Test Report: STEM Moiré GPA

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December 18, 2017

1 Revision History

Date	Version	Notes
18/12/2017	1.0	First incomplete version to meet deadline

2 Symbols, Abbreviations and Acronyms

The same Symbols, Abbreviations and Acronyms as in the SRS, the TestPlan, the MG and the MIS documents (available in STEM Moiré GPA repository) are used in the Test Report document.

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This document is providing information of STEM Moiré GPA implementation by assessing the results of the tests designed in the TestPlan document. Regarding the size of STEM Moiré GPA program, only a small part of the code has been tested in the required time frame therefore, only a few functional requirements have been evaluated. An important update to the document is planed once the implementation of the other tests are done.

For the moment, only a specific focus has been put on the **GPA Module** (M 6 in the MG document and section 10 in the MIS document) and the modules used by GPA which are:

- the **Data Structure Module** (M 15 in MG document and section 19 in the MIS document)
- the **Mask Module** (M 7 in the MG document and section 11 in the MIS document)
- the **Fourier Transform Module** (M 11 in MG document and section 15 in the MIS document)
- the **Gradient Module** (M 12 in MG document and section 16 in the MIS document)
- the **Phase Calculation Module** (M 14 in MG document and section 18 in the MIS document)

3 Functional Requirements Evaluation

3.1 Test R 7 in IM 2: Correctness of the GPA method application

TestRep 1 Test 2 from TestPlan document

Test 2 was designed to check if the gpa function of the GPA module outputs no strain with a simulated input signal with no strain. As a reminder, the GPA module is calculating $\Delta\vec{g}$ the variation of the wave vector $\vec{g}$ by isolating the spatial frequency $\vec{g}$ in Fourier space to extract the phase component. The variation of the phase is then related to the variation of the $\vec{g}$ wave vector using the gradient operation.

For Test 2 to run, one SMH and the mask have to be provided. The SMH has been simulated using the numpy library by generating a 2D array of (256,256) in size with a single spatial frequency. Each element of the array (call pixel in the following of the document) represents the value of the sine function taken at the location of the array. The 2D array as a whole represents the sampled version of the 2D sine function and is a good representation of what is considered a STEM Moire hologram with a single frequency. The mask is set up to be centred on the simulated frequency of the Fourier transform of the SMH with a radius of one pixel^{-1} (elementary unit in Fourier space). The mask array is performed by the function mask_gaussian in the Mask Module. The maask_gaussian function is executed inside the gpa function of the GPA module.

Figure 1 is highlighting the results of Test 2 for the particular case described below:

- $I_{SMH_{exp}} = \sin(2\pi \overrightarrow{g} \cdot \overrightarrow{r})$, with $\overrightarrow{g} = \frac{1}{16} \overrightarrow{u_x}$ pixel^{-1} which represents a periodicity of 16 pixels in the horizontal direction of $I_{SMH_{exp}}$.
- Mask M of one pixel^{-1} in radius and centred on $\overrightarrow{g} = (g_x, g_y)$ in $\widetilde{I}_{SMH_{exp}}$
- $\overrightarrow{g} = \overrightarrow{g_{\text{ref}}} + \overrightarrow{\Delta g}$. Since $\overrightarrow{g}$ is constant and $\overrightarrow{g_{\text{ref}}}$ represents the value of $\overrightarrow{g}$ at a chosen pixel, $\overrightarrow{\Delta g} = \overrightarrow{0}$ everywhere in $I_{SMH_{exp}} = \sin(2\pi g)$ (case of no strain).

A visual summary of the test case can be read in fig. 1. The I_SMH plot is the representation of $I_{SMH_{exp}}$ and the Fourier Transform of I_SMH plot is showing the location of $\overrightarrow{g}$ in Fourier space (maximum intensity) where the mask M is positioned. The Raw Phase plot is highlighting the result of the GPA algorithm corresponding to the phase component related to the spatial frequency $\overrightarrow{g}$ and the Phase corrected plot is displaying the variation of the related to the spatial frequency $\overrightarrow{g}$. The vertical and horizontal components of $\overrightarrow{\Delta g}$ showing the gradient of the phase corrected and are related to the variation of the wave vector $\overrightarrow{g}$. More details can be found in the SRS document (T 2 and DD 2).

