8-gVirtualXRay_vs_VHP

March 2, 2022

[1]:
```
from IPython.display import display
from IPython.display import Image
import os
from utils import * # Code shared across more than one notebook
```

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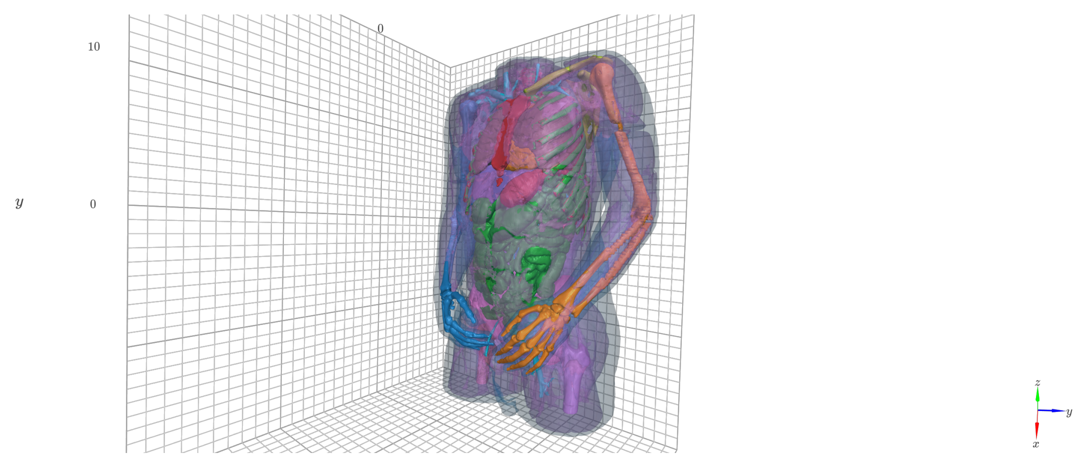
Purpose: In this notebook, we aim to demonstrate that gVirtualXRay is able to generate analytic simulations on GPU comparable to real images from the Visible Human Project (VHP). We register the data provided by VoxelMan segmented from the cadaver's CT and cryosections onto a pelvis radiograph of the human participant. All the acquisition parameters are unknown and would need to be estimated.

Material and Methods: We use the definitions of tissue substitutes provided in the ICRU Report 44 by the International Commission on Radiation Units and Measurements.

[2]:
```
fname = "plots/VHP_model.png"
if os.path.exists(fname):
    display(Image(fname))
```



Results: The **zero-mean normalised cross-correlation is 58.48%**. The **Structural Similarity Index (SSIM) is 0.2985**.

The calculations were performed on the following platform:

[3]:

```
printSystemInfo()
```

```
OS:
        Linux 5.3.18-150300.59.49-default
        x86_64

CPU:
        AMD Ryzen 7 3800XT 8-Core Processor

RAM:
        63 GB
GPU:
        Name: GeForce RTX 2080 Ti
        Drivers: 455.45.01
        Video memory: 11 GB
```

1 Import packages

[4]:

```
%matplotlib inline

import os # Locate files
from time import sleep

import datetime
import math
import numpy as np # Who does not use Numpy?
import pandas as pd # Load/Write CSV files

import matplotlib
# old_backend =  matplotlib.get_backend()
# matplotlib.use("Agg")  # Prevent showing stuff

from matplotlib.cm import get_cmap
import matplotlib.pyplot as plt # Plotting
from matplotlib.colors import LogNorm # Look up table
import matplotlib.colors as mcolors

font = {'family' : 'serif',
        #'weight' : 'bold',
         'size'   : 22
       }
matplotlib.rc('font', **font)
matplotlib.rc('text', usetex=True)

from scipy.stats import pearsonr # Compute the correlatio coefficient
```

```
from skimage.util import compare_images # Checkboard comparison between two␣
↪images

from skimage.util import compare_images # Checkboard comparison between two␣
↪images
from skimage.metrics import structural_similarity as ssim
from sklearn.metrics import mean_absolute_percentage_error as mape
# from skimage.metrics import structural_similarity as ssim
from sklearn.metrics import mean_absolute_error, mean_squared_error
import cv2

from tifffile import imread, imwrite # Load/Write TIFF files

import viewscad # Use OpenSCAD to create STL files

# import pyvista as pv # 3D visualisation
# from pyvista import themes

# import cma # Optimise the parameters of the noise model

import k3d
import random
import base64
from stl import mesh

import urllib, gzip # To download the phantom data, and extract the␣
↪corresponding Z file


import gvxrPython3 as gvxr # Simulate X-ray images
import json2gvxr # Set gVirtualXRay and the simulation up
from utils import * # Code shared across more than one notebook
import cma # Optimisation

from pymoo.algorithms.moo.nsga2 import NSGA2
from pymoo.factory import get_problem
from pymoo.optimize import minimize
from pymoo.visualization.scatter import Scatter

import plotly.express as px
import plotly.graph_objects as go
from plotly.subplots import make_subplots

import sys
```

```
SimpleGVXR 1.0.1 (2022-02-22T14:00:25) [Compiler: GNU g++] on Linux
gVirtualXRay core library (gvxr) 1.1.5 (2022-02-22T14:00:25) [Compiler: GNU g++]
```

