue.

Hue wraps at 360° / 2π rads, making it a good choice for phase.



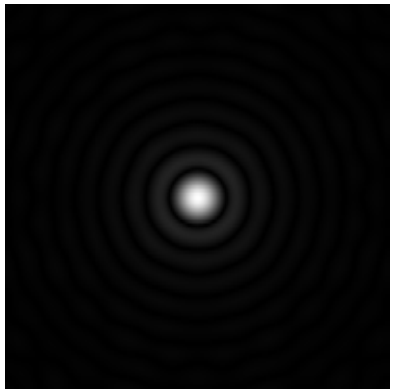
Zero phase color is arbitrary

Building Physics into Figure Generation

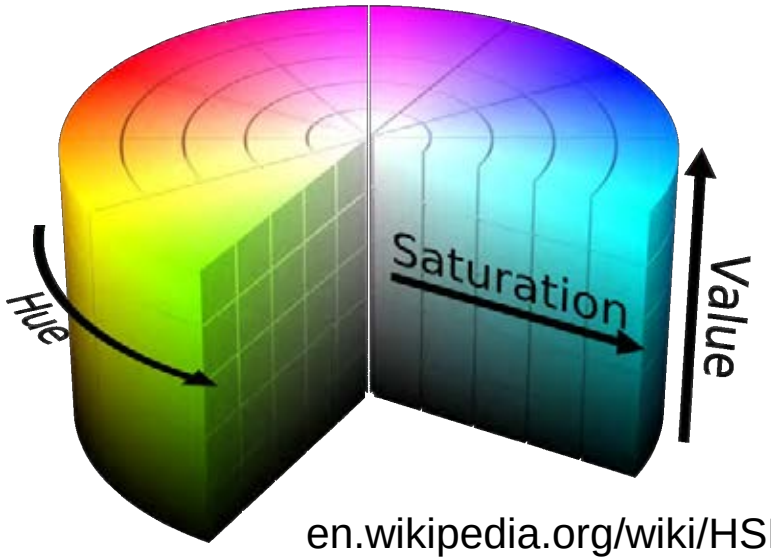
How can we represent complex numbers?

Two values per pixel requires a vector representation with at least 2 coordinates:

absolute



phase



en.wikipedia.org/wiki/HSL_and_HSV

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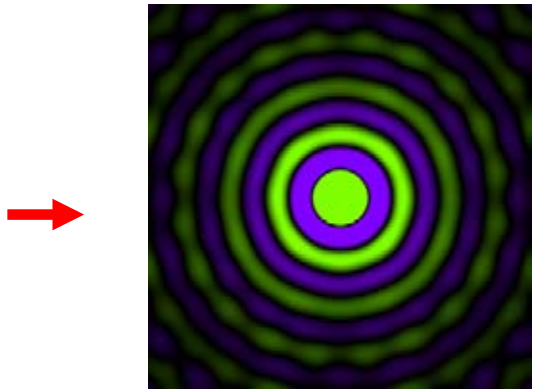
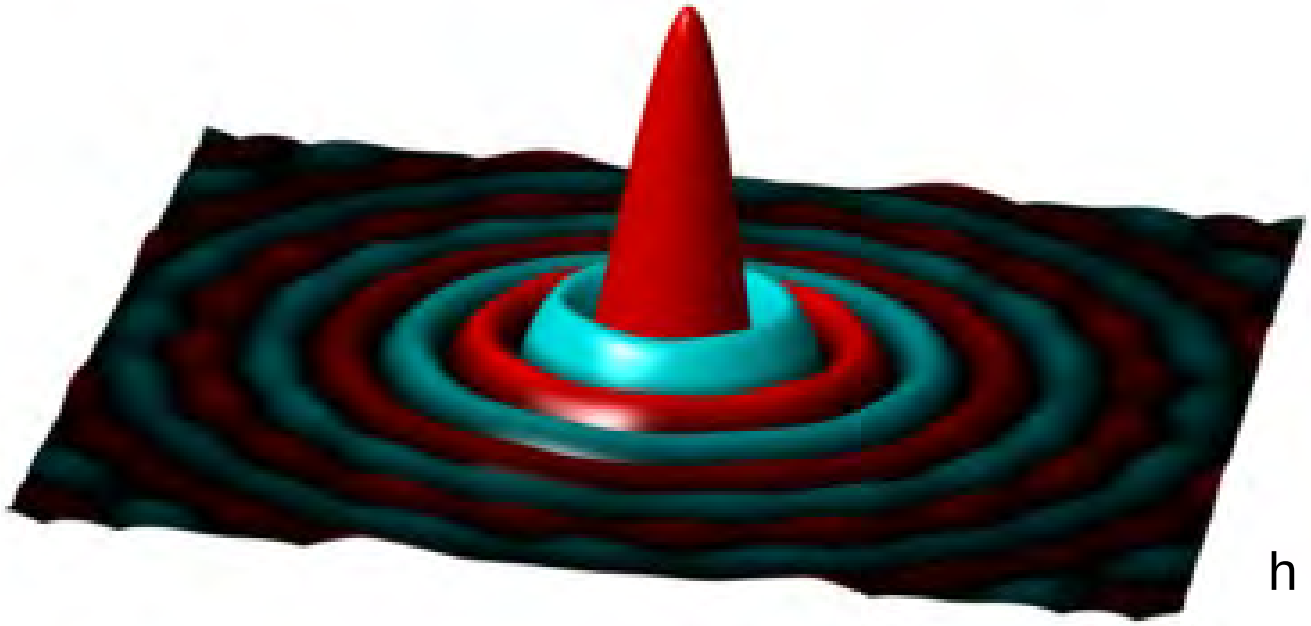
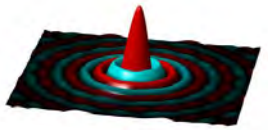


Zero phase color is arbitrary

Building Physics into Figure Generation

To make it easier to visualize the wave amplitude, we can add height:



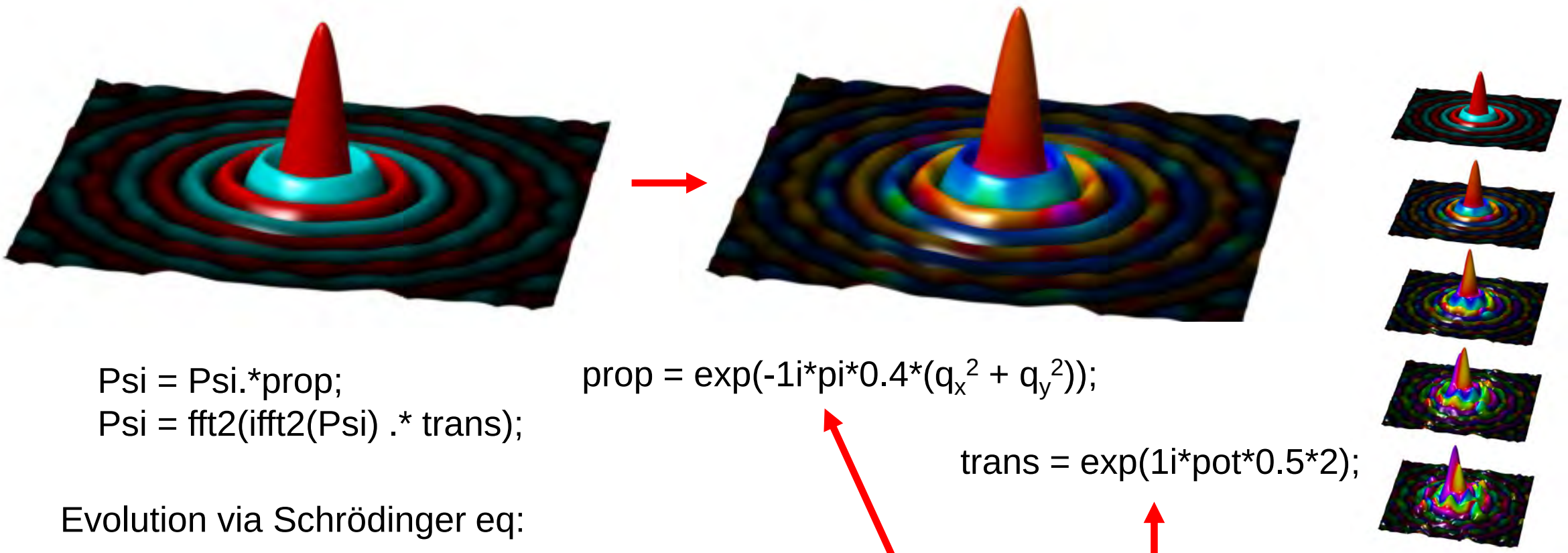


h = abs(psi).^0.8 * 100 * scale(a0);

Scaling is tweaked until it looks good – goal is to visualize the complex wavefunction in one image.

