NanoSIMS Preprocessing

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1 NanoSIMS Preprocessing

[2]:
```
import os
import copy
import tifffile
import numpy as np
from matplotlib import pyplot as plt

import sims # For reading Cameca NanoSIMS data files (.im)
from pystackreg import StackReg # Image registration based on Thevenaz et al.
from pystackreg.util import to_uint16
```

```
Matplotlib created a temporary cache directory at /tmp/matplotlib-z7g9pun6
because the default path (/.config/matplotlib) is not a writable directory; it
is highly recommended to set the MPLCONFIGDIR environment variable to a writable
directory, in particular to speed up the import of Matplotlib and to better
support multiprocessing.
```

1.1 Read raw data

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We use the SIMS python module to read Cameca nanoSIMS data files.

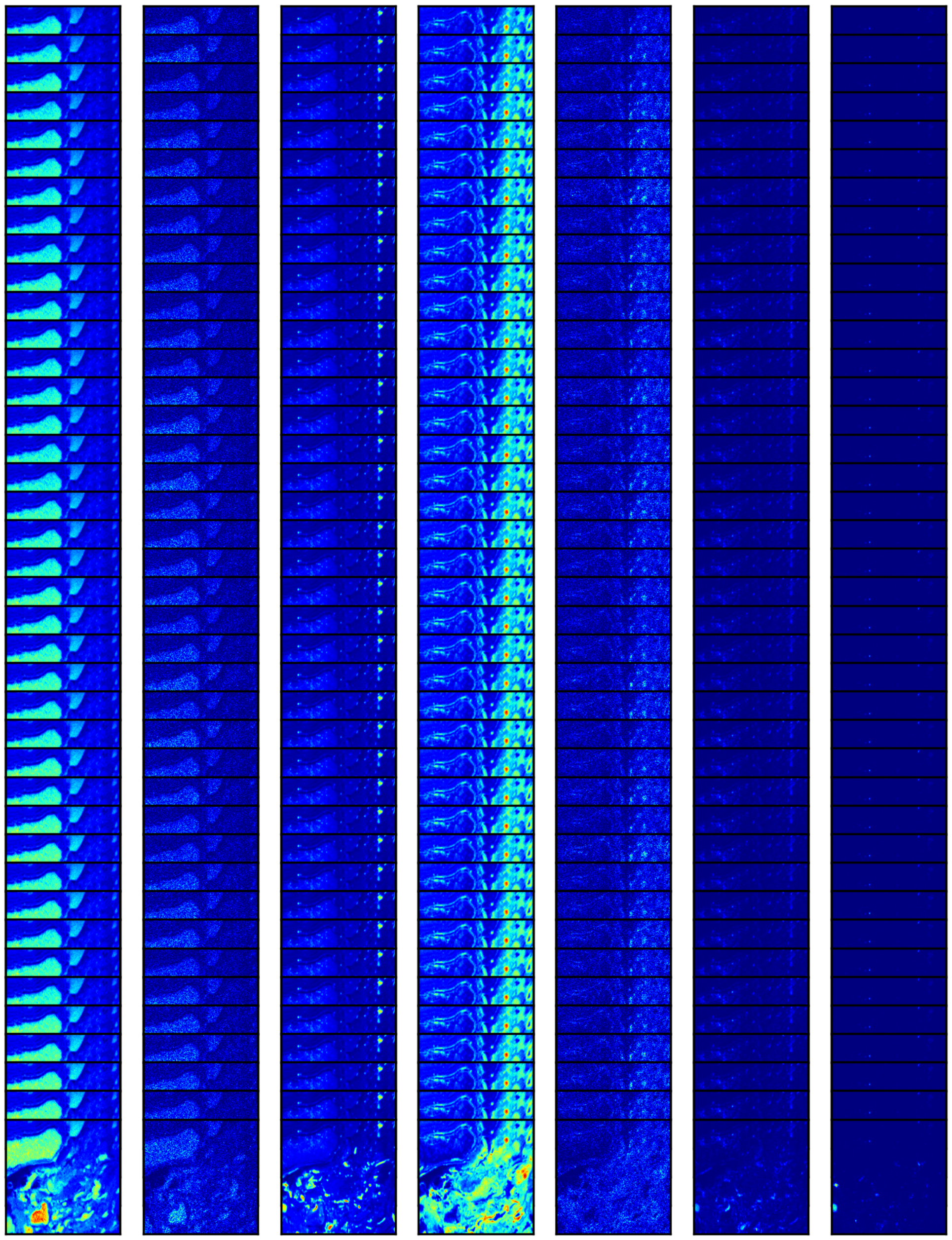
[6]:
```
# Choose a ".im" file from the "Black_sand_soils" dataset to process
# Remember to add the root directory "/tf" to the path
path = "/path/to/data.im"
```

