Applying the Lawler-Fujita algorithm and distortion subtraction by Gao et al. (2017) to real STM images

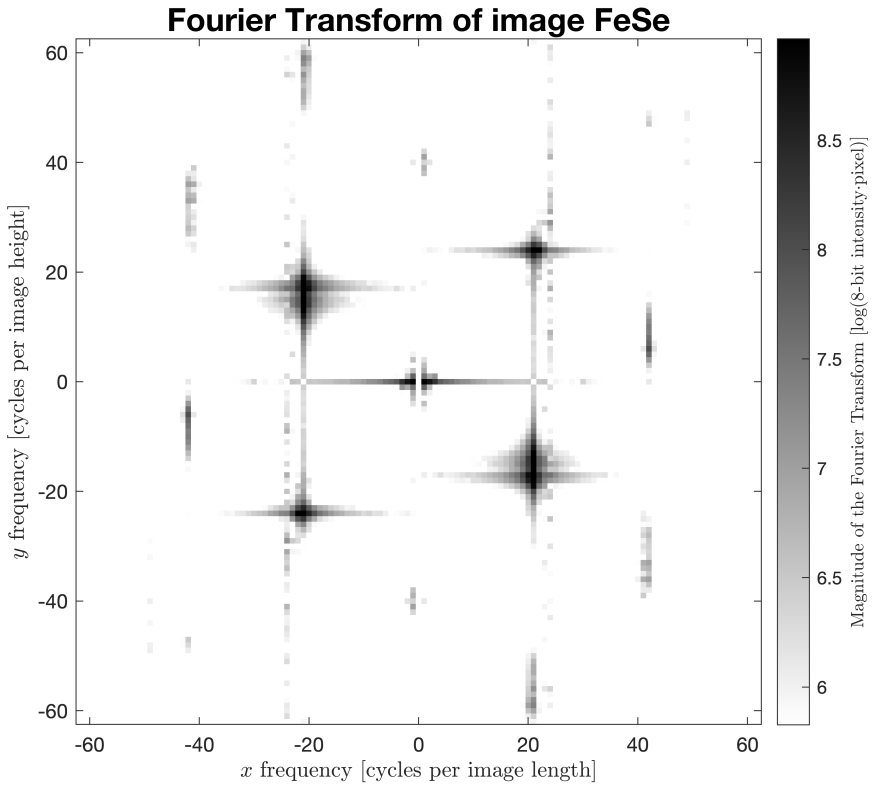
This is another attempt in calculating the displacement field in real STM images with the specific goal of examining the performance of the Lawler-Fujita algorithm and distortion subtraction to elucidate the physical strain present in the real sample.

1 Importing an image

```
[~, lattice] = loadsxm('FeSe_Topos_025.sxm', 1);
```

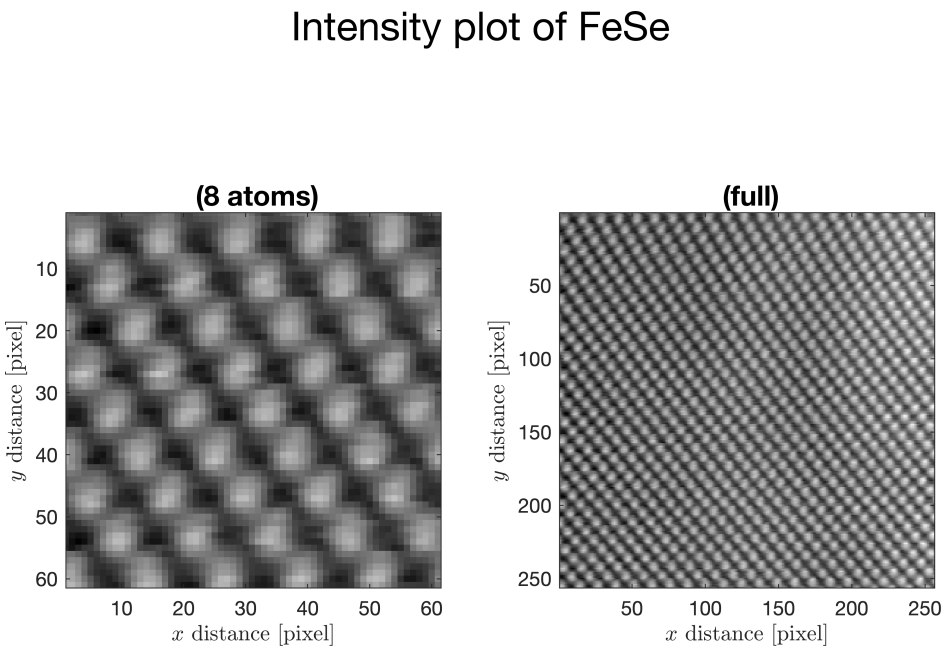
Image specifications

```
[image_height, image_length] = size(lattice);
lattice = reshape(normalize(lattice(:)),image_height,image_length);

lattice = (lattice-mean(lattice,2))./std(lattice,1,2);
% normalize per row. Adapted from Kirsty's topo042401.m

[lattice_fft, Q_x] = myFFT(lattice,"FeSe");
```




```
% xlim([-68 68]);
% ylim([-68 68]);

atom_diameter = 1/sqrt((Q_x(1)/image_length)^2+(Q_x(2)/image_height)^2); % [pixel]
```

```
comboPlot(lattice,"FeSe",atom_diameter);
```




```
lambda_scoring_weights = [1 1 0.05];
% distortion, noise, proportion weights in selecting lambda

% Q_x = [70 54]; % [atom^-1]
Q_y = [-Q_x(2) Q_x(1)]; % just to ensure orthogonality

confidence_level = 0.9999999;
```