Building Physics into Figure Generation

Next up is evolution of the wavefunction during scattering / propagation:



```
Psi = Psi.*prop;
Psi = fft2(ifft2(Psi) .* trans);
```

prop = exp(-1i*pi*0.4*(q_x^2 + q_y^2));

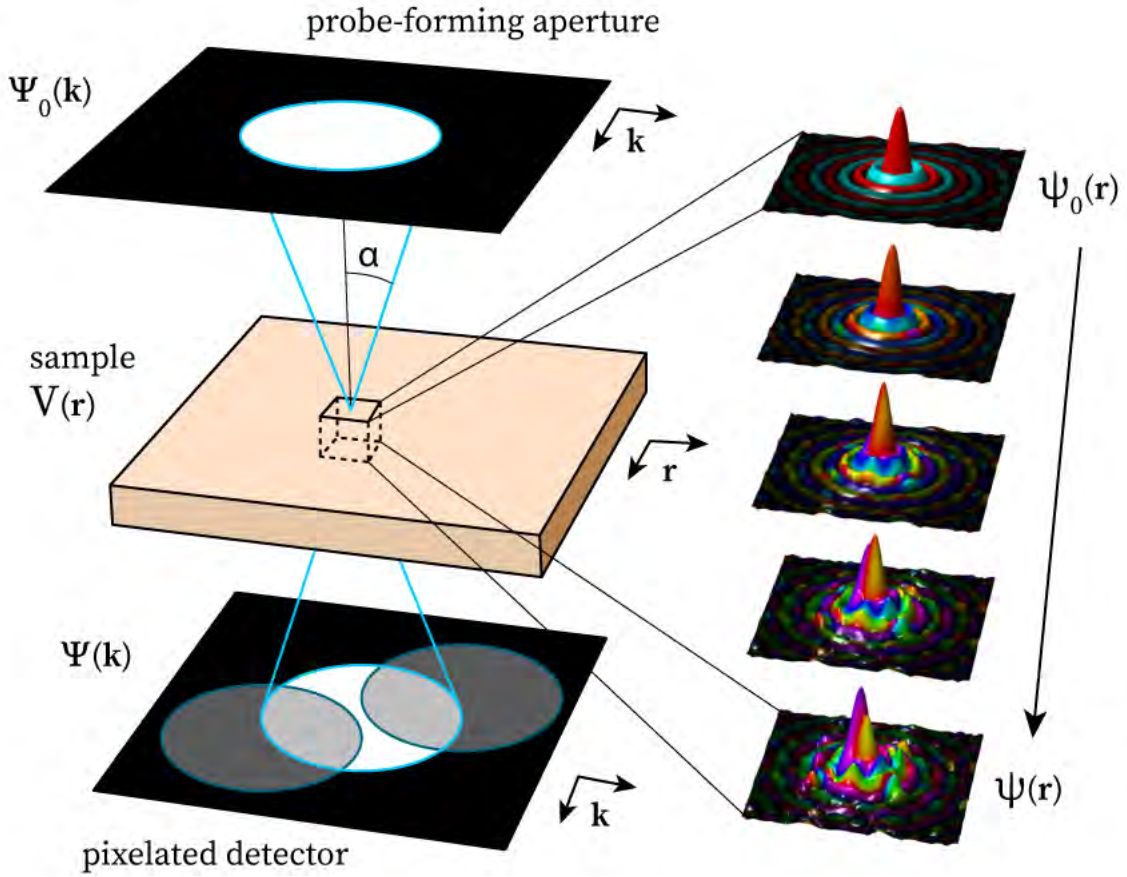
trans = exp(1i*pot*0.5*2);

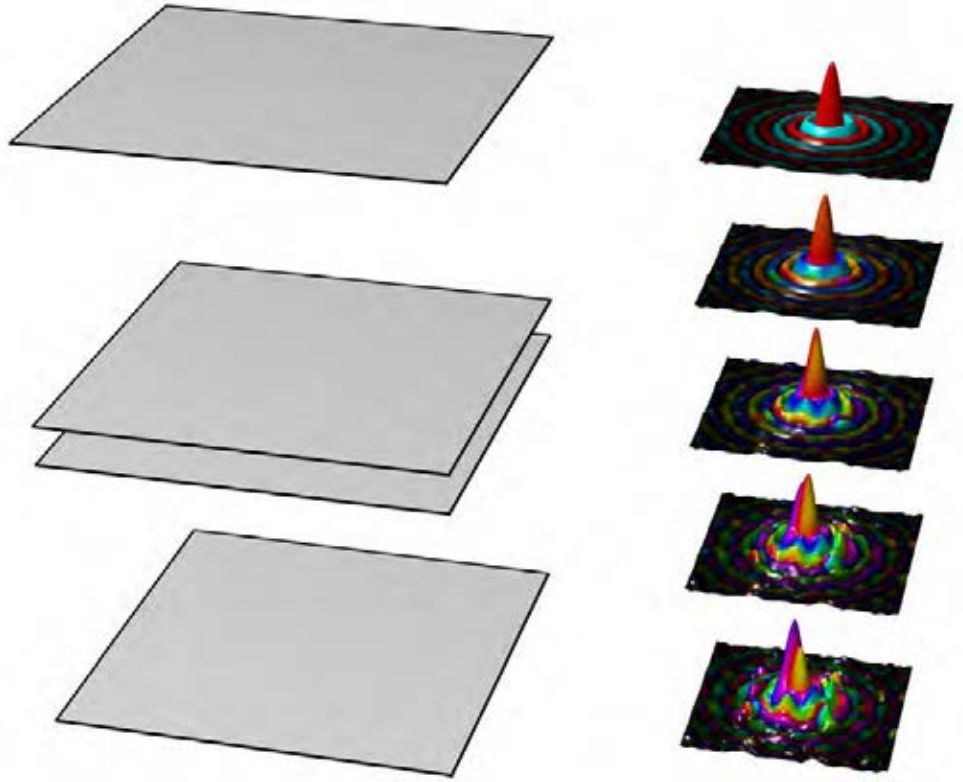
Evolution via Schrödinger eq:

$$i\hbar \frac{\partial}{\partial t}\psi(\vec{r}) = \hat{H}(\vec{r})\,\psi(\vec{r}) \rightarrow \frac{\partial}{\partial z}\psi(\vec{r}) = \frac{i\lambda}{4\pi}\nabla_{xy}{}^2\psi(\vec{r}) + i\sigma V(\vec{r})\psi(\vec{r})$$

Building Physics into Figure Generation

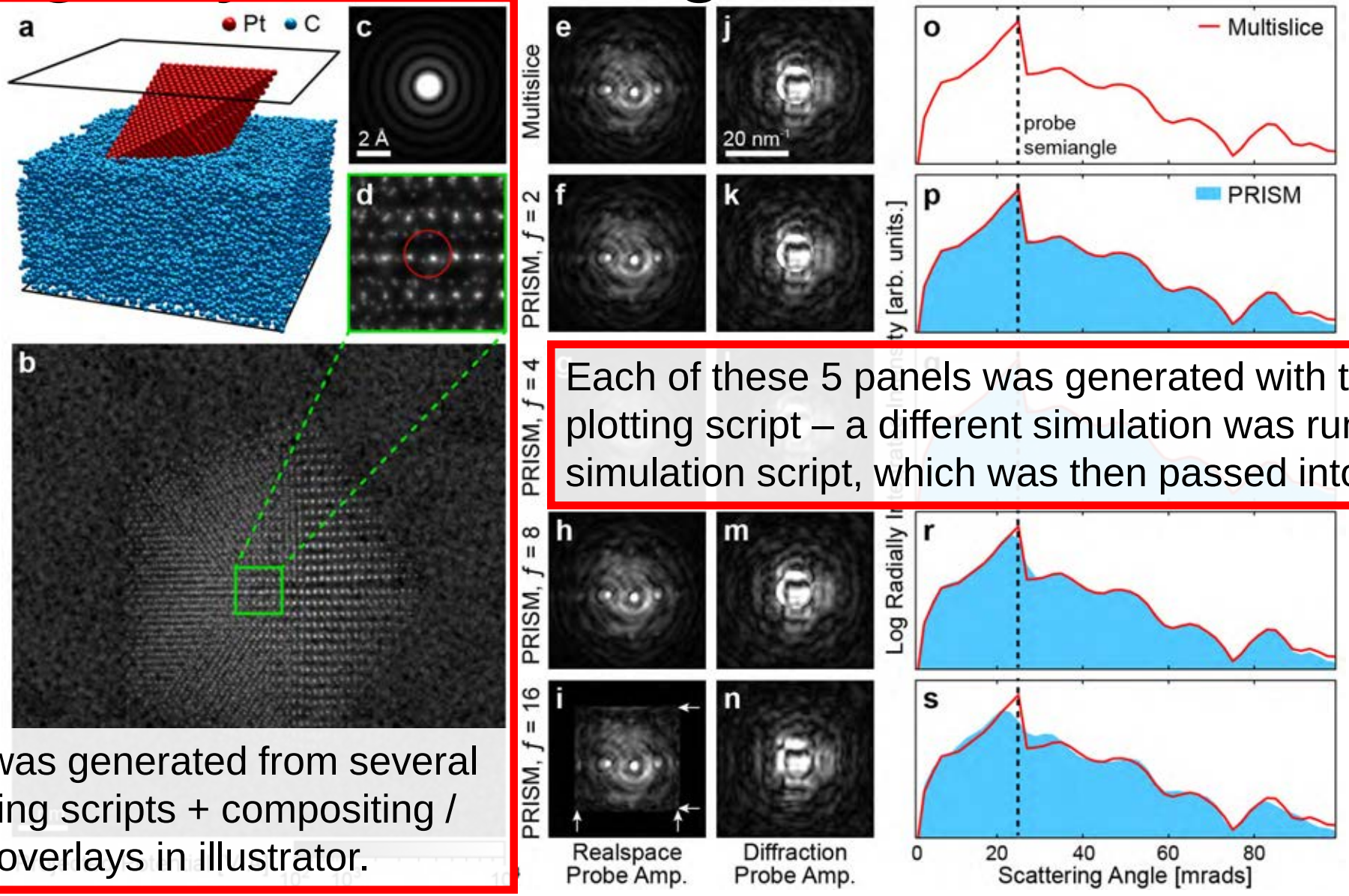
Add 5 time points, composite in illustrator:





Labels and text added, saved in PDF format

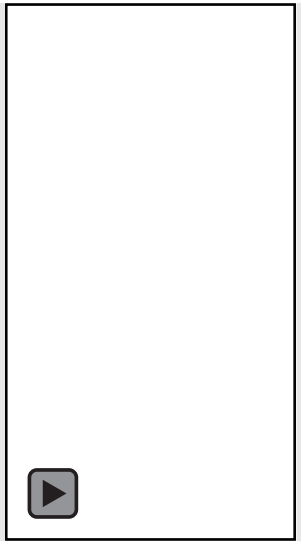
Building Physics into Figure Generation

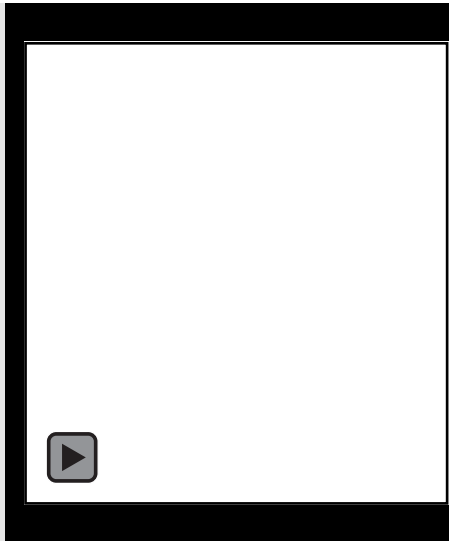


Each of these 5 panels was generated with the same plotting script – a different simulation was run in the simulation script, which was then passed into plotting code.

