In [1]:

```
!wget https://raw.githubusercontent.com/ML4SCI/ML4SCI_GSoC/main/Messenger/Mercury/mercur
y-albedo-top-half.png.csv
!wget https://raw.githubusercontent.com/ML4SCI/ML4SCI_GSoC/main/Messenger/Mercury/mercur
y-albedo-resized-bottom-half.png.csv
!wget https://raw.githubusercontent.com/ML4SCI/ML4SCI_GSoC/main/Messenger/Mercury/alsima
p_smooth_032015.png.csv
!wget https://raw.githubusercontent.com/ML4SCI/ML4SCI_GSoC/main/Messenger/Mercury/casima
p_smooth_032015.png.csv
!wget https://raw.githubusercontent.com/ML4SCI/ML4SCI_GSoC/main/Messenger/Mercury/fesima
p_smooth_032015.png.csv
!wget https://raw.githubusercontent.com/ML4SCI/ML4SCI_GSoC/main/Messenger/Mercury/mgsima
p_smooth_032015.png.csv
!wget https://raw.githubusercontent.com/ML4SCI/ML4SCI_GSoC/main/Messenger/Mercury/ssimap
_smooth_032015.png.csv
```

```
--2021-03-29 07:41:46--  https://raw.githubusercontent.com/ML4SCI/ML4SCI_GSoC/main/Messen
ger/Mercury/mercury-albedo-top-half.png.csv
Resolving raw.githubusercontent.com (raw.githubusercontent.com)... 185.199.108.133, 185.1
99.109.133, 185.199.110.133, ...
Connecting to raw.githubusercontent.com (raw.githubusercontent.com)|185.199.108.133|:443.
.. connected.
HTTP request sent, awaiting response... 200 OK
Length: 25920000 (25M) [text/plain]
Saving to: ‘mercury-albedo-top-half.png.csv’

mercury-albedo-top- 100%[===================>]  24.72M  82.4MB/s    in 0.3s

2021-03-29 07:41:46 (82.4 MB/s) - ‘mercury-albedo-top-half.png.csv’ saved [25920000/25920
000]

--2021-03-29 07:41:46--  https://raw.githubusercontent.com/ML4SCI/ML4SCI_GSoC/main/Messen
ger/Mercury/mercury-albedo-resized-bottom-half.png.csv
Resolving raw.githubusercontent.com (raw.githubusercontent.com)... 185.199.108.133, 185.1
99.109.133, 185.199.110.133, ...
Connecting to raw.githubusercontent.com (raw.githubusercontent.com)|185.199.108.133|:443.
.. connected.
HTTP request sent, awaiting response... 200 OK
Length: 25920000 (25M) [text/plain]
Saving to: ‘mercury-albedo-resized-bottom-half.png.csv’

mercury-albedo-resi 100%[===================>]  24.72M   113MB/s    in 0.2s

2021-03-29 07:41:47 (113 MB/s) - ‘mercury-albedo-resized-bottom-half.png.csv’ saved [2592
0000/25920000]

--2021-03-29 07:41:47--  https://raw.githubusercontent.com/ML4SCI/ML4SCI_GSoC/main/Messen
ger/Mercury/alsimap_smooth_032015.png.csv
Resolving raw.githubusercontent.com (raw.githubusercontent.com)... 185.199.108.133, 185.1
99.109.133, 185.199.110.133, ...
Connecting to raw.githubusercontent.com (raw.githubusercontent.com)|185.199.108.133|:443.
.. connected.
HTTP request sent, awaiting response... 200 OK
Length: 25920000 (25M) [text/plain]
Saving to: ‘alsimap_smooth_032015.png.csv’

alsimap_smooth_0320 100%[===================>]  24.72M  82.5MB/s    in 0.3s