[7]:
```
raw = sims.SIMS(path)
data = raw.data.data
species = raw.data.species.data
channels, slices, rows, cols = raw.data.data.shape

print("Shape: ", raw.data.data.shape)
print("Species: ", species)
print("Example values: ", data[0,0,0,1], data[0,0,-1,1])
```

```
Shape:  (7, 40, 256, 256)
Species:  ['12C' '13C' '16O' '12C 14N' '12C 15N' '27Al 16O' '56Fe 16O']
```

```
Example values:  56 72
```

```
[8]: fig = plt.figure(dpi=300)
plt.set_cmap('jet')
# You may adjust the spaces here
plt.subplots_adjust(bottom=-0.5, hspace=-0.8)
k=1
for slice in range(slices):
    for channel in range(channels):
        plt.subplot(slices,channels,k)
        k+=1
        plt.imshow(data[channel,slice,:,:])
        plt.tick_params(left =␣
 ↪False,right=False,labelleft=False,labelbottom=False,bottom=False)
```



2 Preprocessing

2.1 1 Dead Time Correction

The dead time is the time after each event when the system cannot record another event. Here, the default value for the Cameca NanoSIMS system is set to 0.000044 seconds.

[9]:
```python
def dtc(data):
    return data/(1-data*0.000044)
```

[10]:
```python
data_dtc = dtc(data)
```

[12]:
```python
print("Shape: ", data_dtc.shape)
print("Example values: ", data_dtc[0,0,0,1], data_dtc[0,0,-1,1])
```

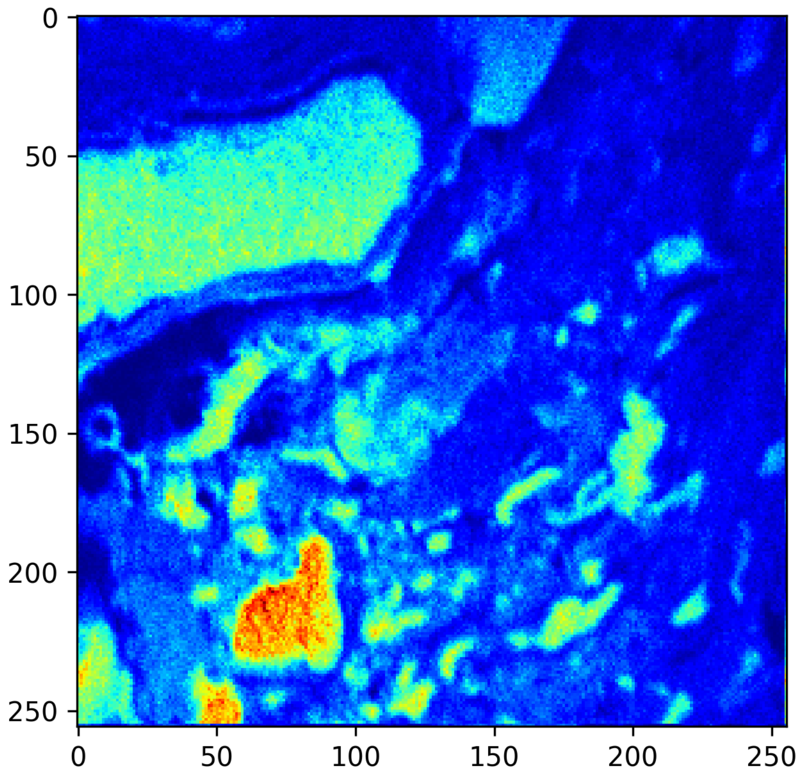
```
Shape:  (7, 40, 256, 256)
Example values:  56.138324832387006 72.22882090462585
```

2.2 2 Correct column and row

Correct column and row of each scan due to a drift, which concerns temperature differences during measurement. The lowermost row should go to the top, and the rightmost column should go to the left while we first correct the column and then the row.