This panel was generated from several Matlab plotting scripts + compositing / adding text overlays in illustrator.

Outline





1

Basic concepts when making figures and movies – raster vs vector.

2

Scaling, coloring and saving scalar and vector **imaging data**.

3

Plotting **points in 3D**, highlight internal features – e.g. atomic coordinates.

4

Animating 3D points, making **movies** – e.g. atomic coordinates.

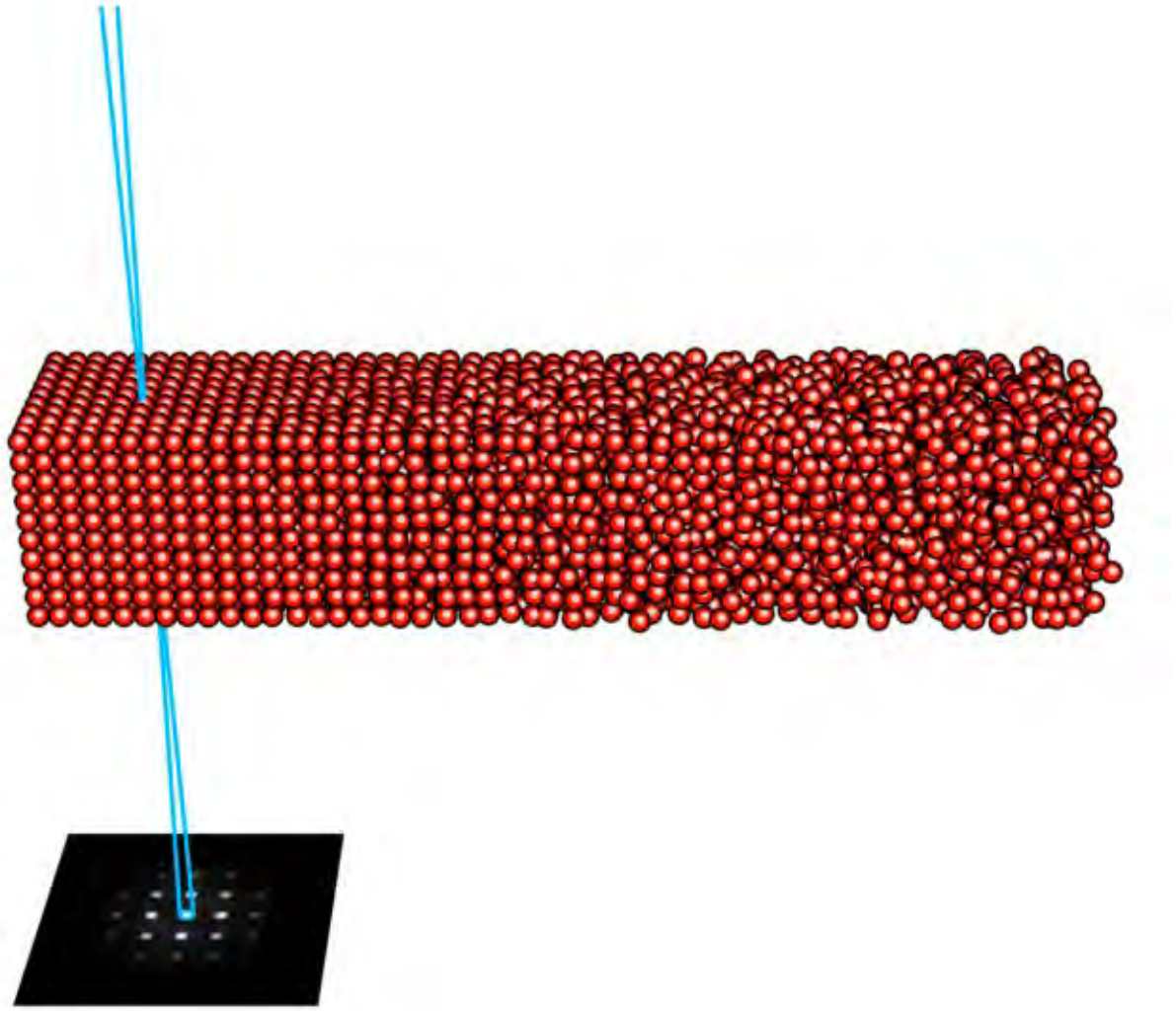
5

Building **physics visualization** and simulation directly into figures.

6

Making simple animations to explain **concepts in physics**.

Examples of Using Movies to Explain Physics

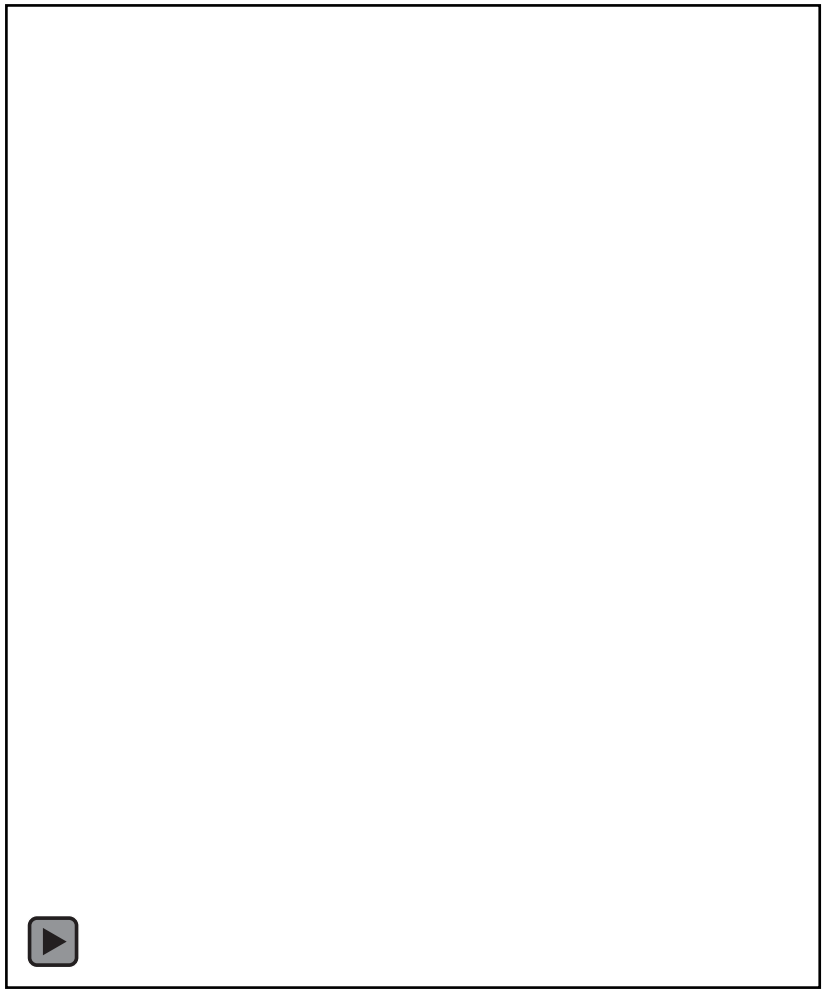


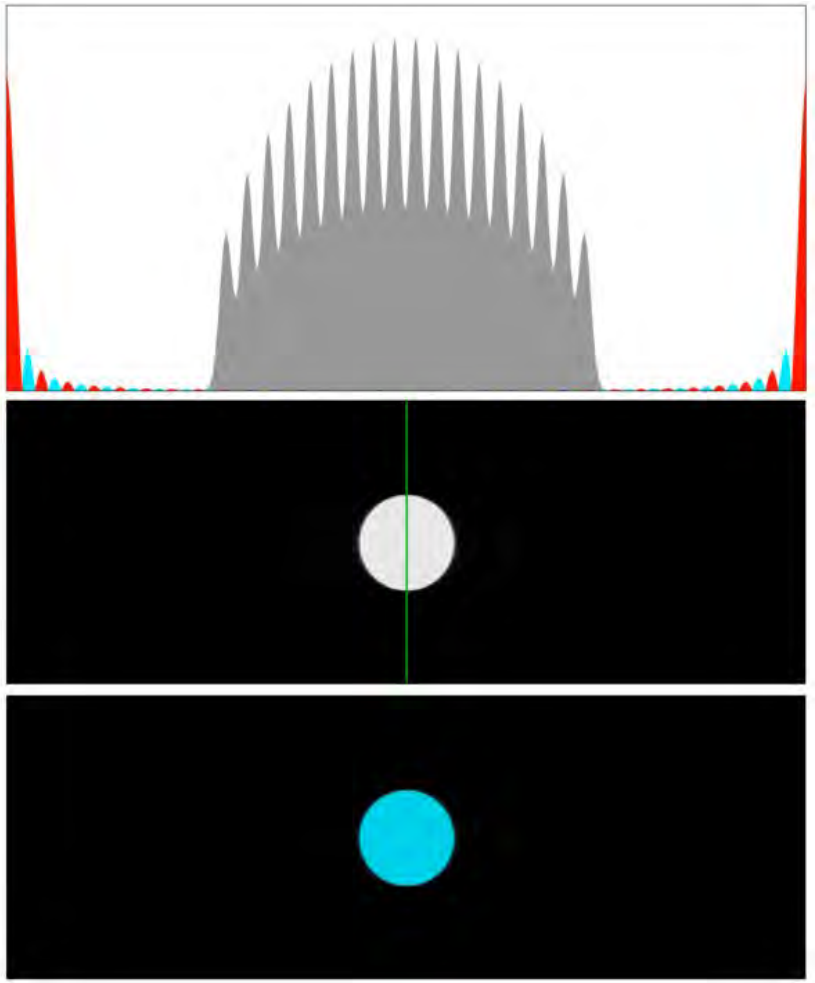
animFEM01(probeSites, rScale)
draws the scene,