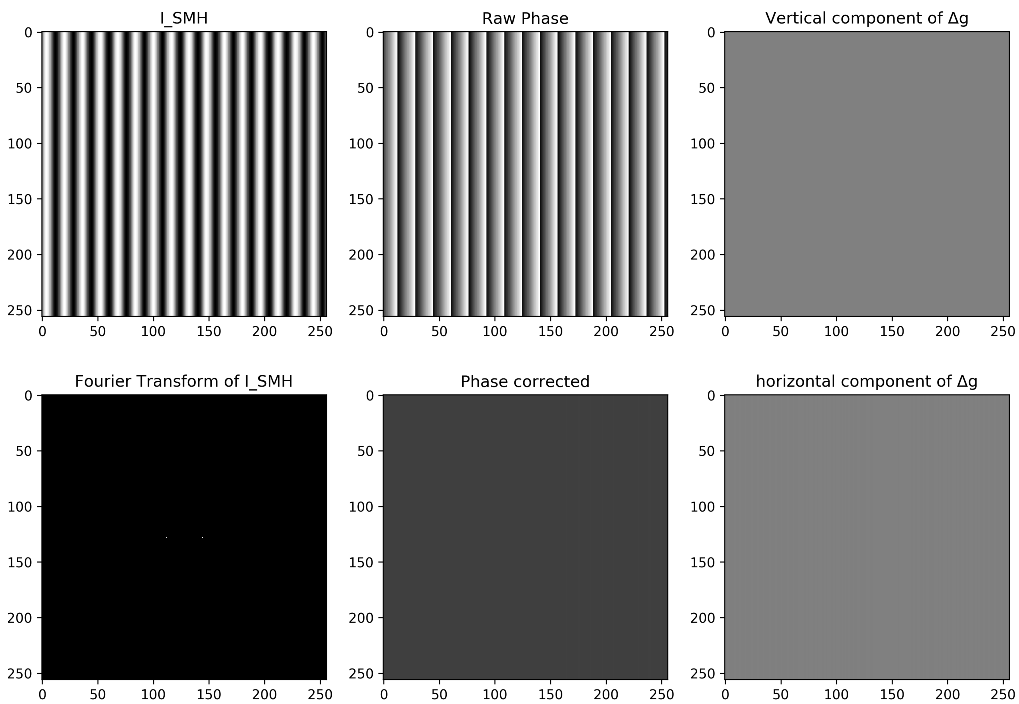

Figure 1: Visual representation of one test case with the input, some intermediate values related to the phase extraction and the output with its horizontal and vertical components.

The expected output is $\overrightarrow{\Delta g} = \overrightarrow{0}$ on each pixel of the array. Since $\overrightarrow{\Delta g}$ is a 2D vector, the horizontal and the vertical components of the vector are shown on each pixel of the array to form the output test images (top and bottom figures on the left side of fig. 1). For the intermediate variables, the phase corrected is expected to be constant, the raw phase to show a sawtooth shape with a constant slope along the horizontal direction. For the initial variables, $I_{SMH_{exp}}$ is a sampled version of a sine function and its Fourier transform should be two delta functions at the frequency $\overrightarrow{g}$ and $-\overrightarrow{g}$. Since the test case is only simulating a frequency in the horizontal direction, all the arrays from fig. 1 can be sliced by extracting only the results from a single vertical array. Such transformation is performed in fig. 2. The 1D representation helps in visualizing the different variables of the test case.