[13]:
```python
plt.figure(dpi=300)
plt.imshow(data[0,0,:,:])
```

[13]:
```
<matplotlib.image.AxesImage at 0x7f73b15e8b90>
```

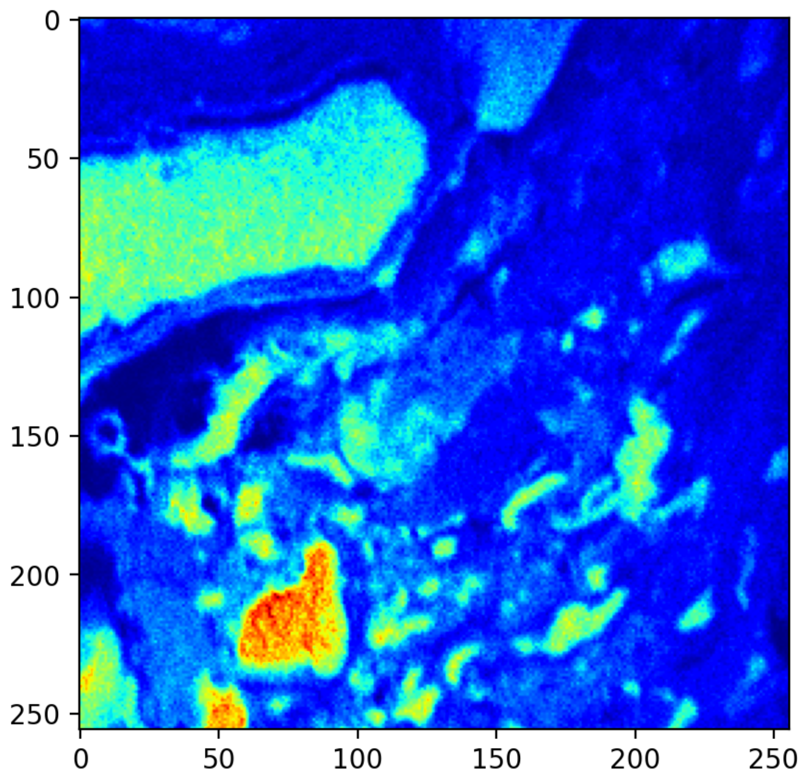


[15]:
```
def roll(data):
    data_rolled = copy.copy(data)
    data_rolled[:, :, :, 0] = np.array(data[:, :, :, -1])
    for col in range(cols-1):
        data_rolled[:, :, :, col+1] = np.array(data[:, :, :, col])

    data_rolled_copy = copy.copy(data_rolled)
    data_rolled[:, :, 0, :] = np.array(data_rolled_copy[:, :, -1, :])
    for row in range(rows-1):
        data_rolled[:, :, row+1, :] = np.array(data_rolled_copy[:, :, row, :])

    return data_rolled
```

[16]:
```
data_roll = roll(data_dtc)
```

[17]:
```
plt.figure(dpi=200)
plt.imshow(data_roll[0,0,:,:])
```

[17]:
```
<matplotlib.image.AxesImage at 0x7f73b0e98ad0>
```



[22]:
```
print("Shape: ", data_roll.shape)
print("Example values: ", data_roll[0,0,0,1], data_roll[0,0,-1,1])
```

```
Shape:  (7, 40, 256, 256)
Example values:  65.18643188476562 167.22137451171875
```

2.3 3 Align

Align (register) scans by auto-track since NanoSIMS might drift during measurement. The image registration algorithm is based on P Thevenaz: A Pyramid Approach to Subpixel Registration Based on Intensity.

We select one mass with distinct boundaries as a reference, which is, in our case, the first one, and run the algorithm on all other "higher" than this.