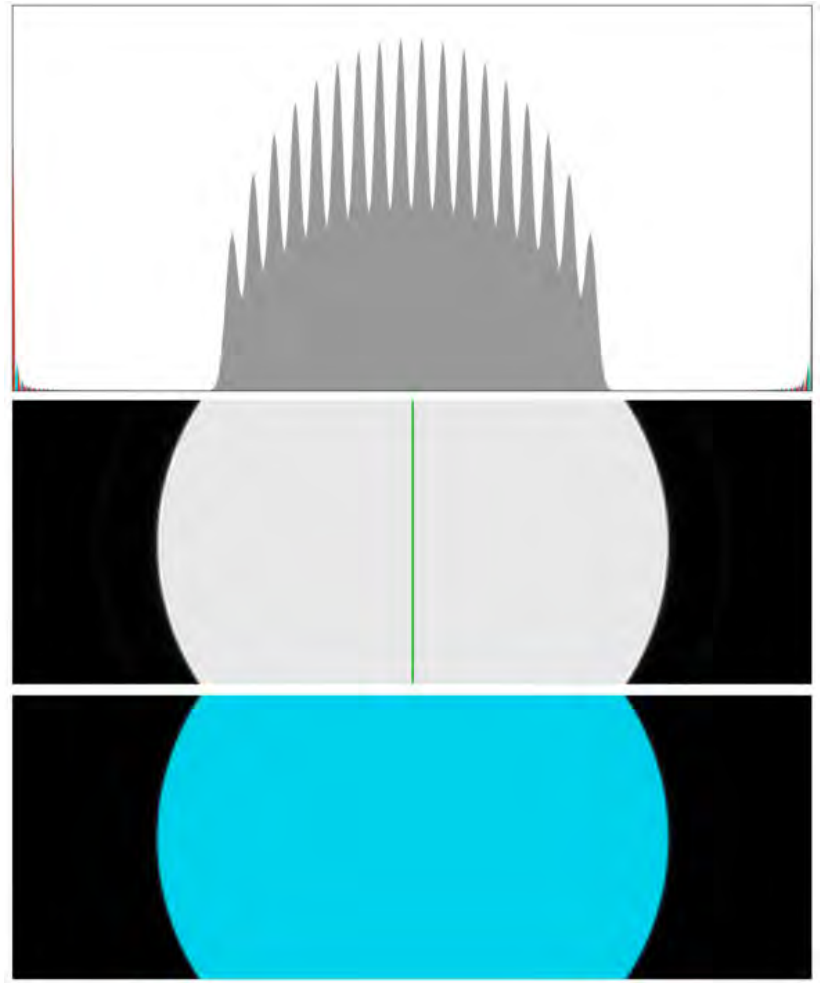
animFEM02()
animates the atoms transforming from ordered → disordered,

animFEM03()
animates STEM probe scanning.

Diff. Phase Contrast – Effect of Probe Semiangle





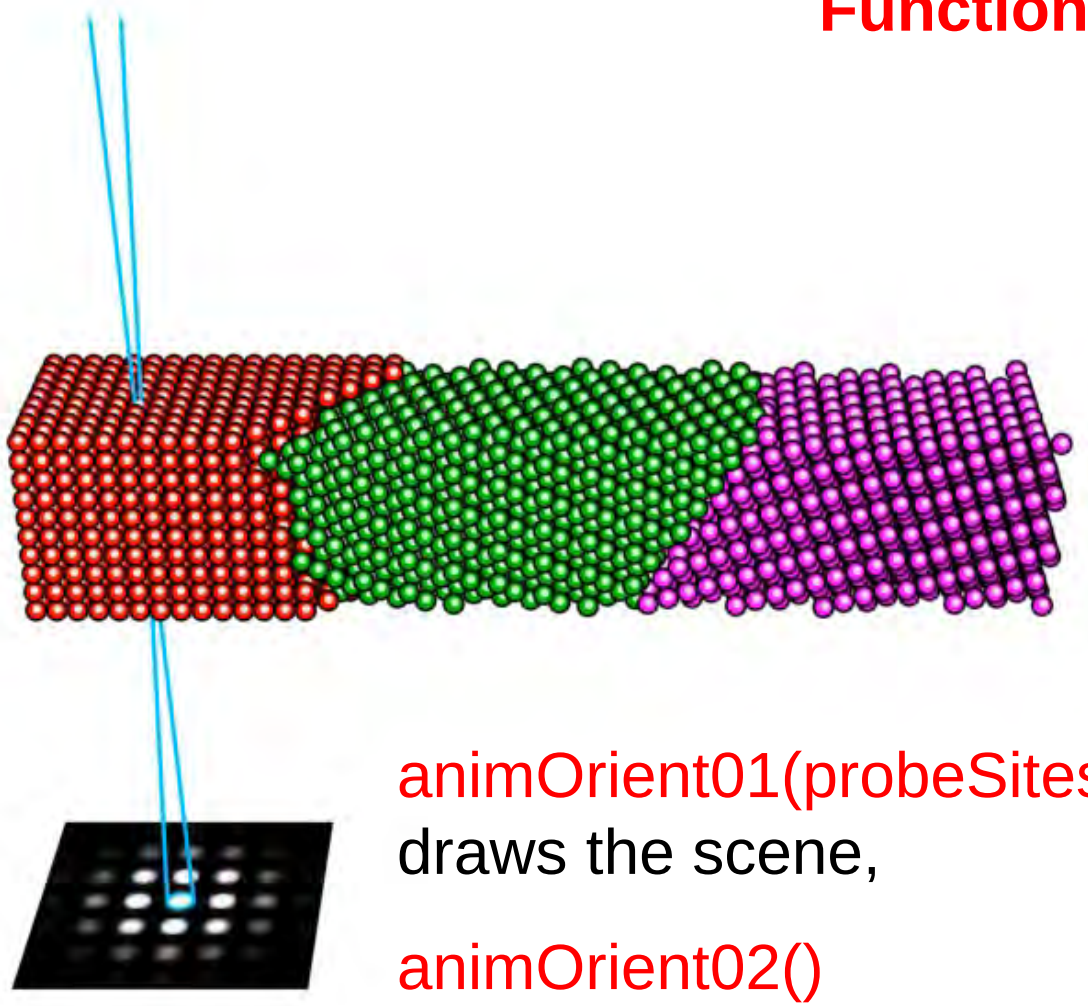


Same sim., plotting and output script for all movies – just change one number!

Try it:

```
>> sDPC = DPC01();
>> DPC02(sDPC);
```

Using a Movie to Explain Diffraction Physics



Functions

line(x,y,z,…)
Probe is just 2 lines and a circle

scatter3(x,y,z,…)
Three grains tiled & rotated, each with 2 scatter plots for the atoms and tints.