2021-03-29 07:41:47 (82.5 MB/s) - ‘alsimap_smooth_032015.png.csv’ saved [25920000/2592000
0]

--2021-03-29 07:41:47--  https://raw.githubusercontent.com/ML4SCI/ML4SCI_GSoC/main/Messen
ger/Mercury/casimap_smooth_032015.png.csv
Resolving raw.githubusercontent.com (raw.githubusercontent.com)... 185.199.111.133, 185.1
99.110.133, 185.199.109.133, ...
Connecting to raw.githubusercontent.com (raw.githubusercontent.com)|185.199.111.133|:443.
.. connected.
HTTP request sent, awaiting response... 200 OK
```

```
Length: 25920000 (25M) [text/plain]
Saving to: 'casimap_smooth_032015.png.csv'

casimap_smooth_0320 100%[===================>]  24.72M  47.4MB/s    in 0.5s

2021-03-29 07:41:48 (47.4 MB/s) - 'casimap_smooth_032015.png.csv' saved [25920000/2592000
0]

--2021-03-29 07:41:48--  https://raw.githubusercontent.com/ML4SCI/ML4SCI_GSoC/main/Messen
ger/Mercury/fesimap_smooth_032015.png.csv
Resolving raw.githubusercontent.com (raw.githubusercontent.com)... 185.199.108.133, 185.1
99.109.133, 185.199.110.133, ...
Connecting to raw.githubusercontent.com (raw.githubusercontent.com)|185.199.108.133|:443.
.. connected.
HTTP request sent, awaiting response... 200 OK
Length: 25920000 (25M) [text/plain]
Saving to: 'fesimap_smooth_032015.png.csv'

fesimap_smooth_0320 100%[===================>]  24.72M  56.5MB/s    in 0.4s

2021-03-29 07:41:48 (56.5 MB/s) - 'fesimap_smooth_032015.png.csv' saved [25920000/2592000
0]

--2021-03-29 07:41:48--  https://raw.githubusercontent.com/ML4SCI/ML4SCI_GSoC/main/Messen
ger/Mercury/mgsimap_smooth_032015.png.csv
Resolving raw.githubusercontent.com (raw.githubusercontent.com)... 185.199.108.133, 185.1
99.109.133, 185.199.110.133, ...
Connecting to raw.githubusercontent.com (raw.githubusercontent.com)|185.199.108.133|:443.
.. connected.
HTTP request sent, awaiting response... 200 OK
Length: 25920000 (25M) [text/plain]
Saving to: 'mgsimap_smooth_032015.png.csv'

mgsimap_smooth_0320 100%[===================>]  24.72M  70.0MB/s    in 0.4s

2021-03-29 07:41:49 (70.0 MB/s) - 'mgsimap_smooth_032015.png.csv' saved [25920000/2592000
0]

--2021-03-29 07:41:49--  https://raw.githubusercontent.com/ML4SCI/ML4SCI_GSoC/main/Messen
ger/Mercury/ssimap_smooth_032015.png.csv
Resolving raw.githubusercontent.com (raw.githubusercontent.com)... 185.199.108.133, 185.1
99.109.133, 185.199.110.133, ...
Connecting to raw.githubusercontent.com (raw.githubusercontent.com)|185.199.108.133|:443.
.. connected.
HTTP request sent, awaiting response... 200 OK
Length: 25920000 (25M) [text/plain]
Saving to: 'ssimap_smooth_032015.png.csv'

ssimap_smooth_03201 100%[===================>]  24.72M  72.7MB/s    in 0.3s

2021-03-29 07:41:49 (72.7 MB/s) - 'ssimap_smooth_032015.png.csv' saved [25920000/25920000
]
```