[18]:
```
def align(data, method='autotrack', clipping=False, ref_channel=0,␣
↪transform='translation'):
    if transform == 'rigid_body':
        sr = StackReg(StackReg.RIGID_BODY)
    if transform == 'translation':
        sr = StackReg(StackReg.TRANSLATION)

    c, _, _, _ = data.shape
    if clipping == True:
        tmats = sr.register_stack((data[ref_channel, :, :, :]-data[ref_channel,␣
↪:, :, :].min()), axis=0, reference='previous', verbose=False)
        for channel in range(c):
            data[channel, :, :, :] = to_uint16(sr.transform_stack(data[channel,␣
↪:, :, :]))

    if clipping == False:
        tmats = sr.register_stack(data[ref_channel, :, :, :], axis=0,␣
↪reference='previous', verbose=False) # axis gives the frame's position
        for channel in range(c):
            data[channel, :, :, :] = sr.transform_stack(data[channel, :, :, :])

    return data
```

[19]:
```
data_align = align(data_roll)
```

[21]:
```
print("Shape: ", data_align.shape)
print("Example values: ", data_align[0,0,0,1], data_align[0,0,-1,1])
```

```
Shape:  (7, 40, 256, 256)
Example values:  65.18643188476562 167.22137451171875
```

2.4 4 Sum images

Create sum images by adding up all slices.

[23]:
```python
def sumim(data):
    c, s, w, h = data.shape
    im = np.zeros((c, w, h))
    for i in range(s):
        im += np.asarray(data[:,i,:,:])
    return im
```

[24]:
```python
im = sumim(data_align)
```

[26]:
```python
print("Shape: ", im.shape)
print("Example values: ", im[0,0,1], im[0,-1,1])
```

```
Shape:  (7, 256, 256)
Example values:  2646.0064849853516 5890.978950500488
```

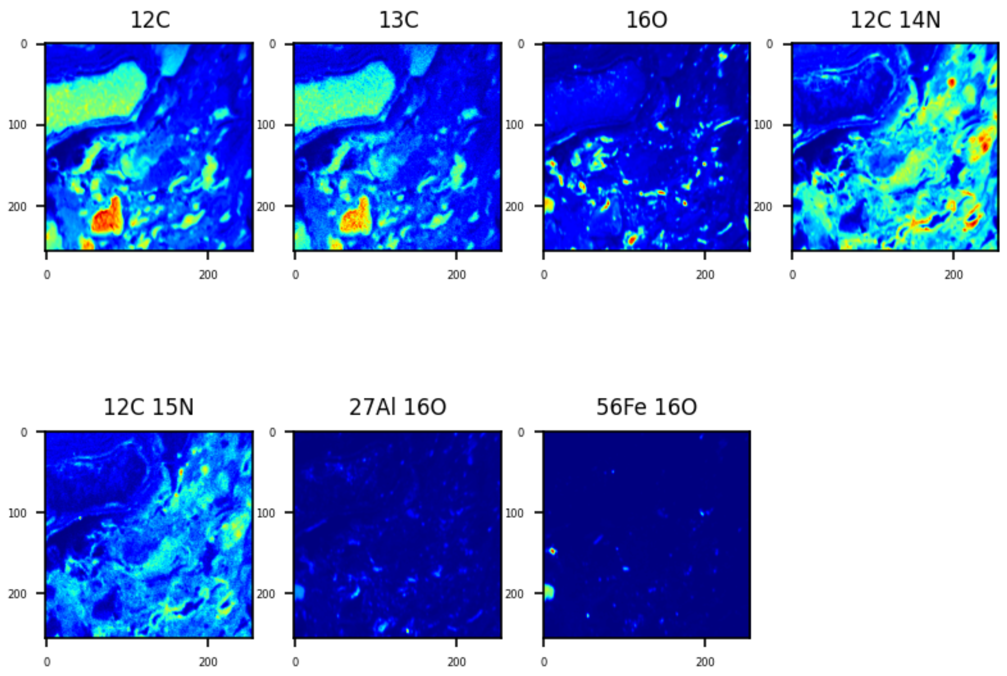
2.5 5 Save

Finally, save the image in ".tif" format.