on Linux

[5]:
```python
def standardisation(img):
    return (img - img.mean()) / img.std()
```

2 Reference image

We first load the reference image from the Visible Human Project. You can find it at https://data.lhncbc.nlm.nih.gov/public/Visible-Human/Male-Images/radiological/xray8/x_vm_pe.Z. When you download it, make sure to gunzip it!

[6]:
```python
if not os.path.exists("VHP"):
    os.mkdir("VHP")

if not os.path.exists("VHP/x_vm_pe.Z"):
    urllib.request.urlretrieve("https://data.lhncbc.nlm.nih.gov/public/
 ↪Visible-Human/Male-Images/radiological/xray8/x_vm_pe.Z", "VHP/x_vm_pe.Z")

if not os.path.exists("VHP/x_vm_pe"):

    gzip_file = gzip.open('VHP/x_vm_pe.Z') # use gzip.open instead of builtin␣
 ↪open function
    file_content = gzip_file.read()
    f = open('VHP/x_vm_pe', 'wb')
    f.write(file_content)
    f.close()
```

[7]:
```python
raw_reference = np.fromfile("VHP/x_vm_pe", dtype=np.uint8)
raw_reference.shape = (1536,1248)
raw_reference = np.rot90(raw_reference)

# Crop
y_max = 1000
raw_reference = raw_reference[:y_max]
```

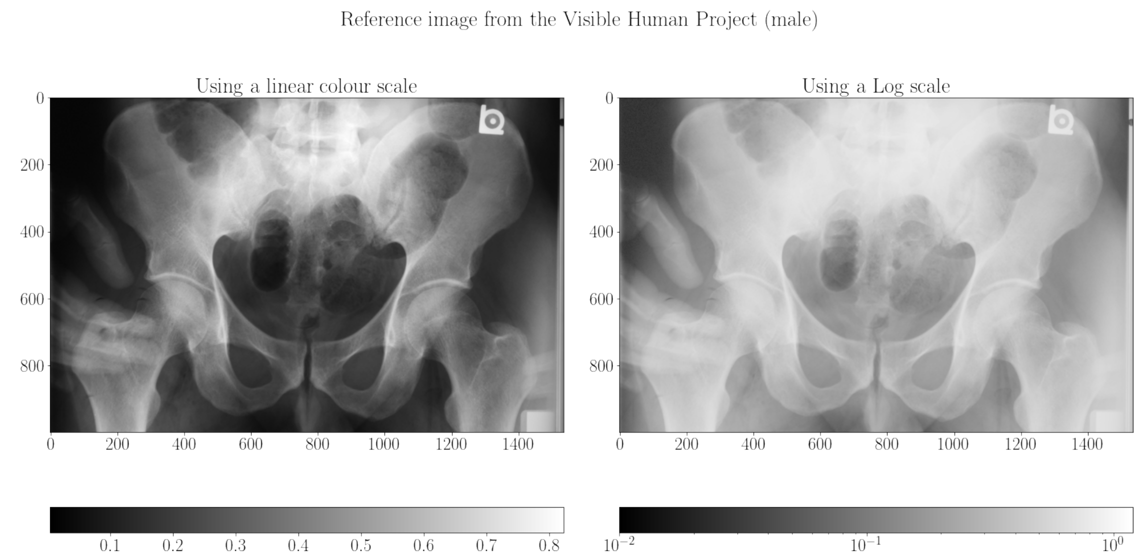
[8]:
```python
imwrite('gVirtualXRay_output_data/real_projection-VHP.tif', raw_reference.
 ↪astype(np.single))
```