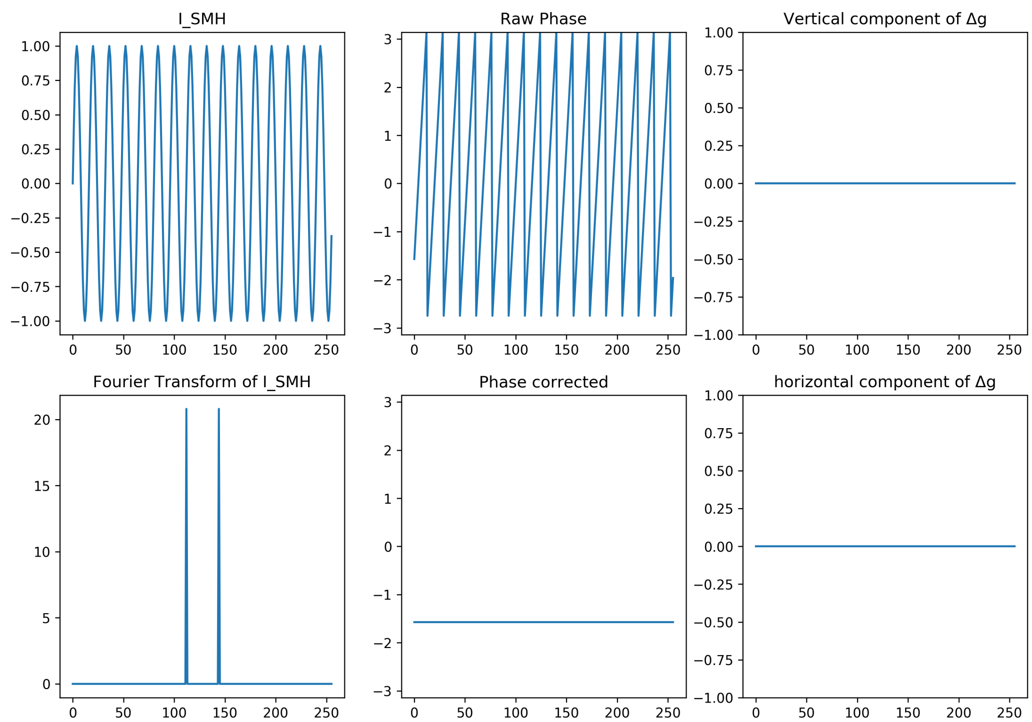

Figure 2

The test can be summarized with the following metrics:

- Statistical **mean** of the elements part of horizontal line profile $\overrightarrow{\Delta g}$
- Statistical **standard deviation** of the elements part of the horizontal line profile $\overrightarrow{\Delta g}$

For the test case described in fig. 2, the metrics are provided in table 1

$\overrightarrow{g}$ (pixel)$^{-1}$	Mean horizontal $\overrightarrow{\Delta g}$ (pixel)$^{-1}$	StDev horizontal $\overrightarrow{\Delta g}$ (pixel)$^{-1}$
16	-2.2768245622195593e-18	3.2869874402072343e-16

Table 1: Table of metrics for

It is reasonable to conclude that the errors are relatively small and can be considered negligible. The behaviour of the gpa function in the GPA module seems to be satisfactory. To check a more variety of test cases similar $I_{SMH_{exp}}$ with different periodicities were also tested. The following different periodicities are proposed: 3, 4, 4.1, 4.2, 4.5, 16 and 100 pixels. For each case, the appropriate mask is used and the radius of the mask is kept to 1 pixel^{-1}. The different test cases are summarized in fig. 3.