In [2]:

```
import numpy as np
import pandas as pd
import seaborn as sns
import matplotlib.pyplot as plt
%matplotlib inline
```

In [3]:

```
try:
  del mer_albedo_top, mer_albedo_bottom
  del mgsi, ssi, fesi, alsi, casi
  print("Cleared previously loaded variables")
except:
  pass
```

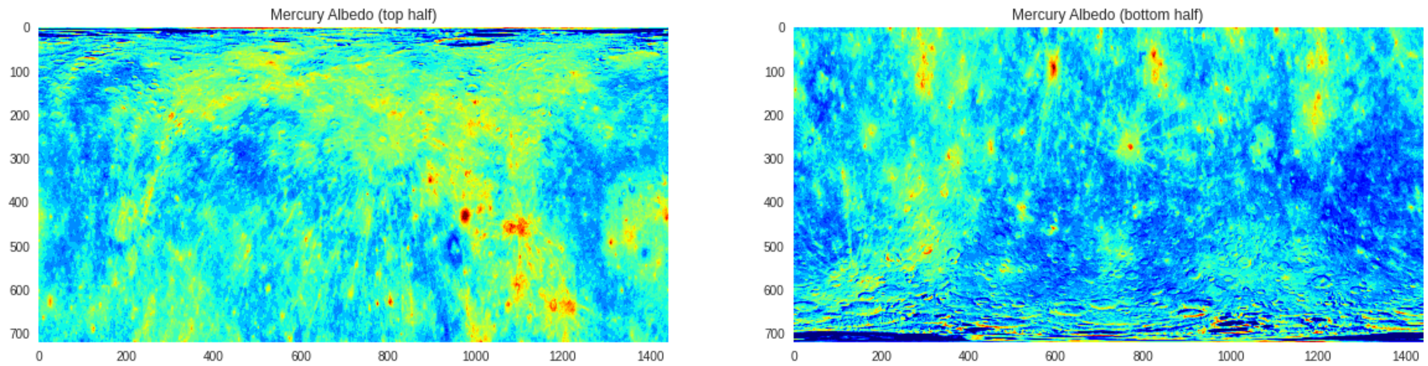
```python
albedo_top = pd.read_csv("mercury-albedo-top-half.png.csv", header=None) # Training part
albedo_bottom = pd.read_csv("mercury-albedo-resized-bottom-half.png.csv", header=None) # Testing part
mgsi = pd.read_csv("mgsimap_smooth_032015.png.csv", header=None)
ssi = pd.read_csv("ssimap_smooth_032015.png.csv", header=None)
fesi = pd.read_csv("fesimap_smooth_032015.png.csv", header=None)
alsi = pd.read_csv("alsimap_smooth_032015.png.csv", header=None)
casi = pd.read_csv("casimap_smooth_032015.png.csv", header=None)
```

In [5]:

```python
# Set plotting parameters
plt.style.use("seaborn")
cmap = plt.get_cmap('jet', 20)
```

In [14]:

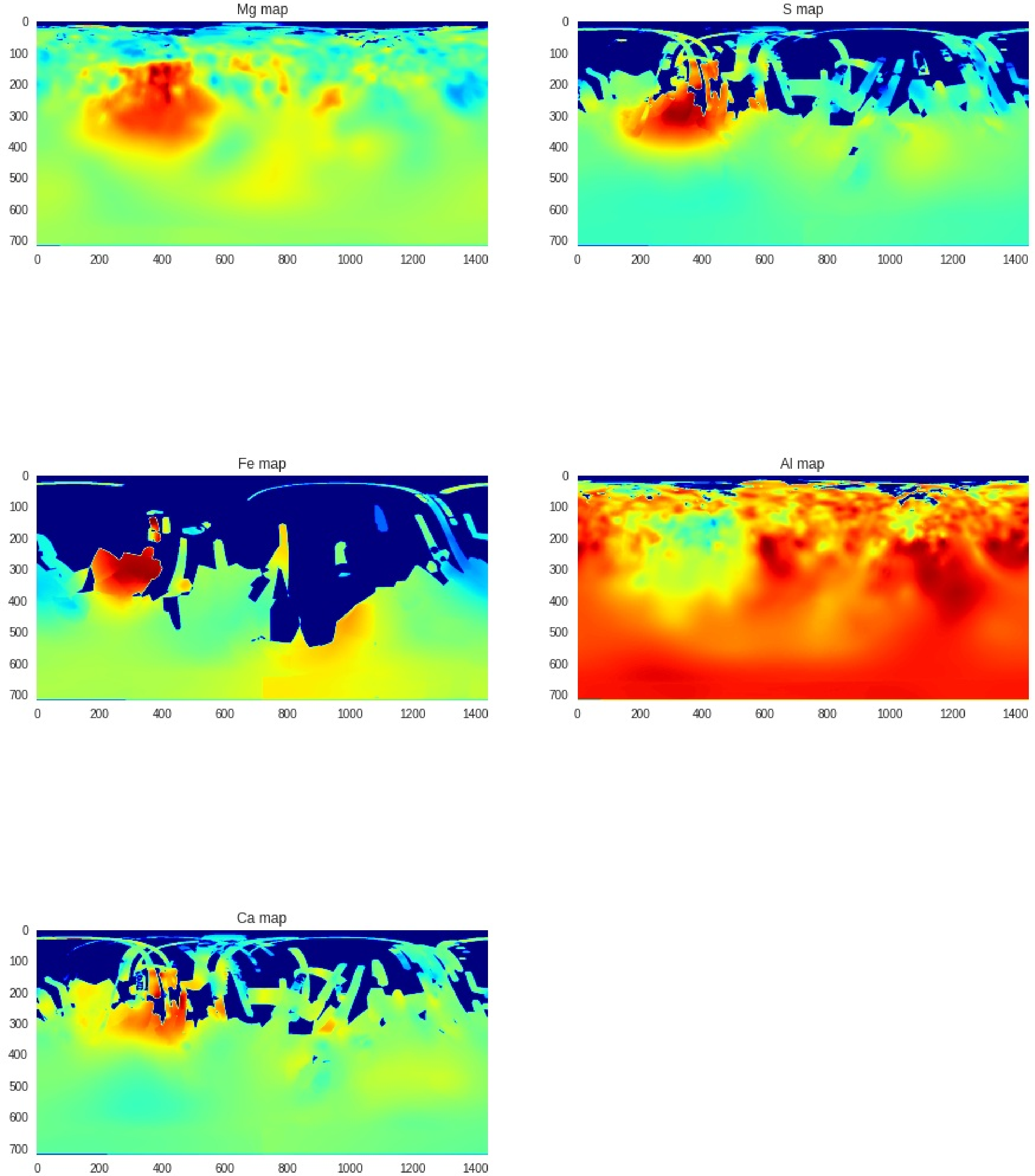
```python
fig, axs = plt.subplots(1, 2, figsize=(20, 10))

axs[0].imshow(albedo_top, cmap=cmap)
axs[0].grid(False)
axs[0].set_title("Mercury Albedo (top half)")

axs[1].imshow(albedo_bottom, cmap=cmap)
axs[1].grid(False)
axs[1].set_title("Mercury Albedo (bottom half)")

plt.show()
```



