Correlation between elevation variation and the strain maps

This live script is used to evaluate the correlation between the defined elevation variation or "noise" and the calculated biaxial and uniaxial strain maps after applying the Lawler-Fujita algorithm and the smooth surface subtraction by Gao et al. (2018).

Image specifications and distortion parameters

All the initializations required for simulating a crystal lattice is included in this preliminary section. Most of the values and variable names are self-explanatory apart from a few which are explained next. The elevation amplitude specifies the amplitude in terms of the lattice constant of the model sinusoids to simulate the elevation change of the STM probe tip. Q_1 is the direction of *one* wavevector in reciprocal space. Lambda is the coarsening constant, Λ_u, used in equation S5 of Lawler et al. (2010)'s paper. Distortion type can be "poly33" which uses a third-degree polynomial surface or "custom" which uses the author-defined distortion equations. For either distortion types, the coordinates (x, y) are defined such that the upper left corner of the image corresponds to the $(0, 0)$ and the lower right corner corresponds to $(1, 1)$. The reciprocal of the strain minimum length encloses one standard deviation of the reciprocals of the widths of strain areas. Strain magnitude is one standard deviation of the magnitude of strain.

```
image height = 67.1911 [nm], 1024 [px]

image length = 67.1911 [nm], 1024 [px]

lattice constant = 0.369 [nm], 5.6236 [px]

elevation amplitude: 0.041667 [lc]

crystal structure: square

Lambda used = 0.2 [lc^-1]

Q_1 = (1.9163, 1.9163) [nm^-1]
Q_2 = (-1.9163, 1.9163) [nm^-1]

Poly33 coefficients:   p00 p10 p01 p20 p11 p02 p30 p21 p12 p03
x component [all in a.u.]
0.0  -3.2  5.6  -4.0  0.4  7.4  -2.6  -3.4  -5.7  3.3
y component [all in a.u.]
0.0  -4.9  7.4  -3.4  -0.5  -3.2  2.8  4.8  2.2  14.1

strain minimum length = 0.5 [lc]; strain magnitude (std) = 0 [lc]
```

Looping with different values of elevation variation

```
    ***** SAMPLE TRIAL *****
```

DISP: the current noise parameters

```
----------Calculating total distortion----------
```

FIGURE: vector fields and their difference

The figure serves as a quick check for the accuracy of the plain Lawler-Fujita algorithm implementation. If for some reason the relative (or absolute) error is too large, then the following blocks for this trial are rendered invalid. The defined displacement field is also shown here (upper left axis).

DISP: the mean and standard deviation of the relative (or absolute) errors of the Lawler-Fujita algorithm

```
----------Calculating physical strain----------
```

DISP: the type of fit being used

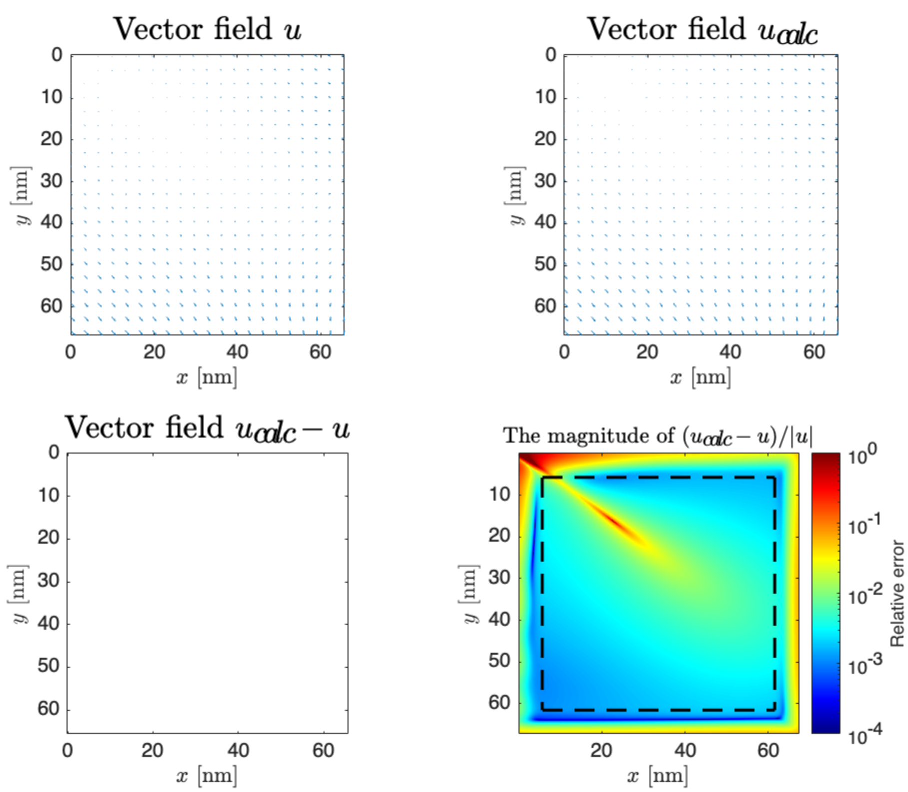
FIGURE: biaxial and uniaxial strain maps