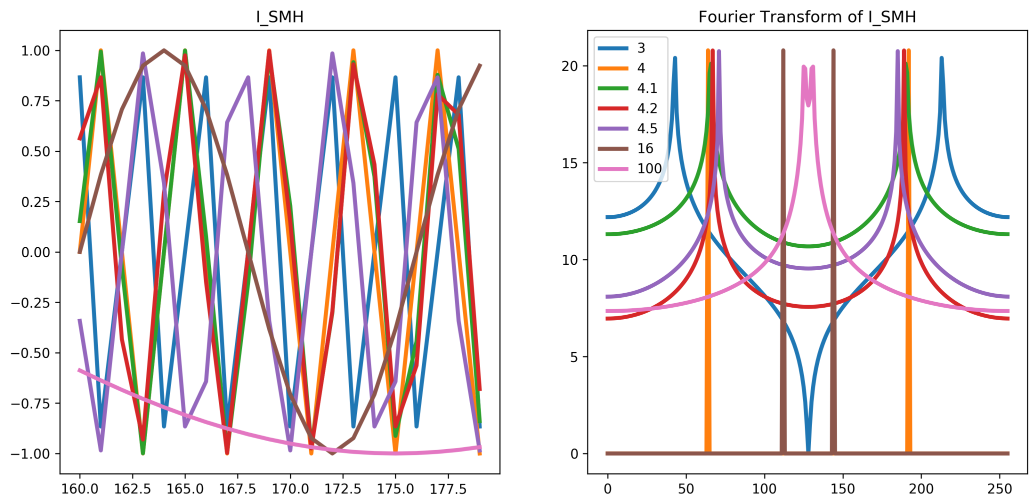

Figure 3

The difference between the different periodicities in the Fourier transform plot can be commented. Only the particular cases with a periodicity of 4 and 16 pixels are highlighting a sharp delta function shape signal at their respective frequency. On all the other cases, the Fourier transform signal is spread on a range of frequency with a maximum at their respective frequency. The cause of the frequency spreading is for the moment unclear. It could be a mix between a sampling artifact and erros from the fast fourier transform algorithm. Those errors are not included in the model described in the SRS document and will have an effect on the gpa algorithm since some artificial frequencies seem to be present in the signal. However, those artifact are still weaker than the main signal coming from periodicity simulated.

The results of the test is highlighted in fig. 4. It is interesting to notice that some non negligible effects are now visible with specific test cases. It is difficult to assess if the numbers shown will have a significant impact on the final strain maps but the variation of the phase (translated into variation of $\overrightarrow{\Delta g}$) will contribute by adding noise in the signal.

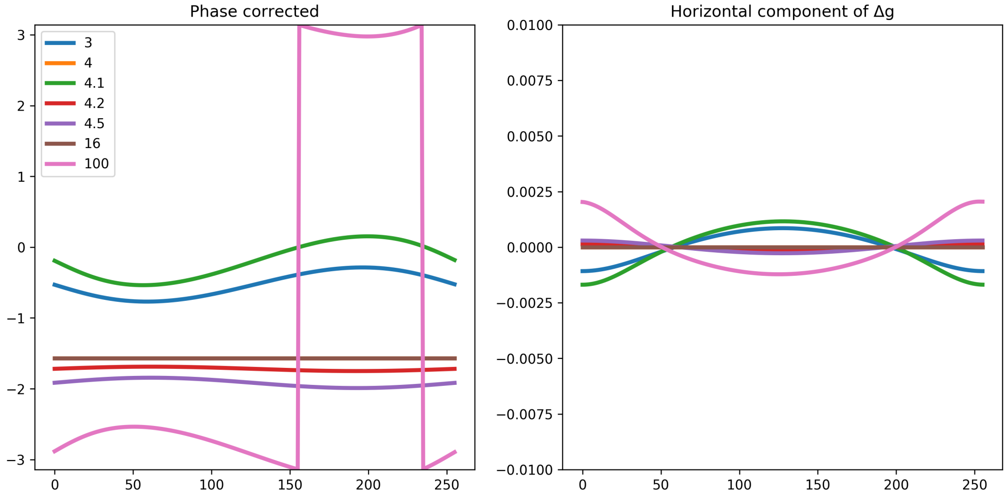

Figure 4

The table of metrics for all the cases is shown in table 2. Those metrics might not be the most appropriate ones to assess GPA performance since the statistics remove the location where the error are minimized or maximized. The error distribution provided by the plot (or the image) are still needed to judge better the precision of the module. The error plot is provided in fig. 5 and corresponds to the absolute value of horizontal component of $\overrightarrow{\Delta g}$ in fig. 4.