Distortion parameters estimates

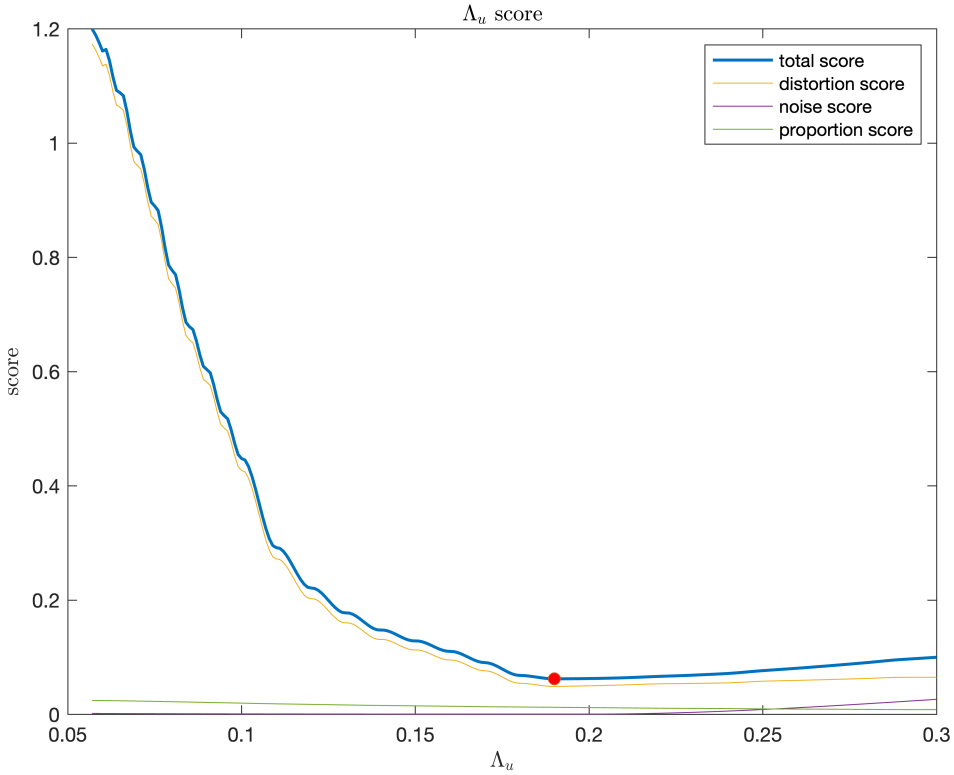
```
drift      =  [5 5; 10 10]; % [atom/scan]
hysteresis =  [2 2; 5 5]; % [atom]
creep      =  [2 2; 5 5]; % [atom]
```

Noise parameters estimates

```
noise_minimumLength = 15; % [atom]
noise_stdMagnitude = 1; % [atom]
```

Pre-processing the inputs, converting units. You might probably would't want to edit these.

```
lambda = lambdaChoose(drift,hysteresis,creep, ...
    noise_minimumLength,noise_stdMagnitude,lambda_scoring_weights); % [atom^-1]
```




```
Optimized lambda = 0.19
```

```
% works only for 256 by 256 images
if ~(image_length==256 && image_height==256)
    lambda = 0.2;
end

disp("Lambda used = " + lambda);
```

```
Lambda used = 0.19
```

```
lambda = lambda*2*pi/atom_diameter;
Q_x = Q_x * 2*pi / (norm(Q_x)*atom_diameter);
Q_y = Q_y * 2*pi / (norm(Q_y)*atom_diameter);
zscore = zscorer(confidence_level);
```