In [22]:

```python
fig = plt.figure(figsize=(15, 20))

# Set some plotting parameters
sm = plt.cm.ScalarMappable(cmap=cmap)
cbar_ax = fig.add_axes([0.75, 0.10, 0.02, 0.40])
fig.colorbar(sm, cax=cbar_ax)

ax1 = plt.subplot2grid((3, 2), (0, 0))
ax1.set_title("Mg map")
ax2 = plt.subplot2grid((3, 2), (0, 1))
ax2.set_title("S map")
ax3 = plt.subplot2grid((3, 2), (1, 0))
ax3.set_title("Fe map")
ax4 = plt.subplot2grid((3, 2), (1, 1))
ax4.set_title("Al map")
ax5 = plt.subplot2grid((3, 2), (2, 0))
ax5.set_title("Ca map")

plt.subplots_adjust()

ax1.imshow(mgsi.to_numpy(), cmap='jet')
ax1.grid(False)

ax2.imshow(ssi.to_numpy(), cmap='jet')
ax2.grid(False)

ax3.imshow(fesi.to_numpy(), cmap='jet')
```

```
ax3.grid(False)

ax4.imshow(alsi.to_numpy(), cmap='jet')
ax4.grid(False)

ax5.imshow(casi.to_numpy(), cmap='jet')
ax5.grid(False)

plt.show()
```



Some claims/points from the paper: https://www.sciencedirect.com/science/article/abs/pii/S001910352030107X that can be verified are:

- **There is a higher detection of S and Ca (orange-red color region) in the regions of high Mg concentration (orange-red section on the Mg map). Moreover, it is partially true also for Fe.**
- **The S and Ca maps look very similar and hence are correlated with each other. This might be an evidence for the presence of the mineral oldhamite (CaS) as stated in the paper.**

for the presence of the mineral oldhamite (CaS) as stated in the paper.

In [45]:

```
if isinstance(albedo_top, pd.DataFrame):
  albedo_top = albedo_top.to_numpy()
if isinstance(albedo_top, pd.DataFrame):
  albedo_bottom = albedo_bottom.to_numpy()

def create_dataset(albedo_ut, s_ut, fe_ut, al_ut, ca_ut, mg_ut):
  """
  Parameters:
  -----------
  Input: NumPy arrays

  Returns a list of dataframe objects
  """

  albedo = albedo_ut.reshape(-1, 1).squeeze()
  s = s_ut.reshape(-1, 1).squeeze()
  fe = fe_ut.reshape(-1, 1).squeeze()
  al = al_ut.reshape(-1, 1).squeeze()
  ca = ca_ut.reshape(-1, 1).squeeze()
  mg = mg_ut.reshape(-1, 1).squeeze()

  return np.array([albedo, s, fe, al, ca, mg])
```