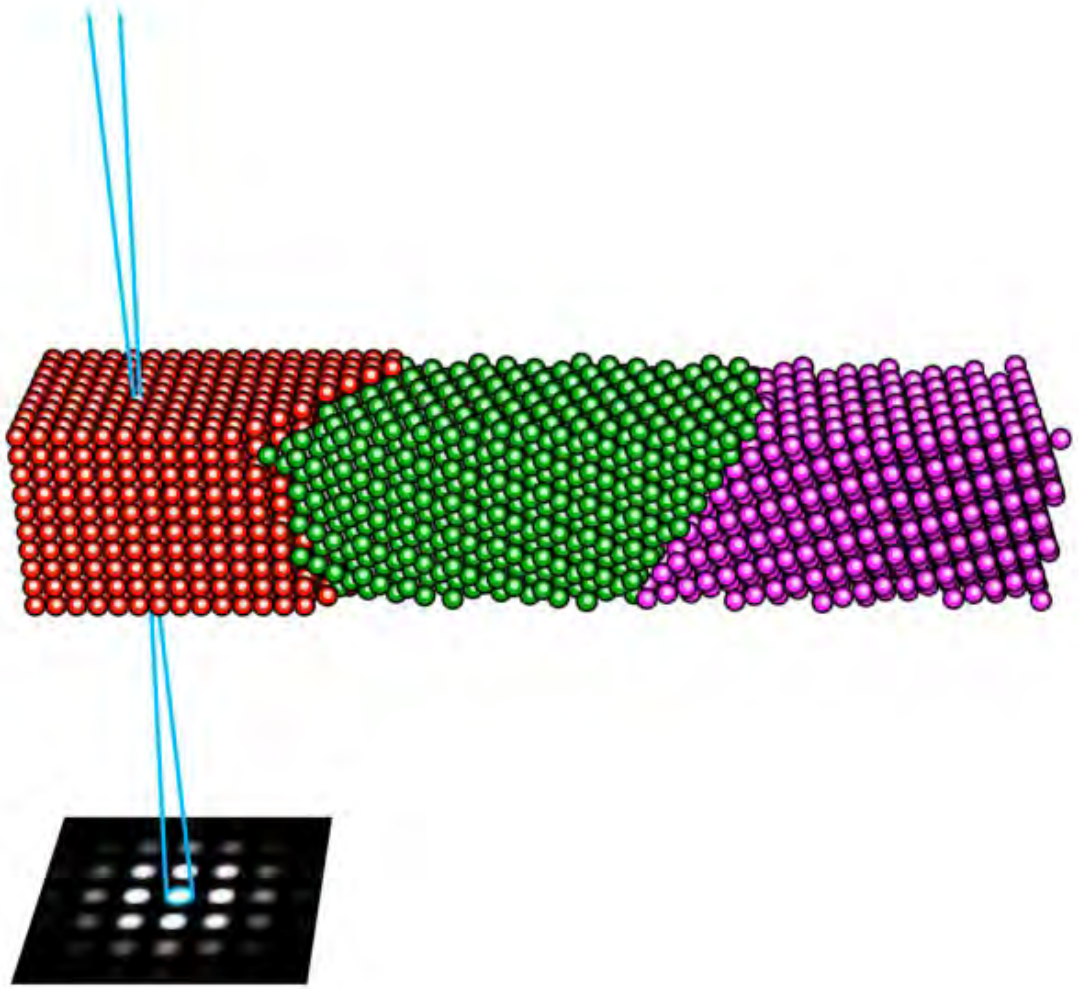
sum(), conv2(), fft2(), …
Images are generated by summing atoms along dim 3, taking the FFT.

warp(), conv2(), fft2(), …
Easy methods for placing a texture-mapped surface in 3D, modifying images.

animOrient01(probeSites)
draws the scene,

animOrient02()
animates it.

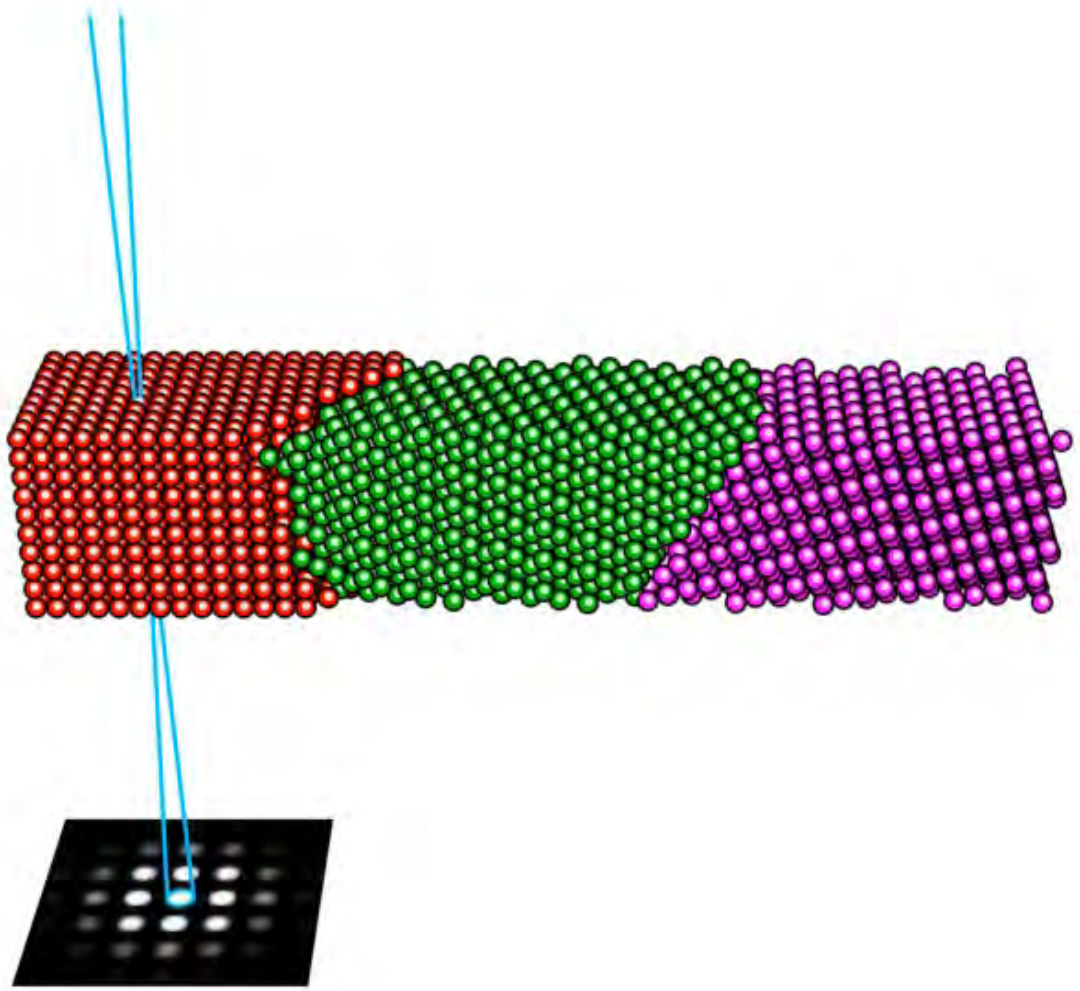
Using a Movie to Explain Diffraction Physics



Building a block of atoms

```
numAtomsMax = max(numAtoms);
v = -round(numAtomsMax/2):round(numAtomsMax/2);
[yy, xx, zz] = meshgrid(v, v, v);
p0 = [xx(:) yy(:) zz(:)];
```

Using a Movie to Explain Diffraction Physics



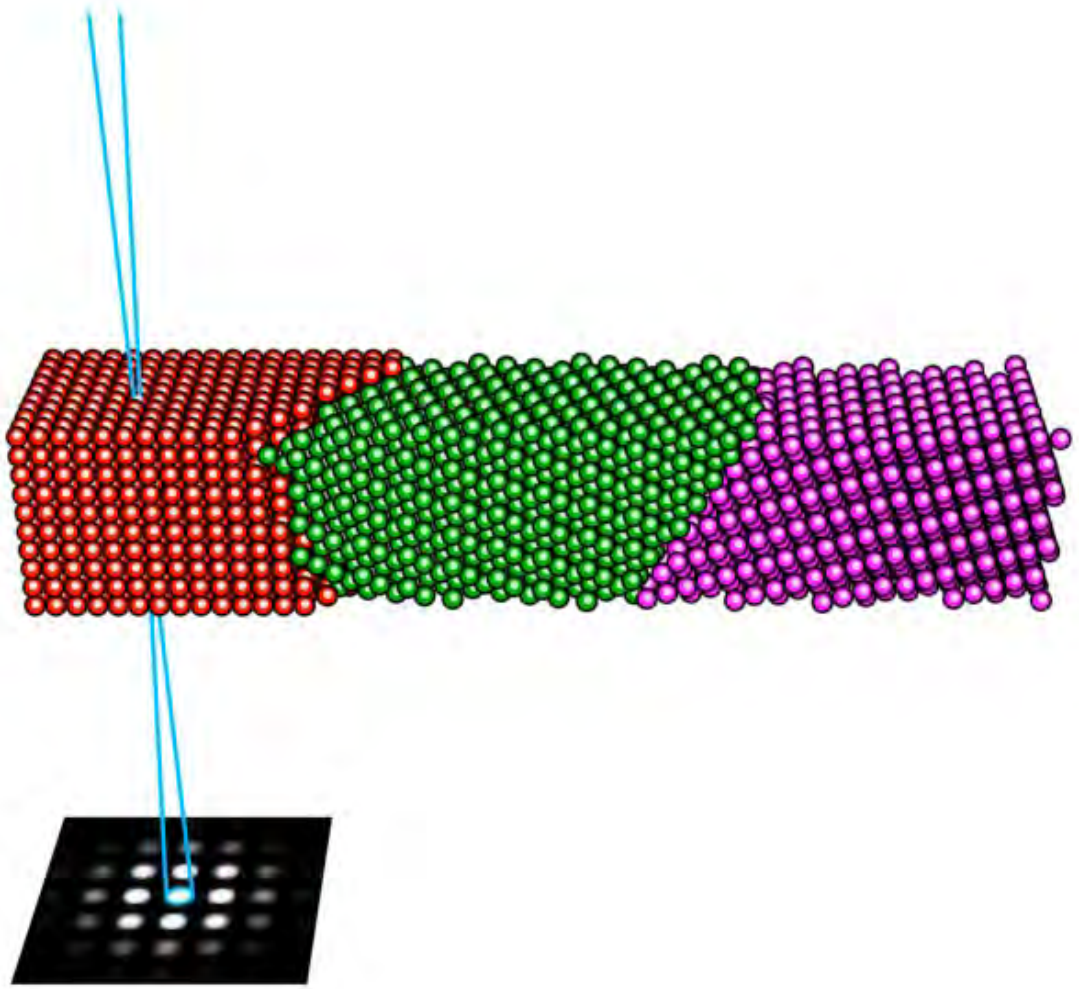
Rotating a block of atoms

```
t = [45 54 -18.43]*pi/180;
m1 = [cos(t(1)) -sin(t(1)) 0;
    sin(t(1)) cos(t(1)) 0;
    0 0 1];
m2 = [1 0 0;
    0 cos(t(2)) -sin(t(2));
    0 sin(t(2)) cos(t(2))];
m3 = [cos(t(3)) -sin(t(3)) 0;
    sin(t(3)) cos(t(3)) 0;
    0 0 1];
p2 = p2 * m1 * m2 * m3;
```