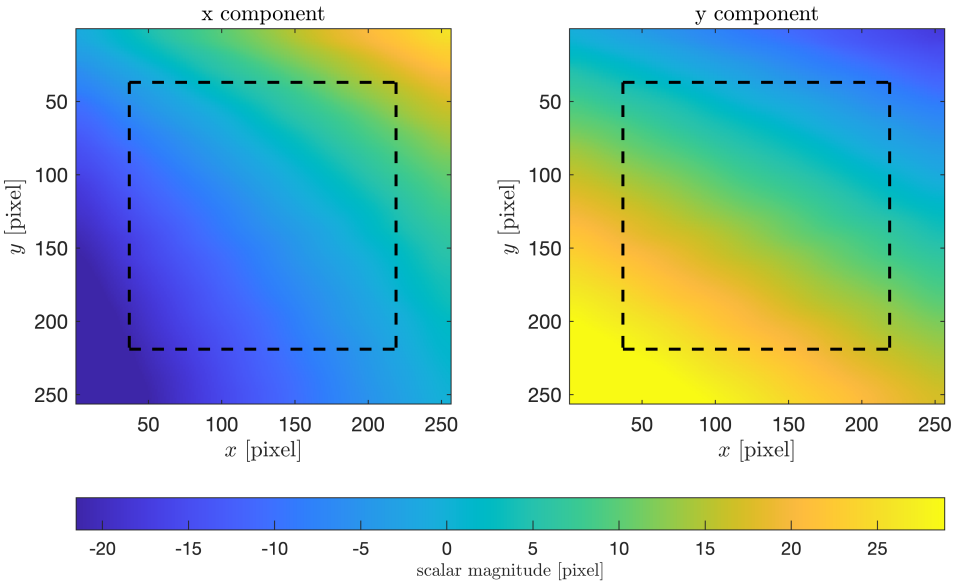
2 Calculating total distortion

Using the Lawler-Fujita algorithm, the total distortion as the sum of the imaging distortion and the physical strain, $\vec{u}_{calc} = \vec{d} + \vec{s}$, is calculated. The effects of noise and the magnitude and type of tolerable distortion could be studied using the previous and the following code.

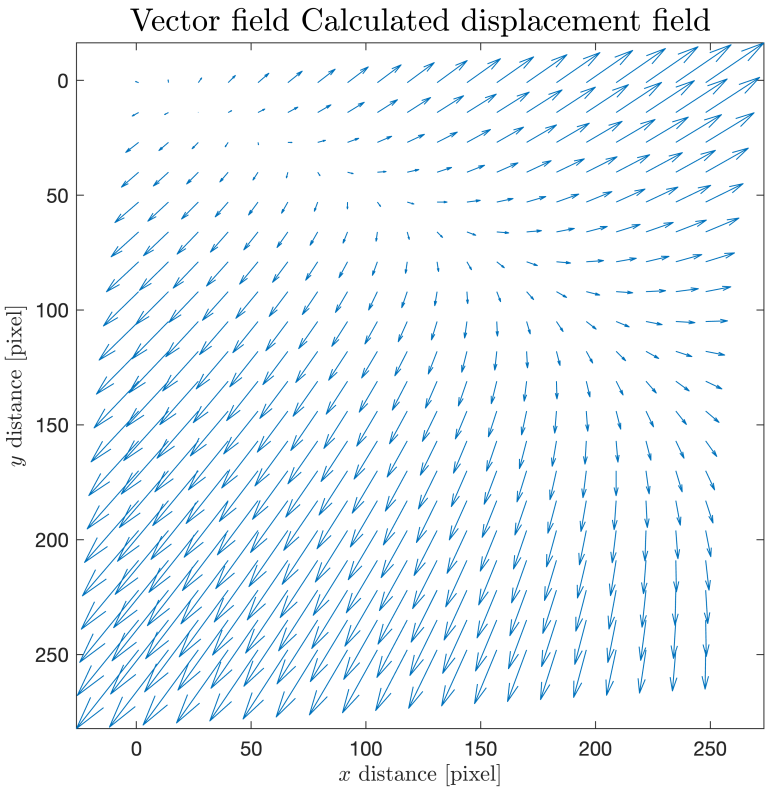
```
ucalc = myConv(lattice,Q_x,Q_y,lambda,zscore,true); % true as last argument to plot u_
```

```
BranchCuts: No residues, length(rowres)=0; sum(abs(residue_charge))=0; sum(abs(residue_charge_masked))=0
BranchCuts: No residues, length(rowres)=0; sum(abs(residue_charge))=0; sum(abs(residue_charge_masked))=0
```