In [46]:

```
ssi_top, fesi_top, alsi_top, casi_top, mgsi_top = np.array(ssi), np.array(fesi), np.arra
y(alsi), np.array(casi), np.array(mgsi)
train_data = pd.DataFrame(create_dataset(albedo_top, ssi_top, fesi_top, alsi_top, casi_t
op, mgsi_top).T)
train_data.rename(columns={0: "Albedo", 1: "S", 2: "Fe", 3: "Al", 4: "Ca", 5: "Mg"}, inp
lace=True)
```

In [47]:

```
test_data = pd.DataFrame(albedo_bottom.reshape(-1, 1).squeeze().T)
test_data.rename(columns={0: "Albedo"}, inplace=True)
```

In [49]:

```
test_data # Feature
```

Out[49]:

	Albedo
0	0.321569
1	0.360784
2	0.392157
3	0.341176
4	0.298039
...	...
1036795	0.188235
1036796	0.188235
1036797	0.192157
1036798	0.196078
1036799	0.200000

1036800 rows × 1 columns

We could try running similar machine learning algorithms (as trained in the first task). It would be interesting to

gauge the performance of those models for this task for a baseline.

In [223]:

```
from sklearn.multioutput import MultiOutputRegressor
# from sklearn.linear_model import LinearRegression
# from sklearn.ensemble import RandomForestRegressor
# from sklearn.svm import LinearSVR
import xgboost as xgb
```

In [224]:

```
x_train = np.array(train_data[train_data.columns[0]])
x_train = x_train.reshape(-1, 1)
y_train = np.array(train_data[train_data.columns[1:]])
x_test = np.array(test_data["Albedo"]).reshape(-1, 1)
```

In [225]:

```
models = [("xgbreg", xgb.XGBRegressor)]

def exp_all_models(x_train, y_train, x_test, models):
  errors = list()
  predictions = list()
  for name, model in models:
    if name == "xgbreg":
      model_ = model(objective="reg:squarederror", colsample_bytree=0.3, learning_rate=0
.1,
                     max_depth=5, alpha=10, n_estimators=400)
    else:
      model_ = model()
    model_ = MultiOutputRegressor(model_)
    model_.fit(x_train, y_train)
    prediction = model_.predict(x_test)
    predictions.append(prediction)

  return predictions
```

In [226]:

```
try:
  del s_list, fe_list, al_list, ca_list, mg_list
except:
  pass
```

In [227]:

```
shape = (720, 1440)

predictions = exp_all_models(x_train, y_train, x_test, models)

s_list = list()
fe_list = list()
al_list = list()
ca_list = list()
mg_list = list()
for pred in predictions:
  s = pred[:, 0].reshape(shape)
  s_list.append(s)
  fe = pred[:, 1].reshape(shape)
  fe_list.append(fe)
  al = pred[:, 2].reshape(shape)
  al_list.append(al)
  ca = pred[:, 3].reshape(shape)
  ca_list.append(ca)
  mg = pred[:, 4].reshape(shape)
  mg_list.append(mg)
```

Observations:

- **Training on a `XGBoost` regressor takes a significant amount of time. As a result, it might be a good idea to**