$\overrightarrow{g}$ (pixel)$^{-1}$	Mean horizontal $\overrightarrow{\Delta g}$ (pixel)$^{-1}$	StDev horizontal $\overrightarrow{\Delta g}$ (pixel)$^{-1}$
3	1.9414415841027127e-09	0.0006730746894985686
4	-9.540979117872439e-18	7.341002270163171e-16
4.1	4.0351392667763858e-09	0.0009728477395757706
4.2	-1.6333255180214085e-10	8.581046509119554e-05
4.5	-3.9869652219449991e-10	0.0002022207376045426
16	-2.2768245622195593e-18	3.2869874402072343e-16
100	-6.0785148749668448e-09	0.0010974597065239072

Table 2: Table of metrics for

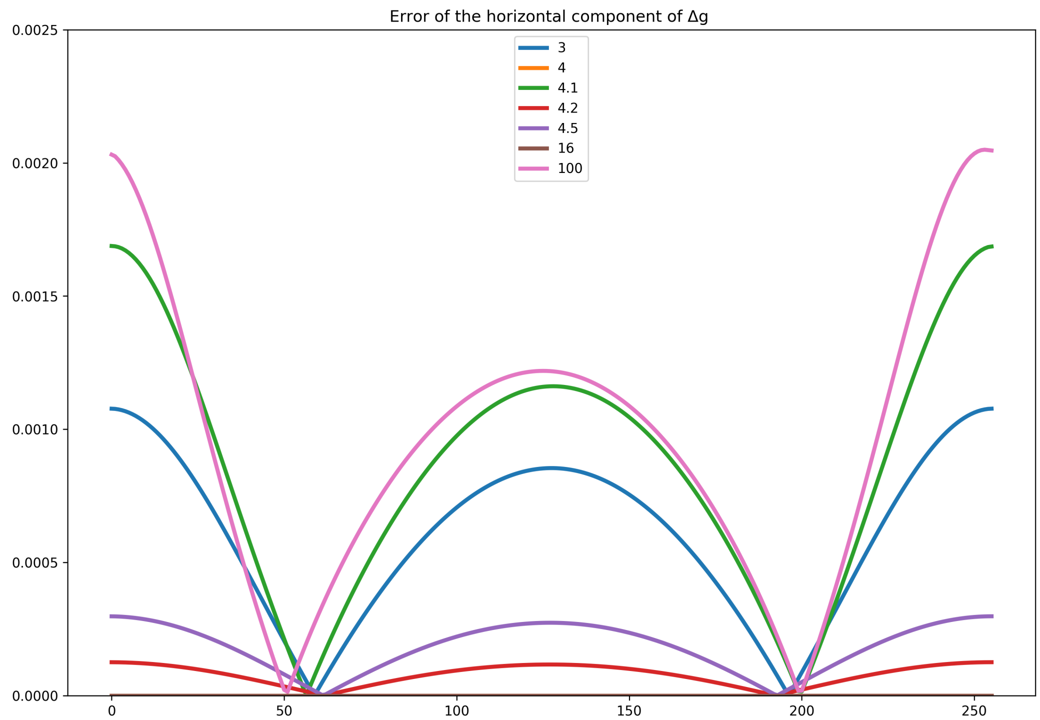

Figure 5

Based on the error plot in fig. 5, the behaviour of the gpa module is not fully satisfactory. Potentially, the error could be small enough to be negligible however, **Test 2** is the simplest test case possible based on generated data. Noise and other artifacts will be included in the experimental data which could also contribute to the error. A system test on the whole program might help in assessing if the errors visible in GPA module have a significant impact on the deformation maps.

TestRep 2 Test 3 from TestPlan document

The same protocol as in TestRep 1 has been used to generate the test cases ofTest 3. The only difference is that the generated data need to have a known strain in an area of the image. For simplicity, the left half of the image has been decided to be the reference state and the right half to be the strained state. An example of test case is shown in fig. 6 with the left side begin modelled by a sin function with a periodicity of 4 pixels and the right side modelled by a sin function with a periodicity of 4.5 pixels. The difference of periodicity correspond to the simulated strain field present on the right side of the image.

The details of the inputs used for test restuls shown in fig. 6 are described below:

- $I_{SMH_{exp}} = \sin\left(2\pi \overrightarrow{g} \cdot \overrightarrow{r} + \overrightarrow{K(x)} \cdot \overrightarrow{r}\right)$, with:

– $\overrightarrow{g} = \frac{1}{4}\overrightarrow{u_x}$ pixel^{-1} which represents a periodicity of 4 pixels in the horizontal direction of $I_{SMH_{exp}}$.