Values of calculated total distortion




```
uPlot(ucalc,"Calculated displacement field");
```



```
if image_length-2*ceil(zscore/lambda)<=0 && image_height-2*ceil(zscore/lambda)<=0
    error("ERROR! No pixels without padded zeros remain.");
else
    npixel = (image_length-2*ceil(zscore/lambda))*(image_height-2*ceil(zscore/lambda))
    % the number of pixels averaged
    disp("Number of pixels averaged: " + npixel + " (" + ...
        npixel/(image_length*image_height)*100 + "%)");
end
```

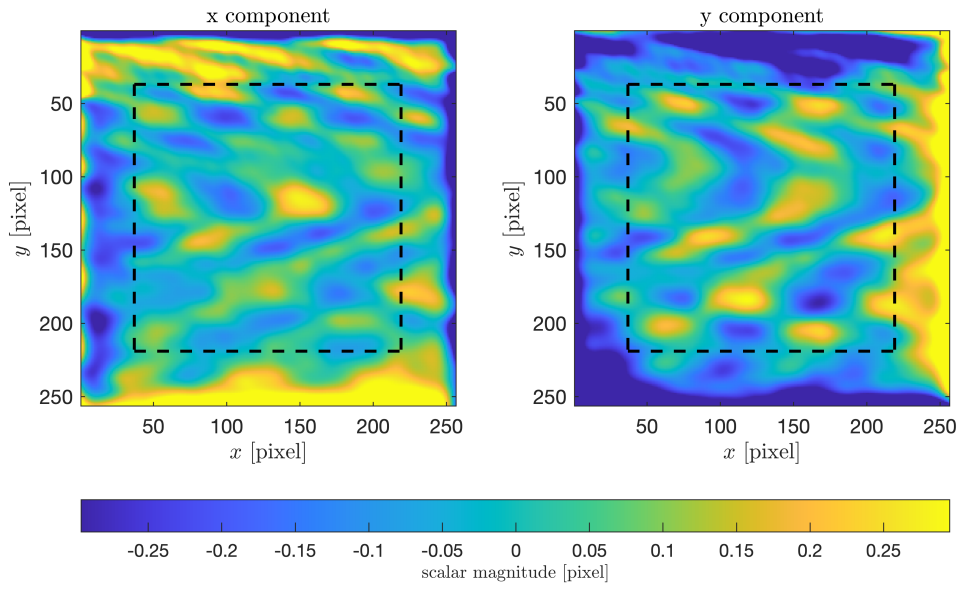
```
Number of pixels averaged: 33124 (50.5432%)
```

3 Calculating physical strain

From the equation given above, the physical strain can be obtained by subtracting the smooth, third-digree polynomial imaging distortion from the total distortion.

```
[fitresultx, gofx,outputx] = createFit(ucalc(:,:,1), lambda,zscore);
% fitPlot(fitresultx, ucalc(:,:,1), "$u_x$", lambda,zscore);
[fitresulty, gofy,outputy] = createFit(ucalc(:,:,2), lambda,zscore);
% fitPlot(fitresulty, ucalc(:,:,2), "$u_y$", lambda,zscore);

resx = reshape(outputx.residuals,image_height-2*ceil(zscore/lambda)+1,[]);
resy = reshape(outputy.residuals,image_height-2*ceil(zscore/lambda)+1,[]);
mu = zeros(2,1); sigma = zeros(2,1);
mu(1) = mean(resx,"all")/atom_diameter; % [lattice constant]
sigma(1) = std(resx,1,"all")/atom_diameter; % [lattice constant]
mu(2) = mean(resy,"all")/atom_diameter; % [lattice constant]
sigma(2) = std(resy,1,"all")/atom_diameter; % [lattice constant]

[xi,yi] = meshgrid(1:image_length,1:image_height);

strain = zeros(size(ucalc));
strain(:,:,1) = ucalc(:,:,1)-fitresultx(xi,yi);
strain(:,:,2) = ucalc(:,:,2)-fitresulty(xi,yi);

convPlot(strain(:,:,1),"calculated physical strain",strain(:,:,2),lambda,zscore);
```

Values of calculated physical strain




```
disp("Physical strain along x = " + (sigma(1)) + " [lattice constant]");
```

```
Physical strain along x = 0.011602 [lattice constant]
```