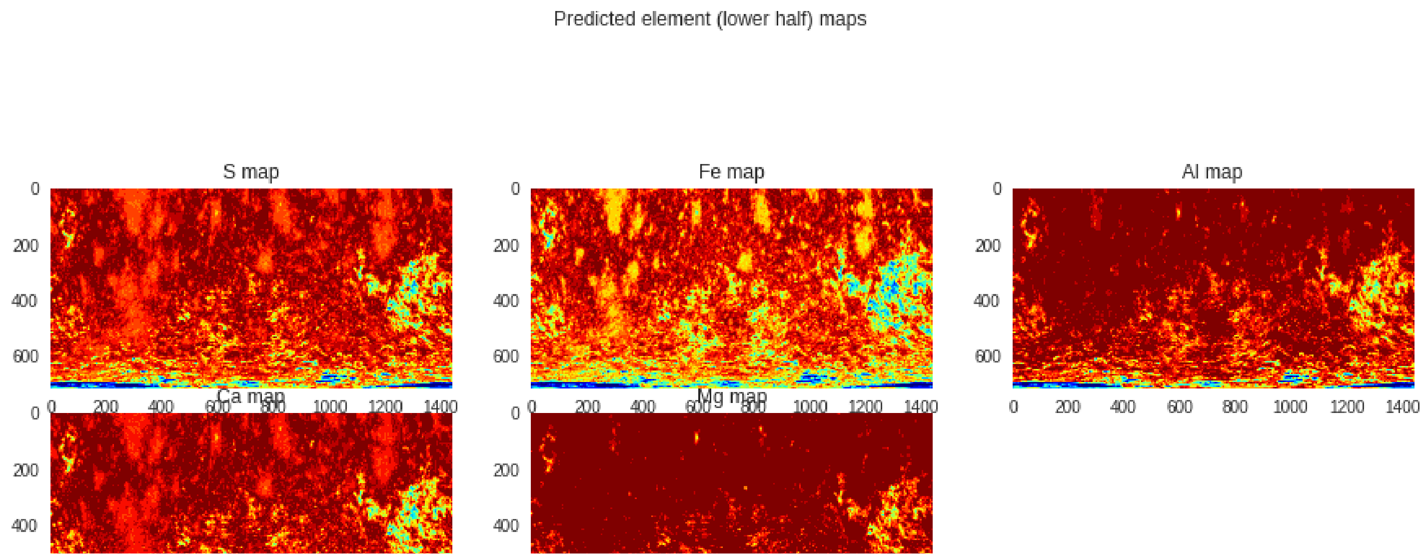
- Training on a `XGBoost` regressor takes a significant amount of time. As a result, it might be a good idea to use xgboost's `DMatrix` data structure which optimizes memory and training time.
- **We could build a more robust model using cross validation on this regressor.**

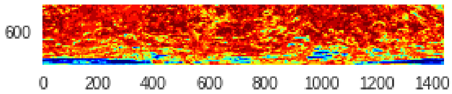
The order of set of plots is: LinearRegression, LinearSVR, XGBoostRegressor, `RandomForestRegressor`.

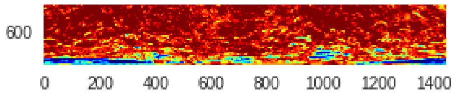
The predictions from the `XGBoostRegressor` are going to be used for the final albedo prediction due to their superior performance in predicting albedo on moon. The predictions from the other regressors are just plotted for analysis.

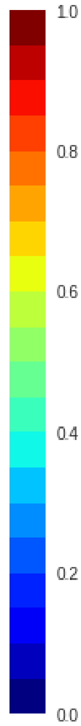
In [231]:

```
fig = plt.figure(figsize=(15, 15))
fig.suptitle("Predicted element (lower half) maps")

# Set some plotting parameters
cmap = plt.get_cmap('jet', 20)
sm = plt.cm.ScalarMappable(cmap=cmap)
cbar_ax = fig.add_axes([0.85, 0.10, 0.02, 0.40])
fig.colorbar(sm, cax=cbar_ax)

# XGBoost Regression
ax1_ = plt.subplot2grid((6, 3), (0, 0))
ax1_.set_title("S map")
ax2_ = plt.subplot2grid((6, 3), (0, 1))
ax2_.set_title("Fe map")
ax3_ = plt.subplot2grid((6, 3), (0, 2))
ax3_.set_title("Al map")
ax4_ = plt.subplot2grid((6, 3), (1, 0))
ax4_.set_title("Ca map")
ax5_ = plt.subplot2grid((6, 3), (1, 1))
ax5_.set_title("Mg map")

plt.subplots_adjust(wspace = 0.2, hspace = 0.1)

ax1_.imshow(s_list[0], cmap=cmap)
ax1_.grid(False)

ax2_.imshow(fe_list[0], cmap=cmap)
ax2_.grid(False)

ax3_.imshow(al_list[0], cmap=cmap)
ax3_.grid(False)

ax4_.imshow(ca_list[0], cmap=cmap)
ax4_.grid(False)

ax5_.imshow(mg_list[0], cmap=cmap)
ax5_.grid(False)

plt.show()
```









As per the paper, the mercury's crust is rich in Mg and S, but poor in the other elements (Al, Ca, Fe).