– $\overrightarrow{K(x)}$ such that $\begin{cases} \overrightarrow{K(x)} = \overrightarrow{0}, \ 0 \leq x \leq 127 \\ \overrightarrow{K(x)} = \frac{4\times4.5}{4.5-4}\ \overrightarrow{u_x} \text{ pixel}^{-1}, \ 128 \leq x \leq 255 \end{cases}$

- Mask M of 20 pixel^{-1} in radius and centred on $\overrightarrow{g} = (g_x, g_y)$ (the unstrained frequency) in $\widetilde{I}_{SMH_{exp}}$

- $\overrightarrow{g} = \overrightarrow{g_{\text{ref}}} + \overrightarrow{\Delta g}$. On the left side, $\overrightarrow{\Delta g} = \overrightarrow{0}$ and on the right side, $\overrightarrow{\Delta g} = (\frac{1}{4.5} - \frac{1}{4})\overrightarrow{u_x} + 0\overrightarrow{u_y}$.

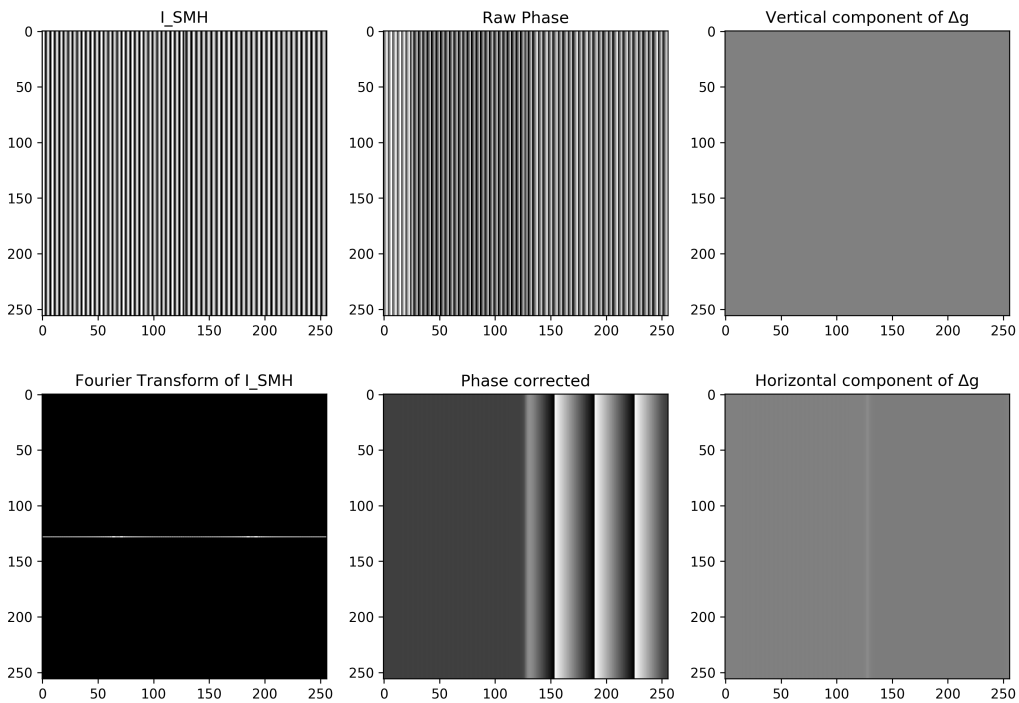

Figure 6

As done in TestRep 1, it is possible to slice the dataset to represent a 1D profile because the periodicity and the strain is only generated along the horizontal axis. The 1D data visualization is done in fig. 7. The presence of two different periodicities is confirmed in both the I_SMH and the Fourier Transform of I_SMH plots. Two areas with their own frequencies are clearly observable. Again similar spreading in frequency of the Fourier Trasform of I_SMH that in fig. 3 are highlighted. The phase corrected plot also shows two different regions with different behaviour. Because of the difference of frequency, the phase is constant on the left side and varying on the right side. These results are expected since the strain corresponds to the slope of the phase. Therefore, with a flat phase, no strain is expected and with a varying phase, a strain is expected. The value of the slope is