Euler angle rotations:

Axis	Matrix
z	m1
x	m2
z	m3

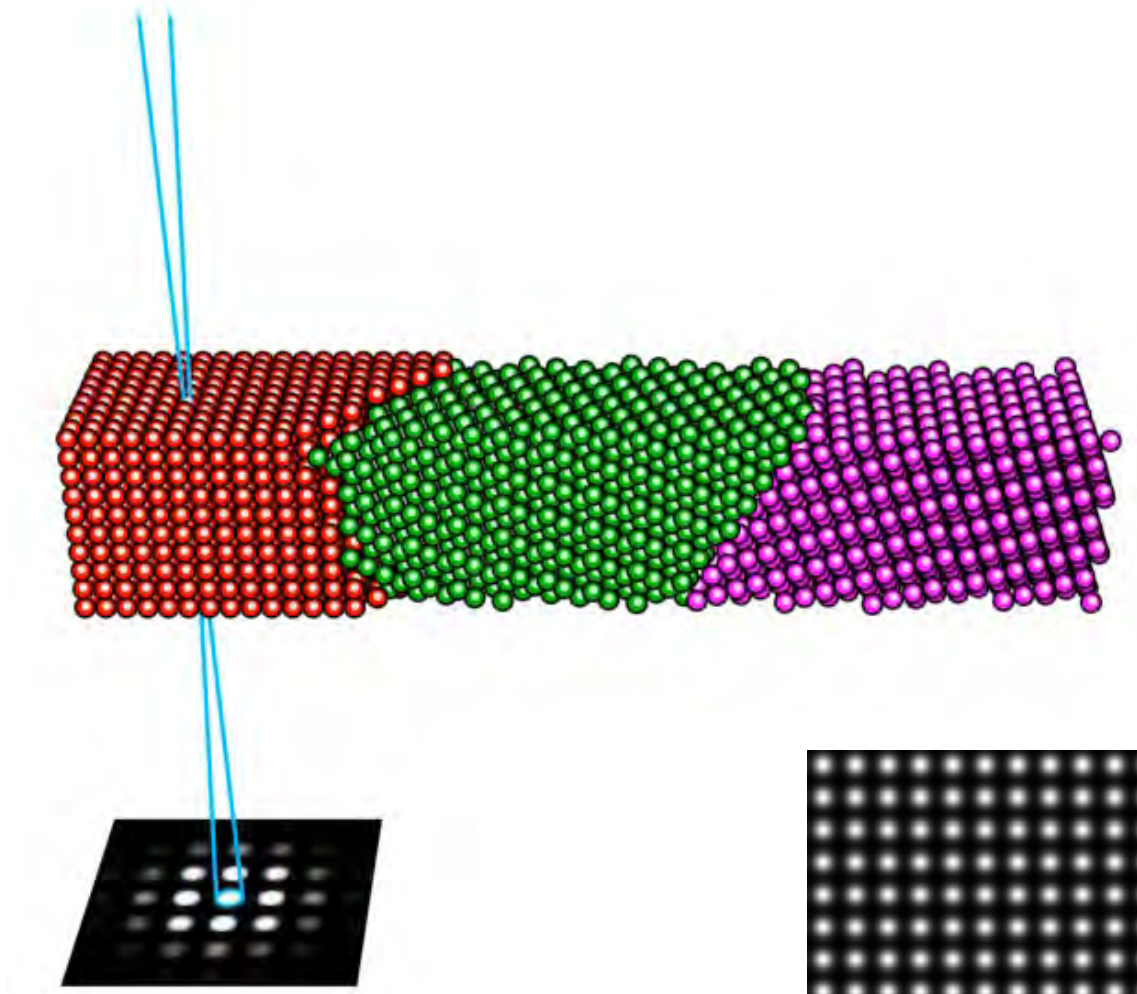
Using a Movie to Explain Diffraction Physics



Deleting atoms on one side of a plane:

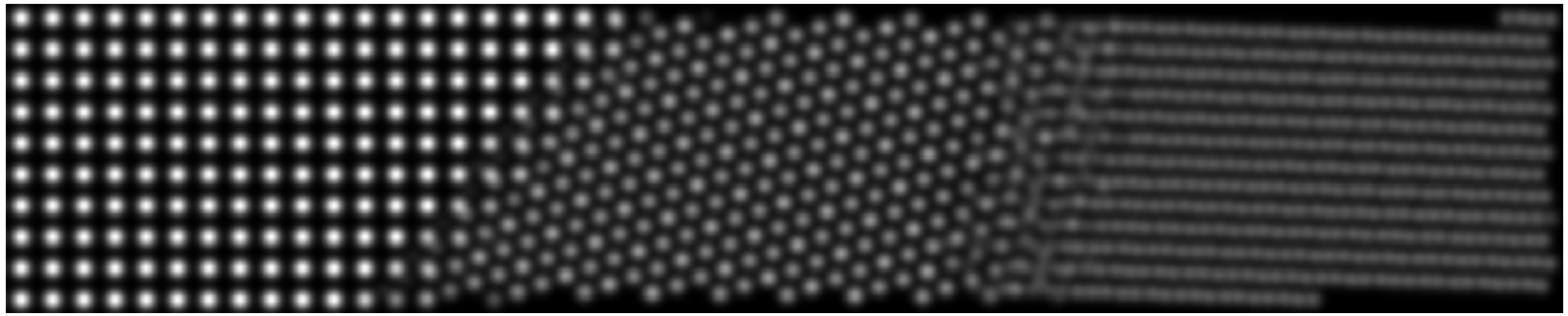
```
abcd12 = [0.2 1 1.2/2 22];
del = p1(:,1) < 1 | p1(:,1) > cellDim(1) ...
    | p1(:,2) < 1 | p1(:,2) > cellDim(2) ...
    | p1(:,3) < 1 | p1(:,3) > cellDim(3) ...
    | p1(:,1)*abcd12(1) + p1(:,2)*abcd12(2) + ...
      p1(:,3)*abcd12(3) > abcd12(4) - 0.1;
p1(del,:) = [];
```

Using a Movie to Explain Diffraction Physics



Create atom image by summing along dim 3, blurring:

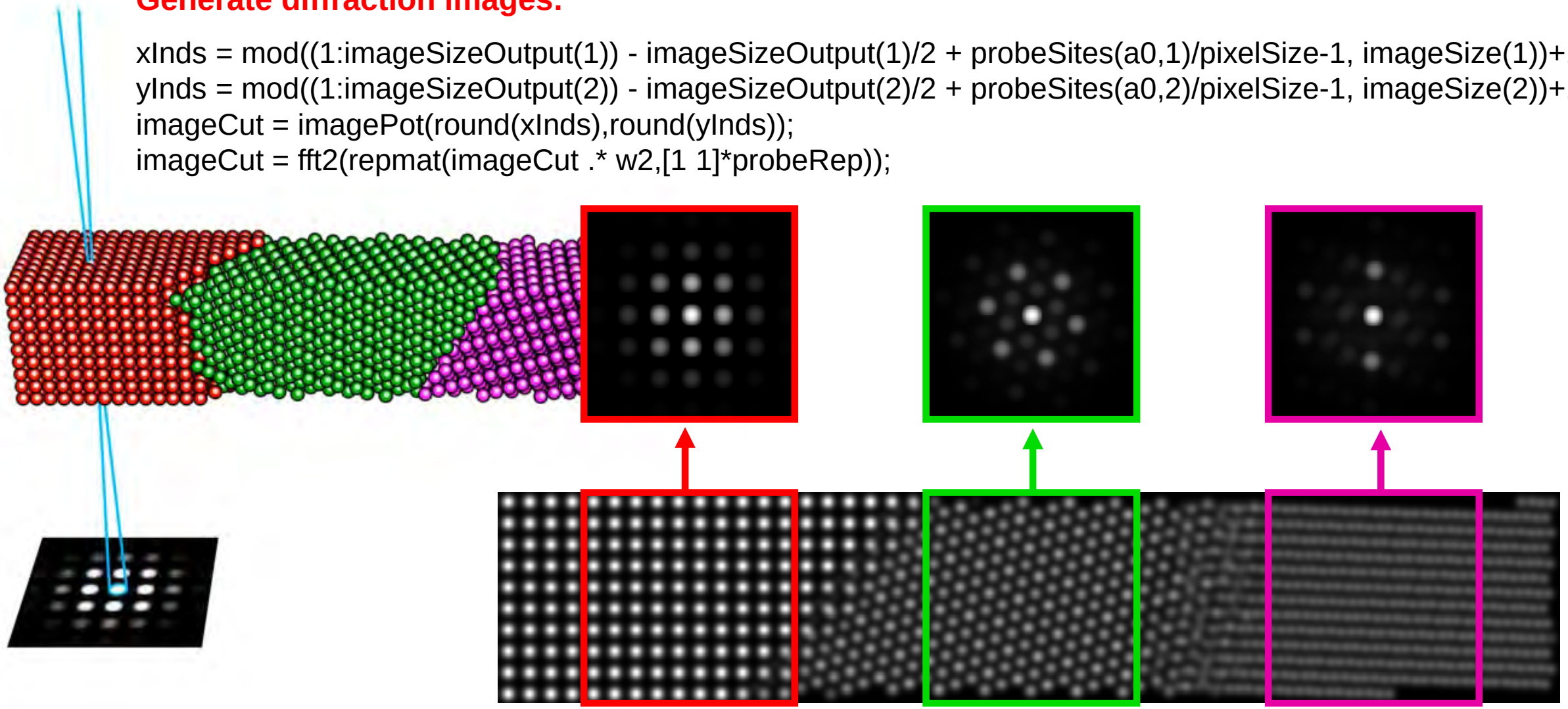
```
k = fspecial('gaussian',2*ceil(4*sigmaAtoms)+1,sigmaAtoms);
imageSize = round(cellDim(1:2) ./ pixelSize);
xInd = (p(:,1) - 0.5) / pixelSize;
yInd = (p(:,2) - 0.5) / pixelSize;
xInd = min(max(round(xInd),1),imageSize(1));
yInd = min(max(round(yInd),1),imageSize(2));
imagePot = accumarray([xInd yInd],...
    ones(length(xInd),1),imageSize);
imagePot(:) = conv2(imagePot,k,'same');
```