[9]:
```python
corrected_real_projection = raw_reference.astype(np.single) / 255.0
```

[10]:
```python
imwrite('gVirtualXRay_output_data/corrected_real_projection-VHP.tif',␣
 ↪corrected_real_projection.astype(np.single))
```

We plot the image using a linear look-up table and a power-law normalisation.

[11]:
```python
displayLinearPowerScales(corrected_real_projection,
                         "Reference image from the Visible Human Project␣
 ↪(male)",
                         "plots/reference-VHP",
                         log=True)
```



Apply a log transformation

[12]:
```python
ground_truth = raw_reference
log_ground_truth = np.log(corrected_real_projection)
normalised_log_ground_truth = standardisation(log_ground_truth)

# imwrite('gVirtualXRay_output_data/ground_truth-VHP.tif', ground_truth.
 ↪astype(np.single))
```

3 Setting up gVirtualXRay

Before simulating an X-ray image using gVirtualXRay, we must create an OpenGL context.

[13]:
```python
json2gvxr.initGVXR("notebook-8.json", "EGL")
```

```
Create an OpenGL context: 800x450
Wed Mar  2 17:56:24 2022 ---- Create window gvxrStatus: Create window

0
1.5
4.5.0 NVIDIA 455.45.01
```

```
Wed Mar  2 17:56:24 2022 ---- EGL version: Wed Mar  2 17:56:24 2022 ---- OpenGL
version supported by this platform OpenGL renderer:   GeForce RTX 2080
Ti/PCIe/SSE2
OpenGL version:    4.5.0 NVIDIA 455.45.01
OpenGL vender:     NVIDIA Corporation
Wed Mar  2 17:56:24 2022 ---- Use OpenGL 4.5.0 0 500 500
0 0 800 450
```

3.1 X-ray source

We create an X-ray source. It is a point source.

[14]:
```
json2gvxr.initSourceGeometry()
```

```
Set up the beam
        Source position: [0.0, -30.5, 150.0, 'cm']
        Source shape: PointSource
```

3.2 Spectrum

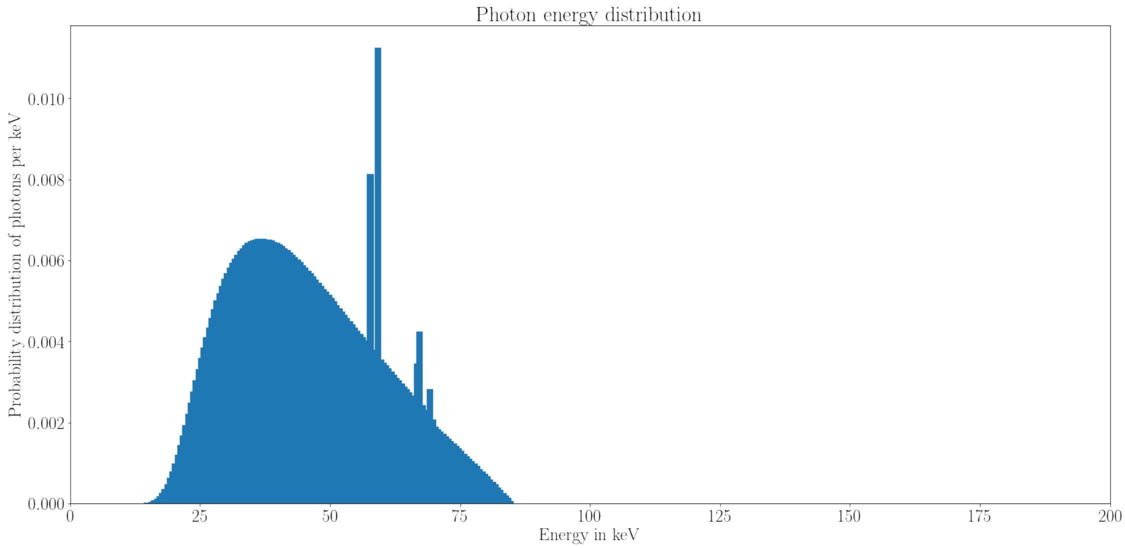
The spectrum is polychromatic.