directly linked to the strength of the strain. The final output $\overrightarrow{\Delta g}$ is confirming a strain observed on the right side of the profile. There is an important spike on the interface between the unstrained and strain region but this is a known weakness of GPA algorithm. One assumption is to not have an abrupt variation of phase in order to model the derivative of the phase as the variation of the wave vector $\overrightarrow{g}$. Any interface won't respect this hypothesis and it is only possible to limit the spiking effect by playing with the mask parameters.

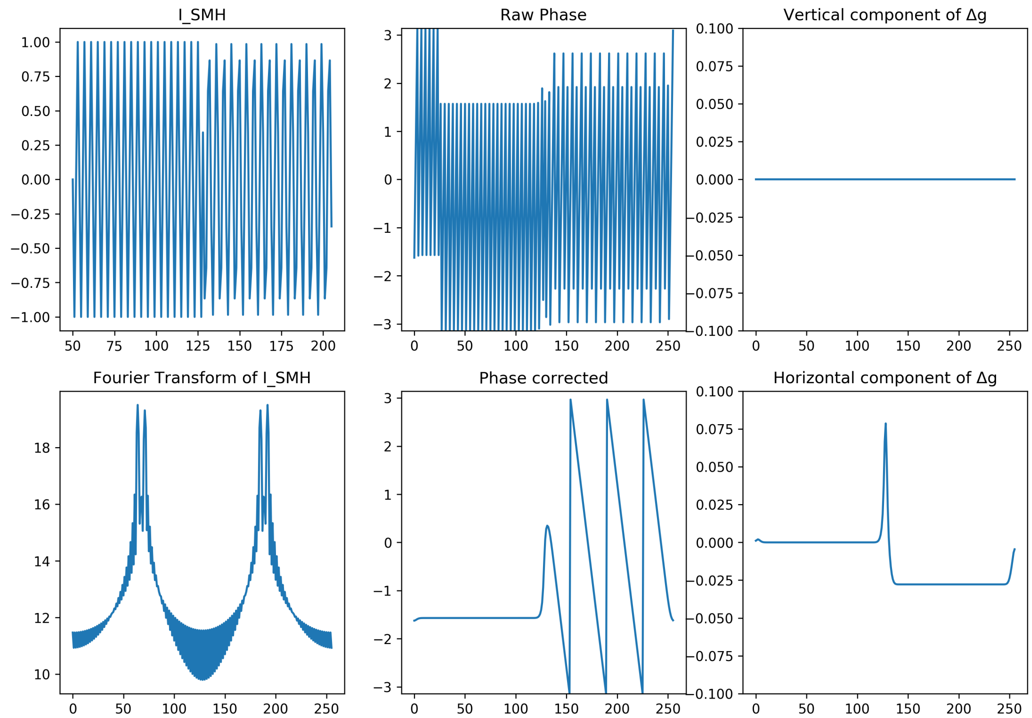

Figure 7

To check the performance of the GPA algorithm the error between the input strain and the output strain can be calculated. Results are shown in table 3 and the error seems to be on the same order of magnitude as the standard deviation of the worst case in TestRep 1.

$\overrightarrow{g}$ (pixel)	$\overrightarrow{K}$ (pixel)	Error = $\lvert\overrightarrow{\Delta g}_{\text{sim}} - \overrightarrow{\Delta g}_{\text{gpa}}\rvert$ (pixel)$^{-1}$
4	4.5	5.55555637e-02

Table 3: Table of metrics for

Several test cases can be designed to see if the error is evolving with the level of strain. The following periodicities on the right side of the image have been tested to verify the GPA algorithm : 3, 3.8, 3.9, 4, 4.1, 4.2 and 5 pixels. The test cases should respectively display the following level of strain : 1/4 - 1/3, 1/4 - 1/3.8, 1/4 - 1/3.9, 0, 1/4 - 1/4.1, 1/4 - 1/4.2 and 1/4 - 1/5 pixel^{-1}. The results of the tests are highlighted in fig. 8 and in the table table 4.