[27]:
```python
outpath = './ppsim/'
if not os.path.exists(outpath):
    os.mkdir(outpath)

filename = raw.filename.split('/')[-1].split('.')[0]
tifffile.imwrite(f'{outpath}{filename}.tif', im)
```

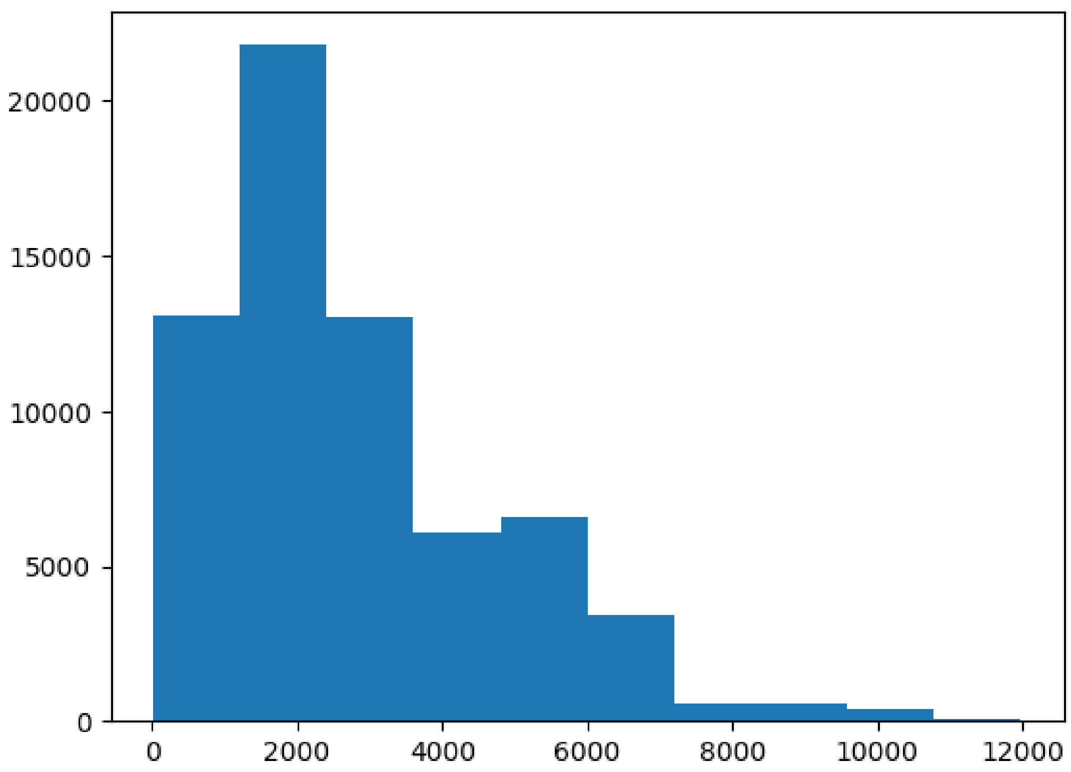
3 Plot

[31]:
```python
fig = plt.figure(dpi=150)
plt.set_cmap('jet')
plt.tight_layout()
for channel in range(im.shape[0]):
    plt.subplot(2,4,channel+1)
    plt.imshow(im[channel,:,:])
    plt.yticks(fontsize=4)
    plt.xticks(fontsize=4)
    plt.title(species[channel], size=8)
#plt.colorbar(fraction=0.046, pad=0.04)
```



```
[37]: plt.hist(im[0].flatten(), bins=10)
```

```
[37]: (array([13075., 21798., 13024.,  6064.,  6560.,  3444.,   597.,   566.,
           358.,    50.]),
       array([   17.09061329,  1212.82730391,  2408.56399454,  3604.30068516,
               4800.03737579,  5995.77406641,  7191.51075704,  8387.24744766,
               9582.98413828, 10778.72082891, 11974.45751953]),
       <BarContainer object of 10 artists>)
```


20000
15000
10000
5000
0
0
2000
4000
6000
8000
10000
12000

```
[ ]:
```