[15]:
```
spectrum, unit, k, f = json2gvxr.initSpectrum(verbose=0)
energy_set = sorted(spectrum.keys())

count_set = []

for energy in energy_set:
    count_set.append(spectrum[energy])
```

```
params["Source"]["Beam"] {'kvp': 85, 'tube angle': 12, 'filter': [['Al', 3.2]]}
['Al', 3.2]
```

Plot the spectrum

[16]:
```
plotSpectrum(k, f, 'plots/spectrum-VHP')
```



3.3 Detector

Create a digital detector

[17]:
```
json2gvxr.initDetector()
```

```
Set up the detector
        Detector position: [0.0, -30.5, -20.5, 'cm']
        Detector up vector: [0, -1, 0]
        Detector number of pixels: [1536, 1248]
        Pixel spacing: [0.026347682927083334, 0.026347683, 'cm']
```

3.4 Sample

We now load the models segmented from the Visible Human.

Load the samples. `verbose=2` is used to print the material database for Gate. To disable it, use `verbose=0` or `verbose=1`.

[18]:
```
json2gvxr.initSamples(verbose=0)
```

```
VHP/meshes/armR.stl     nb_faces:       33838   nb_vertices:    101514
bounding_box (in cm):   (-10.0264, -10.1334, -2.8384)   (0.294166, 10.694,
6.13302)
VHP/meshes/armL.stl     nb_faces:       33475   nb_vertices:    100425
bounding_box (in cm):   (1.14313, -10.7634, -3.28228)   (9.46749, 11.1713,
5.74204)
```

```
VHP/meshes/chest.stl    nb_faces:       89235   nb_vertices:    267705
bounding_box (in cm):   (-5.19216, -2.22134, -4.18652)  (5.28961, 12.0778,
3.51821)
VHP/meshes/chest2.stl   nb_faces:       75408   nb_vertices:    226224
bounding_box (in cm):   (-5.20763, -2.213, -4.16399)    (5.26581, 12.0682,
4.06685)
VHP/meshes/femurL.stl   nb_faces:       9660    nb_vertices:    28980
bounding_box (in cm):   (2.2332, -14.6571, -1.851)      (5.5281, -8.86371,
0.57499)
VHP/meshes/femurR.stl   nb_faces:       9660    nb_vertices:    28980
bounding_box (in cm):   (-5.60176, -14.6576, -1.48193)  (-2.25352, -8.82717,
0.79766)
VHP/meshes/hips.stl     nb_faces:       56575   nb_vertices:    169725
bounding_box (in cm):   (-4.86403, -12.1307, -4.17882)  (4.97615, -4.45668,
1.91861)
VHP/meshes/bladder.stl  nb_faces:       2706    nb_vertices:    8118
bounding_box (in cm):   (-1.47306, -10.5873, -0.88731)  (0.947542, -9.09488,
1.8016)
VHP/meshes/bronch.stl   nb_faces:       1658    nb_vertices:    4974
bounding_box (in cm):   (-1.94132, 5.95348, -1.32576)   (1.82832, 8.46616,
0.070288)
VHP/meshes/circulatory.stl      nb_faces:       28012   nb_vertices:    84036
bounding_box (in cm):   (-4.15496, -13.5437, -2.42441)  (3.83071, 11.9091,
2.33955)
VHP/meshes/gallbladder.stl      nb_faces:       1172    nb_vertices:    3516
bounding_box (in cm):   (-3.57645, 0.788212, 0.717928)  (-2.14436, 2.12213,
3.22025)
VHP/meshes/heart.stl    nb_faces:       19290   nb_vertices:    57870
bounding_box (in cm):   (-1.82649, 3.34164, -0.817277)  (3.04628, 8.98106,
3.46046)
VHP/meshes/intestine.stl        nb_faces:       111010  nb_vertices:    333030
bounding_box (in cm):   (-4.22381, -9.67662, -1.68918)  (4.91206, 3.18448,
4.39048)