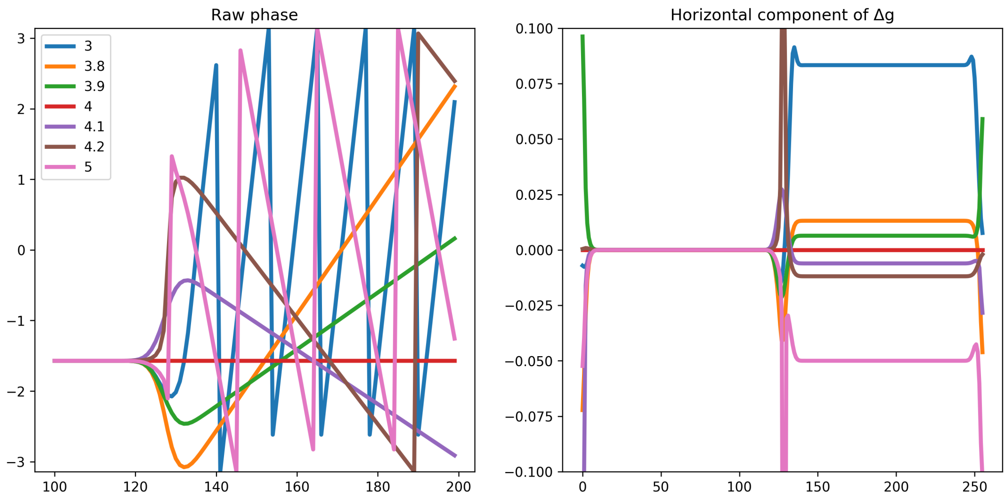

Figure 8

$\overrightarrow{g}$ (pixel)	$\overrightarrow{K}$ (pixel)	Error = $\lvert\overrightarrow{\Delta g}_{\mathrm{sim}} - \overrightarrow{\Delta g}_{\mathrm{gpa}}\rvert$ (pixel)$^{-1}$
4	3	1.66666626e-01
4	3.8	2.63157758e-02
4	3.9	1.28205175e-02
4	4	8.32667268e-16
4	4.1	1.21951224e-02
4	4.2	2.38095207e-02
4	5	9.99999872e-02

Table 4: Table of metrics for

The error seems to increase slowly with the level of strain. Nevertheless, the higher the level of strain, the higher the radius of the mask should be. In this case, we kept the radius of the mask constant which can be at the disadvantage of higher strain level. The effect of the mask radius should be also assessed to give a more complete picture of the error evolution.

4 Nonfunctional Requirements Evaluation

Nonfunctional Requirements have not been addressed for the moment.

5 Comparison to Existing Implementation

No other equivalent open-access software has been identified for a comparison. sMoiré program (available on HREM website) is a good candidate but a licence must be bought in order to use the software. The licence purchase is not an option, moreover all aspects of STEM Moiré GPA are not covered by sMoiré.

The GPA algorithm used in STEM Moiré GPA could be however compared to other open-access GPA software and is planned to be performed. Nevertheless, most of them are plug-ins for Digital Micrograph software therefore an interface must be designed to perform a comparison with STEM Moiré GPA.

6 Unit Testing

A couple of unit tests were performed in order to verify the proper behaviour of a few functions. The amount of tests are still not sufficient to qualify the reliability of STEM Moiré GPA nevertheless, the Data Structure Module has been tested such as a few properties of the Mask module. The test can be run using pytest testing framework and the content of the test can be found in the python files with the designation test_*.py (the * replacing the name of the module tested).

7 Changes Due to Testing

Mask function

8 Automated Testing

For the moment, only a manual testing approach has been considered.

9 Trace to Requirements

Not enough tests have been performed to assess the requirement of STEM Moiré GPA.

10 Trace to Modules

Not enough tests have been performed to assess the proper behaviour of the modules in STEM Moiré GPA.

11 Code Coverage Metrics