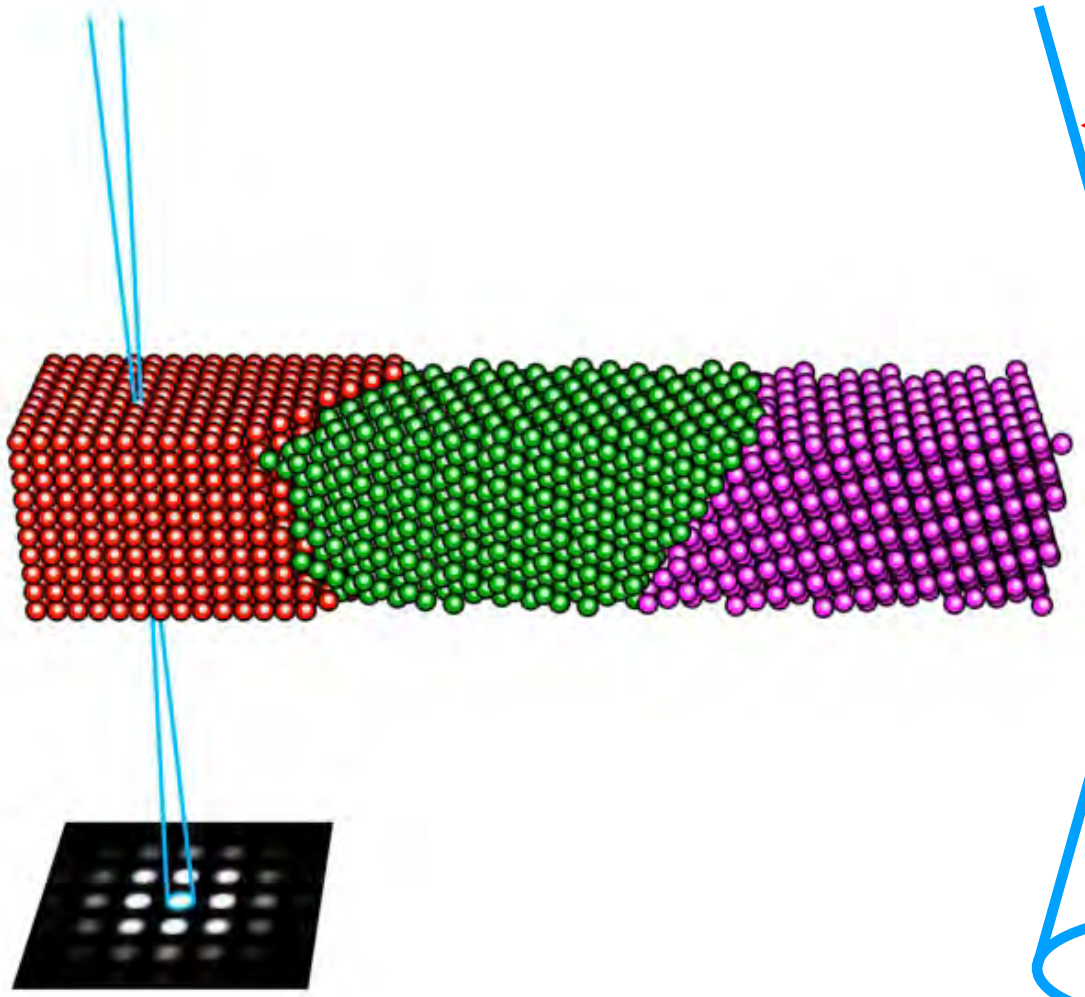
Using a Movie to Explain Diffraction Physics

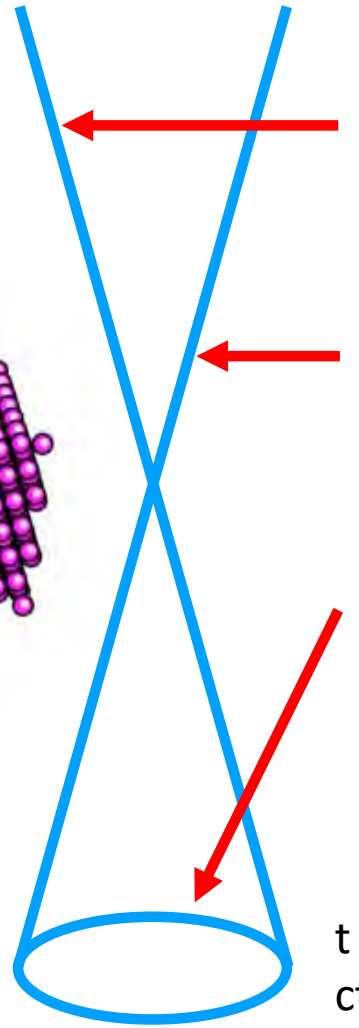
Generate diffraction images:

```
xInds = mod((1:imageSizeOutput(1)) - imageSizeOutput(1)/2 + probeSites(a0,1)/pixelSize-1, imageSize(1))+1;
yInds = mod((1:imageSizeOutput(2)) - imageSizeOutput(2)/2 + probeSites(a0,2)/pixelSize-1, imageSize(2))+1;
imageCut = imagePot(round(xInds),round(yInds));
imageCut = fft2(repmat(imageCut .* w2,[1 1]*probeRep));
```



Using a Movie to Explain Diffraction Physics





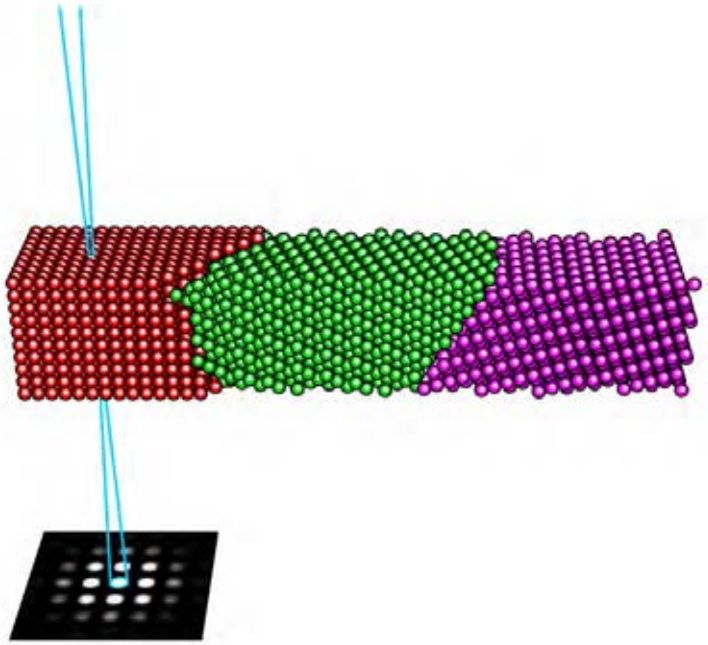
Draw the STEM probe:

```
line([-1 1]*probeRadius+probeSites(a0,2),...
        [0 0]+probeSites(a0,1),...
        probePos([1 3]),...
        'linewidth',linewidthProbes,'color',[0 0.8 1])
line([1 -1]*probeRadius+probeSites(a0,2),...
        [0 0]+probeSites(a0,1),...
        probePos([1 3]),...
        'linewidth',linewidthProbes,'color',[0 0.8 1])
line(ct*probeRadius+probeSites(a0,2),...
        st*probeRadius+probeSites(a0,1),...
        probePos(3)+ct*0,...
        'linewidth',linewidthProbes,'color',[0 0.8 1])
```

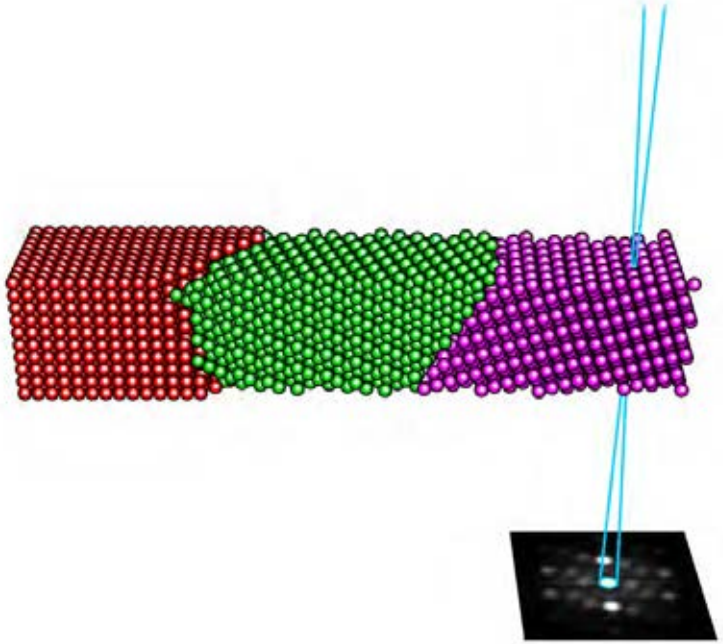
```
t = linspace(0,2*pi,180+1);
ct = cos(t);
st = sin(t);'linewidth',linewidthProbes,'color',[0 0.8 1])
```