VHP/meshes/kidney.stl   nb_faces:       18283   nb_vertices:    54849
bounding_box (in cm):   (-3.52353, -2.96092, -2.65465)  (3.8139, 1.46367,
0.675229)
VHP/meshes/liver.stl    nb_faces:       29688   nb_vertices:    89064
bounding_box (in cm):   (-4.89368, -1.17826, -3.13392)  (2.02827, 5.00414,
3.76076)
VHP/meshes/lungs.stl    nb_faces:       68674   nb_vertices:    206022
bounding_box (in cm):   (-4.61199, 2.87393, -3.52451)   (4.57452, 10.5346,
3.27177)
VHP/meshes/muscles.stl  nb_faces:       553157  nb_vertices:    1659471
bounding_box (in cm):   (-10.1643, -14.6703, -4.70584)  (9.63791, 12.0829,
5.65443)
VHP/meshes/pancreas.stl nb_faces:       5638    nb_vertices:    16914
bounding_box (in cm):   (-1.25805, -0.822349, -1.27119) (2.71833, 2.29143,
1.78095)
```

```
VHP/meshes/shoulderL.stl        nb_faces:       12548   nb_vertices:    37644
bounding_box (in cm):   (0.437246, 5.94084, -4.08889)   (6.5641, 12.0494,
1.94009)
VHP/meshes/shoulderR.stl        nb_faces:       12454   nb_vertices:    37362
bounding_box (in cm):   (-7.24934, 5.67127, -4.06742)   (-0.804483, 11.5342,
1.83824)
VHP/meshes/skin.stl     nb_faces:       64068   nb_vertices:    192204
bounding_box (in cm):   (-10.2747, -14.6631, -5.1876)   (9.70979, 12.1115,
6.36175)
VHP/meshes/spine.stl    nb_faces:       22205   nb_vertices:    66615
bounding_box (in cm):   (-1.63024, -5.87568, -3.46047)  (1.92212, 0.863915,
0.495364)
VHP/meshes/spleen.stl   nb_faces:       6096    nb_vertices:    18288
bounding_box (in cm):   (0.76985, -0.12949, -3.09199)   (4.73059, 3.94038,
0.045474)
VHP/meshes/stomach.stl  nb_faces:       8928    nb_vertices:    26784
bounding_box (in cm):   (-0.162305, 0.659165, -2.26369) (3.41186, 4.32818,
3.96684)
```

[19]:

```
number_of_triangles = 0

for sample in json2gvxr.params["Samples"]:
    label = sample["Label"]
    number_of_triangles_in_mesh = gvxr.getNumberOfPrimitives(label)
    number_of_triangles += number_of_triangles_in_mesh

    print(label, \
          "has", \
          f"{number_of_triangles_in_mesh:,}", \
          "triangles.")

print("\nThere are", f"{number_of_triangles:,}", "triangles in total")
```

```
armR has 33,838 triangles.
armL has 33,475 triangles.
rib cage has 89,235 triangles.
sternum has 75,408 triangles.
femurL has 9,660 triangles.
femurR has 9,660 triangles.
hips has 56,575 triangles.
bladder has 2,706 triangles.
bronch has 1,658 triangles.
circulatory has 28,012 triangles.
gallbladder has 1,172 triangles.
heart has 19,290 triangles.
intestine has 111,010 triangles.
kidney has 18,283 triangles.
liver has 29,688 triangles.
```

```
lungs has 68,674 triangles.
muscles has 553,157 triangles.
pancreas has 5,638 triangles.
shoulderL has 12,548 triangles.
shoulderR has 12,454 triangles.
skin has 64,068 triangles.
spine has 22,205 triangles.
spleen has 6,096 triangles.
stomach has 8,928 triangles.

There are 1,273,438 triangles in total
```

3.5 Visualise the virtual patient

First, apply the scaling factor from voxels to cm.