From the predicted chemical composition it seems that all the maps have some similarity between them, and although it predicted the high concentration of Mg and S, it also modeled the composition of the other elements in a similar fashion, thus failing to reproduce lower concentrations of Al, Ca, and Fe:

Unlike for the case of moon, a more sophisticated architecture might be needed to split the degeneracy of element maps and to match the observational ground-truth.

Using this chemical composition map, we could predict the albedo and compare with the observed albedo map. Since machine learning techniques rely on data heavily, we could expect the final results to be slightly sub-optimal.

Some analysis that was not shown here:

- **If a `LinearSVR` model is fitted, it does seem to converge for this data (unlike for the moon maps).**
- **The resulting maps from different regressors (`LinearSVR`, `LinearRegression`) seem to be similar to the `XGBoostRegressor` version.**

In [232]:

```
test_elements = pred # lower half
test_albedo = albedo_bottom # lower half
train_elements = train_data[train_data.columns[1:]].to_numpy() # upper half
train_albedo = train_data[train_data.columns[0]]
```

Tree based regressors have proven their ability to identify relationship between chemical composition and albedo. Hence, we are using a `XGBoostRegressor` for the final albedo prediction.

In [233]:

```
xgbmodel = xgb.XGBRegressor(objective="reg:squarederror", colsample_bytree=0.3, learning_
rate=0.1,
```

```
                     max_depth=5, alpha=10, n_estimators=400)
xgbmodel.fit(train_elements, train_albedo)
```

Out[233]:

```
XGBRegressor(alpha=10, base_score=0.5, booster='gbtree', colsample_bylevel=1,
             colsample_bynode=1, colsample_bytree=0.3, gamma=0,
             importance_type='gain', learning_rate=0.1, max_delta_step=0,
             max_depth=5, min_child_weight=1, missing=None, n_estimators=400,
             n_jobs=1, nthread=None, objective='reg:squarederror',
             random_state=0, reg_alpha=0, reg_lambda=1, scale_pos_weight=1,
             seed=None, silent=None, subsample=1, verbosity=1)
```

In [234]:

```python
from sklearn.metrics import mean_squared_error, mean_absolute_error

def metric_eval(y_test, prediction, metric="rmse"):
  """
  metric: 'mse' or 'mae' or 'rmse', default to 'rmse'
  """

  if metric == "mse":
    error = mean_squared_error(y_test, prediction)
  elif metric == "mae":
    error = mean_absolute_error(y_test, prediction)
  else:
    error = mean_squared_error(y_test, prediction, squared=False)

  return error
```

In [235]:

```python
final_albedo_pred = xgbmodel.predict(test_elements)
error = metric_eval(test_albedo, final_albedo_pred.reshape(shape))
```

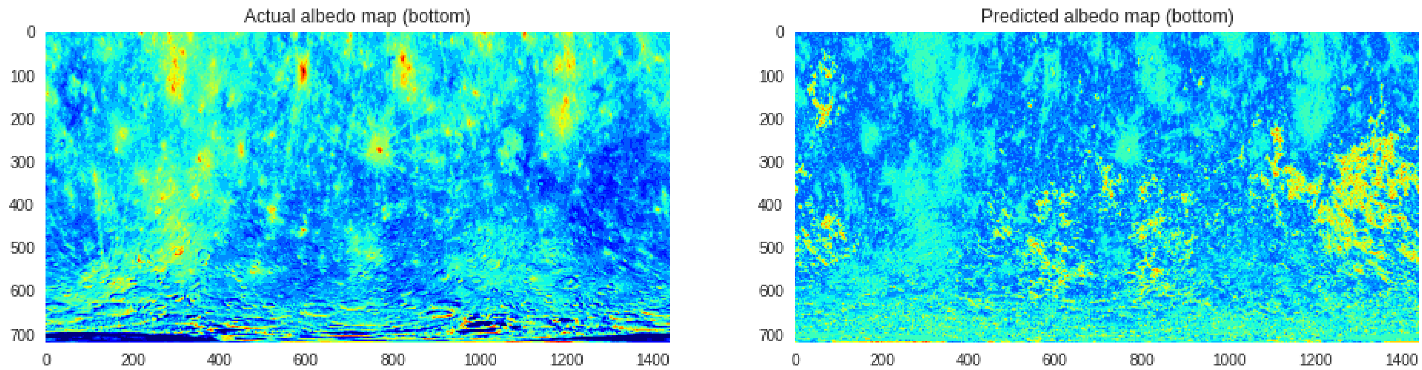
In [236]:

```python
print(f"rmse: {error}")
```

```
rmse: 0.16065340318377683
```