Using a Movie to Explain Diffraction Physics

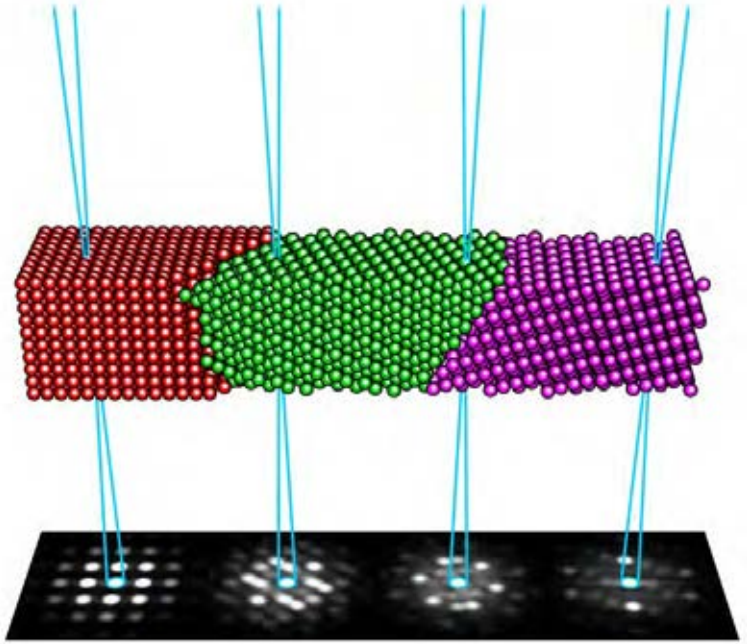
>> animOrient01([5 45]);



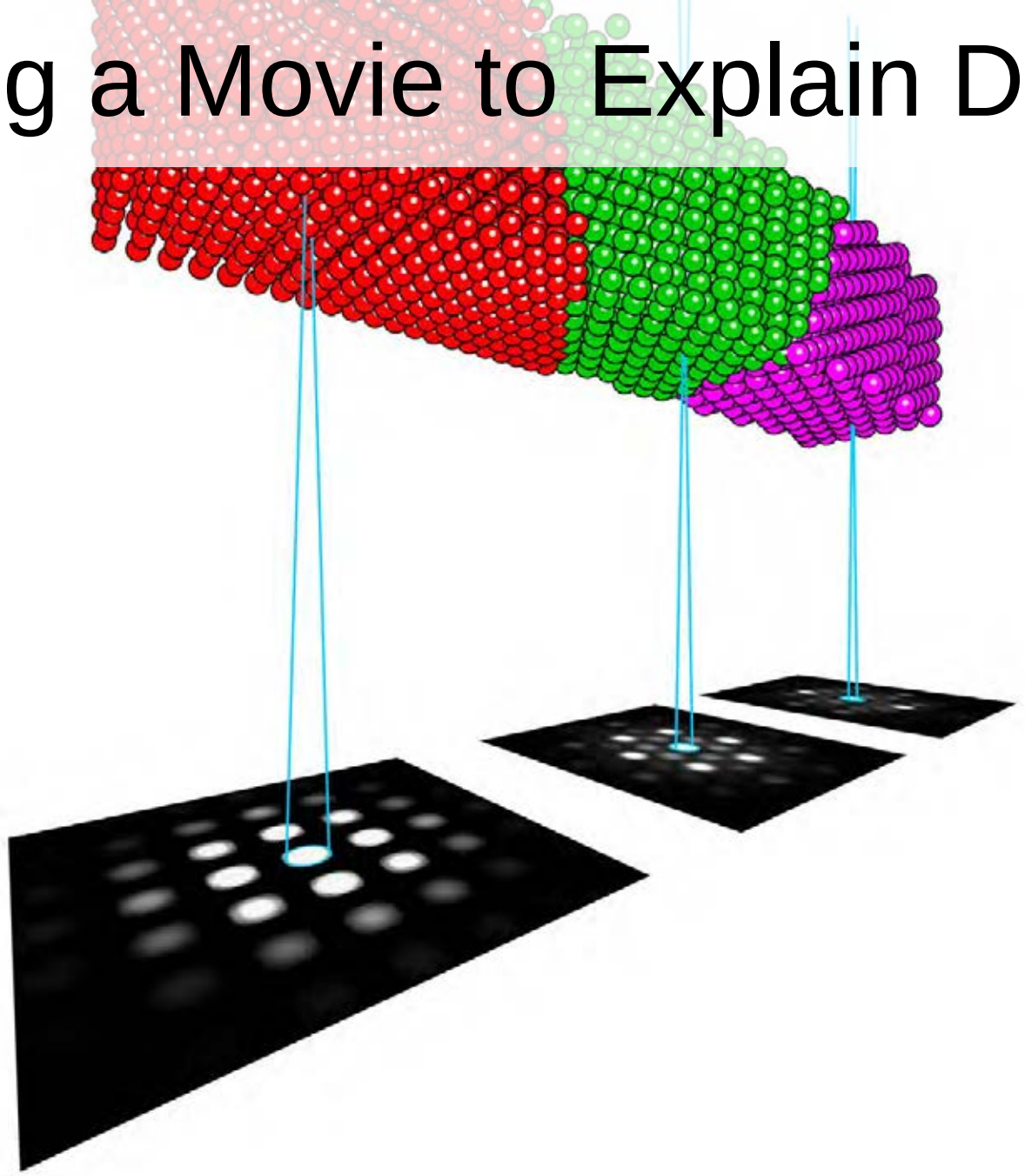
>> animOrient01([5 5]);



>> animOrient01([5 4; 5 18;5 32;5 46]);



Using a Movie to Explain Diffraction Physics

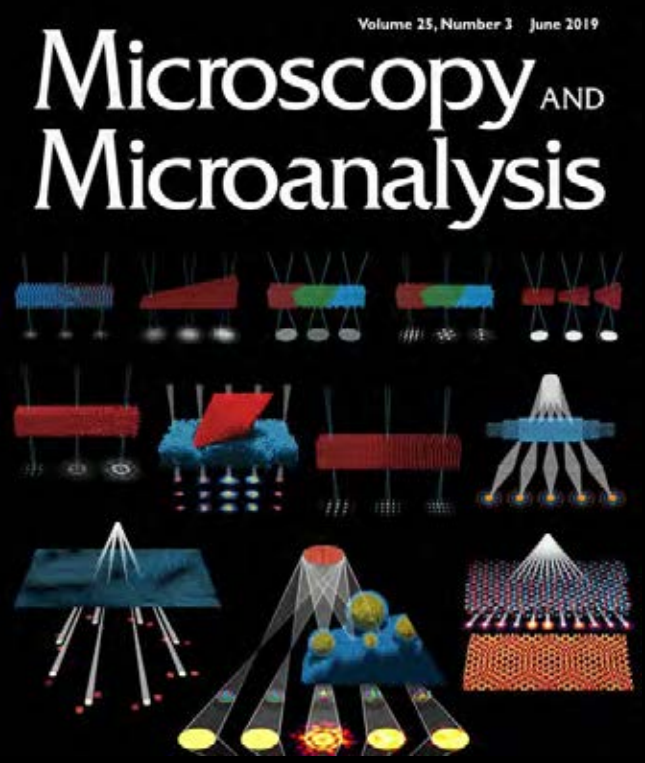


Just play with the camera, plot, image settings until you are happy with the result!

For example:

```
cTar = [0 0 0] + cellDim * 0.5 + [10 5 -15];
cPos = [-2.25 1.75 0]*13;
cAngle = 75;
```

Colin Research Stuff – clophus@lbl.gov

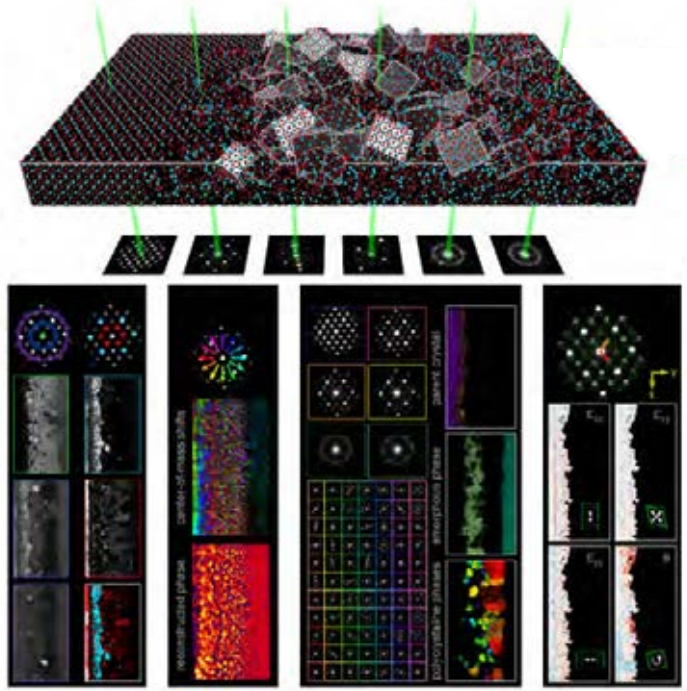


4D-STEM Review

C Ophus, Microscopy and Microanalysis **25**, 563 (2019)

4D-STEM analysis: **py4DSTEM**

www.github.com/py4dstem



www.prism-em.com

Fast 4D-STEM Simulation Code

Source code, GUI programs for Windows, OSX, Linux, tutorials