FIGURE: 8-atom and full intensity plots of the simulated lattice

The colorbar for the strain maps is maintained at 5×10^{-3} [a.u.] to remain close to the original one presented by Gao et al. (2018) and Zhao et al. (2021). The intensity plot is placed here so that it would be easier to visually look for correlations between the strain maps and the elevation variations in the simulated lattice.

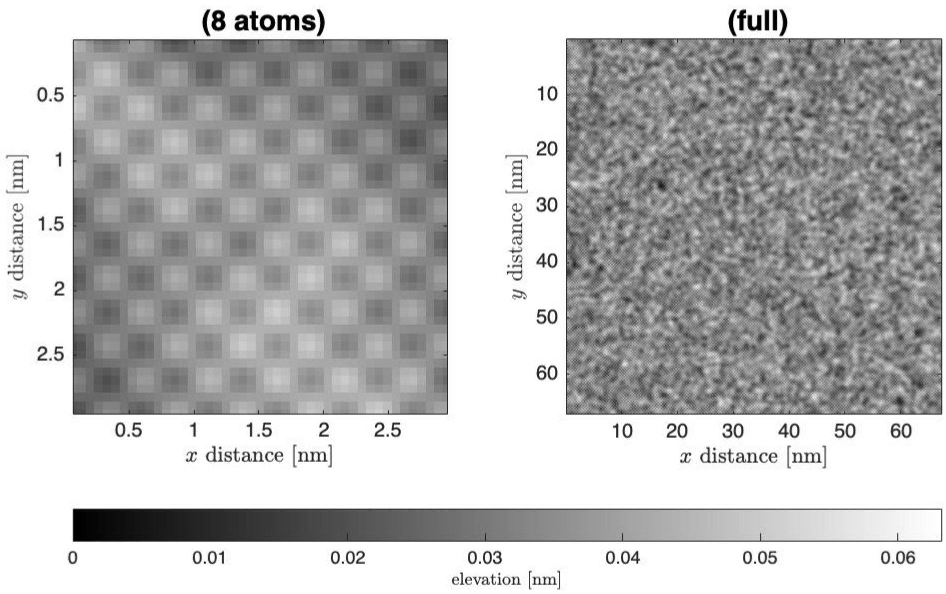
DISP: mean and standard deviations of the magnitudes of the strain maps and their correlation with the elevation variation or "noise"

```
   ***** NEXT TRIAL *****
noise minimum length = 0.2 [lc]; noise magnitude (std) = 0.015625 [lc]
----------Calculating total distortion----------
```