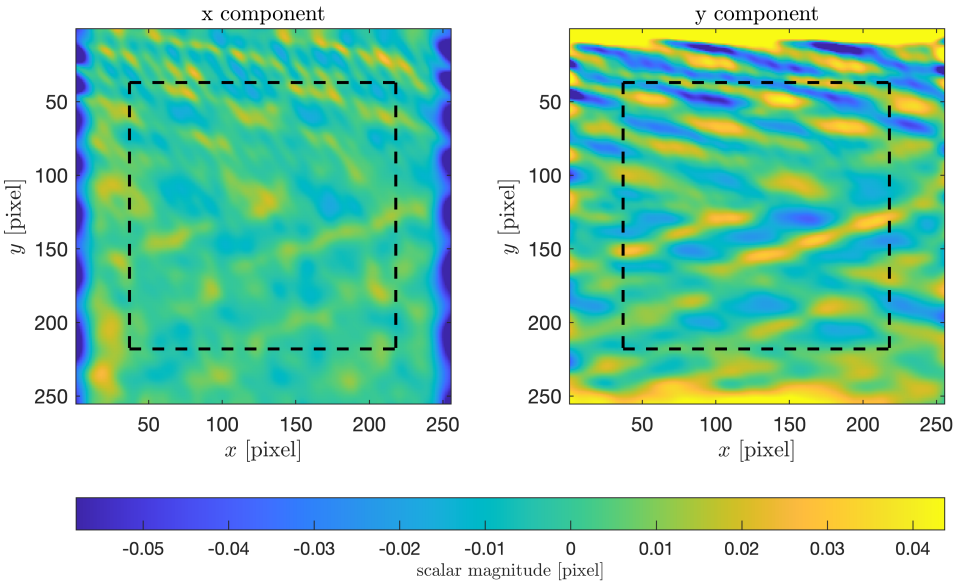
```
disp("Physical strain along y = " + (sigma(2)) + " [lattice constant]");
```

```
Physical strain along y = 0.014271 [lattice constant]
```

The strain and it's first order partial derivatives are calculated and plotted. Biaxial and approximate uniaxial strain maps are also generated from the previous calculations.

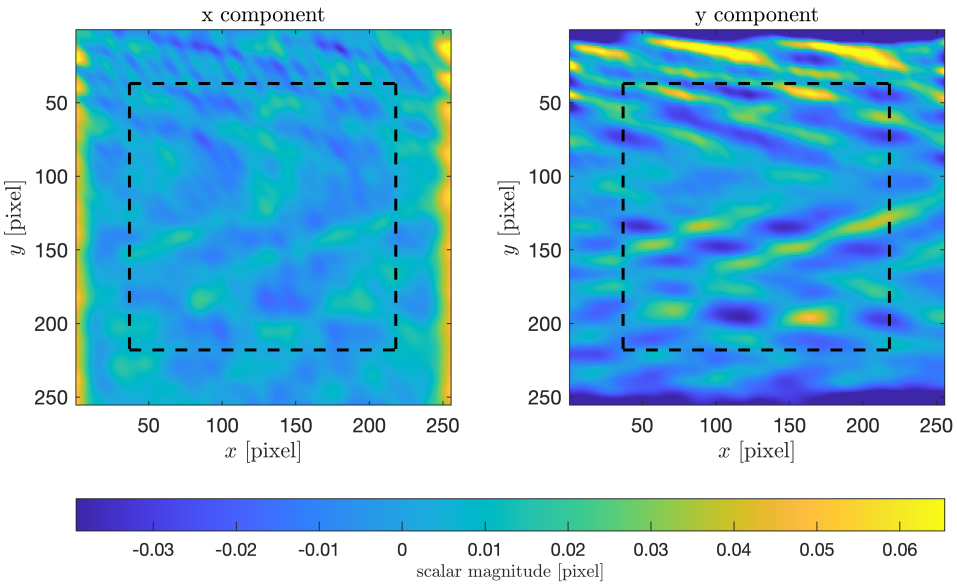
```
Sxdx = diff(strain(1:end-1,:,1),1,2);
Sxdy = diff(strain(:,1:end-1,1));
Sydx = diff(strain(1:end-1,:,2),1,2);
Sydy = diff(strain(:,1:end-1,2));
convPlot(Sxdx,"derivative of physical strain in x",Sxdy,lambda,zscore);
```

Values of derivative of physical strain in x




```
convPlot(Sydx,"derivative of physical strain in y",Sydy,lambda,zscore);
```

Values of derivative of physical strain in y



```
convPlot((Sxdx+Sydy)/2,"biaxial and uniaxial strain",(Sxdx-Sydy)/2,lambda,zscore);
```

Values of biaxial and uniaxial strain