In [237]:

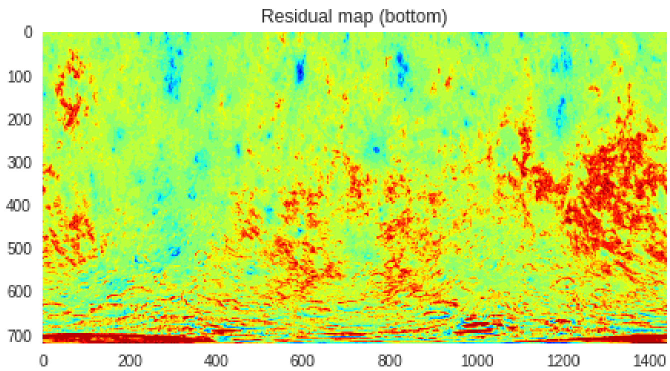
```python
fig_, axes_ = plt.subplots(1, 2, figsize=(16, 8))

axes_[0].imshow(albedo_bottom, cmap=cmap)
axes_[0].grid(False)
axes_[0].set_title("Actual albedo map (bottom)")

axes_[1].imshow(final_albedo_pred.reshape(shape), cmap=cmap)
axes_[1].grid(False)
axes_[1].set_title("Predicted albedo map (bottom)")

plt.show()
```

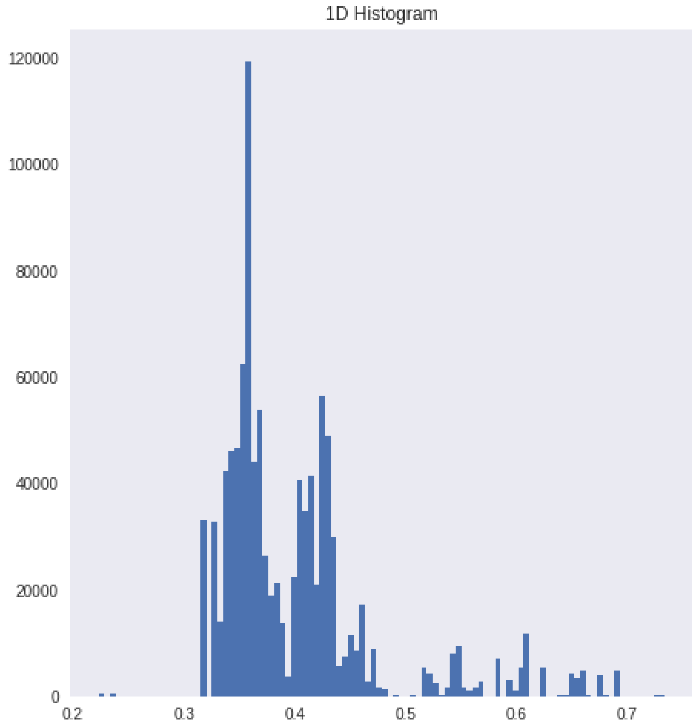


In [238]:

```python
residual_albmap = final_albedo_pred.reshape(shape) - albedo_bottom
```

```
residual_albmap = final_albedo_pred.reshape(shape) - albedo_bottom
n_bins = 100

fig_, axes_ = plt.subplots(1, 2, figsize=(16, 8))

axes_[0].imshow(residual_albmap, cmap=cmap)
axes_[0].grid(False)
axes_[0].set_title("Residual map (bottom)")

axes_[1].hist(final_albedo_pred.reshape(shape).flatten(), bins=n_bins)
axes_[1].grid(False)
axes_[1].set_title("1D Histogram")

plt.show()
```





Analysis

The result above is a consequence of the inaccurate prediction of the chemical composition maps.

Deep learning architectures can potentially be able to find and learn patterns between features and albedo on mercury. It is also evident that learning patterns on mercury maps is slightly difficult for traditional machine learning architectures (unlike moon maps), especially because the element ratio maps didn't had full coverage throughout the field.