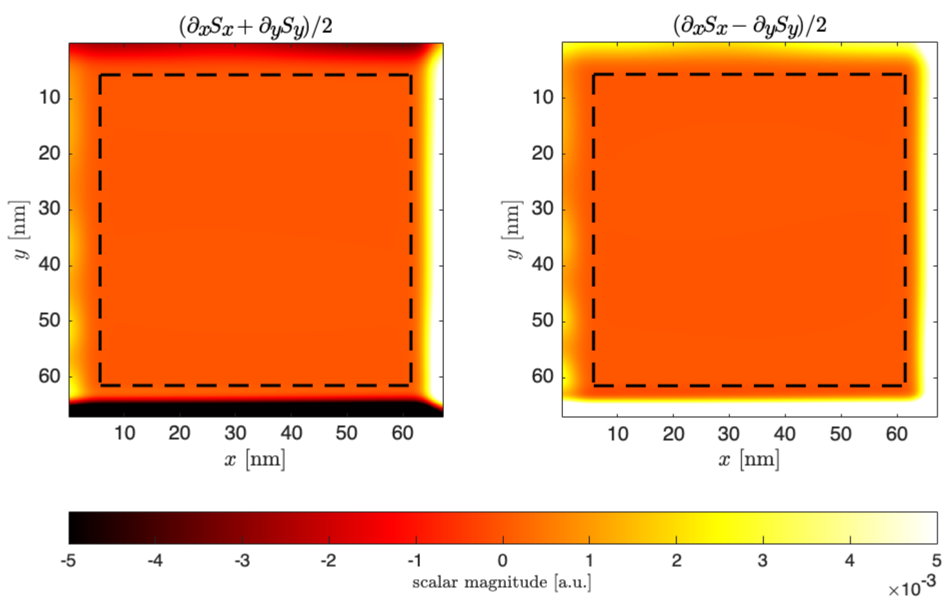



```
Number of pixels averaged: 725904 (69.2276%)
Error is: 0.0053874+/-0.072413
Total error is: 0.077801
Errors are relative unless stated otherwise.
----------Calculating physical strain----------
Doing polynomial fit using MATLAB's poly33.
Warning: Iteration limit reached for robust fitting.
Doing polynomial fit using MATLAB's poly33.
```

Intensity plot of DNaS

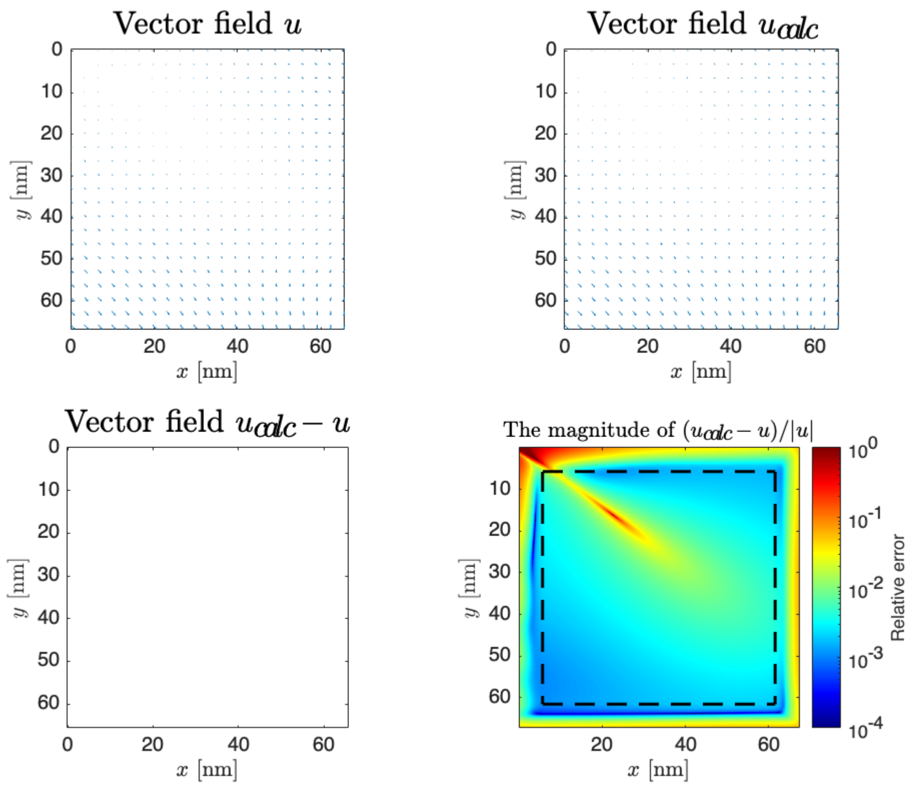


Biaxial and uniaxial strain



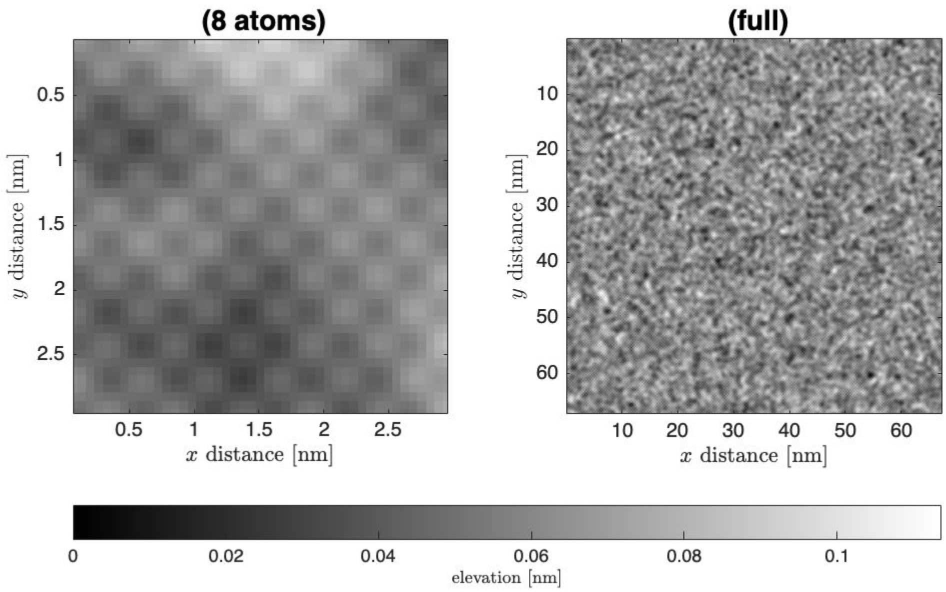

```
biaxial mean = 1.1267e-06; biaxial std = 8.0506e-06
uniaxial mean = 1.1214e-06; uniaxial std = 8.1227e-06
----------Correlations----------
biaxial vs noise correlation, r^2 = 2.7931e-05
```

```
uniaxial vs noise correlation, r^2 = 9.948e-05
------------------------------------------------------------------
   ***** NEXT TRIAL *****
noise minimum length = 0.2 [lc]; noise magnitude (std) = 0.03125 [lc]
----------Calculating total distortion----------
```

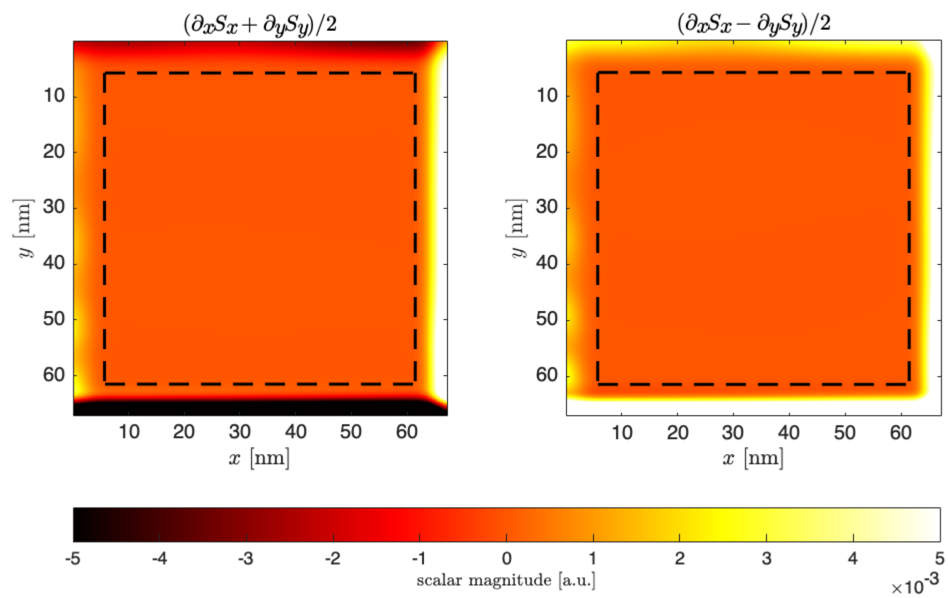



```
Number of pixels averaged: 725904 (69.2276%)
Error is: 0.0053874+/-0.072413
Total error is: 0.077801
Errors are relative unless stated otherwise.
----------Calculating physical strain----------
Doing polynomial fit using MATLAB's poly33.
Warning: Iteration limit reached for robust fitting.
Doing polynomial fit using MATLAB's poly33.
```

Intensity plot of DNaS



Biaxial and uniaxial strain




```
biaxial mean = 1.1267e-06; biaxial std = 8.0506e-06
uniaxial mean = 1.1214e-06; uniaxial std = 8.1227e-06
----------Correlations----------
biaxial vs noise correlation, r^2 = 0.00092768
```

```
uniaxial vs noise correlation, r^2 = 5.2752e-06
---------------------------------------------------------------------
```