[20]:
```
for anatomy in json2gvxr.params["Samples"]:
    label = anatomy["Label"]
    gvxr.scaleNode(label, 3.3, 3.3, 3.3)
    gvxr.applyCurrentLocalTransformation(label)
```

Visualise the virtual patient

[21]:
```
plot = k3d.plot()
plot.background_color = 0xffffff

for sample in json2gvxr.params["Samples"]:

    label = sample["Label"]

    fname = sample["Path"]

    r, g, b, a = gvxr.getAmbientColour(label)
    R = math.floor(255*r)
    G = math.floor(255*g)
    B = math.floor(255*b)
    A = math.floor(255*a)

    k3d_color = 0;
    k3d_color |= (R & 255) << 16;
    k3d_color |= (G & 255) << 8;
    k3d_color |= (B & 255);

    mesh_from_stl_file = mesh.Mesh.from_file(fname)

    if label == "skin":
        opacity = 0.2
```

```
    elif label == "muscles":
        opacity = 0.3
    else:
        opacity = 1
    geometry = k3d.mesh(mesh_from_stl_file.vectors.flatten(),
                        range(int(mesh_from_stl_file.vectors.flatten().
 ↪shape[0] / 3)),
                        color=k3d_color,
                        wireframe=False,
                        flat_shading=False,
                        name=fname,
                        opacity=opacity)

    plot += geometry

plot.display()
plot.camera = [17.757085561576094, -0.5941481609904308, 25.327896522760597, -0.
 ↪2824745178222656, -1.2793889045715332, 0.587073564529419, -0.
 ↪00450313545724278, 0.9990136450056702, 0.044175319620058 56]
```

Output()

[22]:
```
fname = 'plots/VHP_model.png'
if not os.path.isfile(fname):

    sleep(10)
    plot.fetch_screenshot() # Not sure why, but we need to do it twice to get␣
 ↪the right screenshot
    sleep(10)

    data = base64.b64decode(plot.screenshot)
    with open(fname,'wb') as fp:
        fp.write(data)
```

3.6 Simulation with the default values

[23]:
```
# Backup the transformation matrix
global_matrix_backup = gvxr.getSceneTransformationMatrix()
```

[24]:
```
def getXRayImage():
    global total_energy_in_MeV

    # Compute the X-ray image
    xray_image = np.array(gvxr.computeXRayImage())

    # Apply the ROI
```

```
    xray_image = xray_image[:y_max]

    # Flat-field
#     xray_image /= total_energy_in_MeV

    # Negative
    # x_ray_image = 1.0 - x_ray_image
    return xray_image #np.ones(xray_image.shape).astype(np.single) - xray_image
```

[25]:

```
xray_image = getXRayImage()
```

[26]:

```
# gvxr.enableArtefactFilteringOnCPU()
gvxr.enableArtefactFilteringOnGPU()
# gvxr.disableArtefactFiltering() # Spere inserts are missing with GPU␣
↪integration when a outer surface is used for the matrix
```

[27]:

```
# total_energy_in_keV = 0.0
# for energy, count in zip(energy_set, count_set):
#     effective_energy = find_nearest(detector_response[:,0], energy / 1000,␣
↪detector_response[:,1])

#     total_energy_in_keV += effective_energy * count

total_energy_in_MeV = gvxr.getTotalEnergyWithDetectorResponse()
```

[28]:

```
xray_image = getXRayImage()
```

[29]:

```
gvxr.displayScene()
gvxr.useNegative()

gvxr.setZoom(1569.6787109375)
gvxr.setSceneRotationMatrix([-0.3190782964229584,  -0.15100032091140747, -0.
↪9356207251548767,  0.0,
                              0.002036974299699068, 0.987101674079895,   -0.
↪16000667214393616, 0.0,
                              0.9477221369743347,  -0.05296054854989052, -0.
↪31466084718704224, 0.0,
                              0.0,                  0.0,                  0.0, ␣
↪               1.0])

gvxr.setWindowBackGroundColour(0.5, 0.5, 0.5)

gvxr.displayScene()
```

[30]:

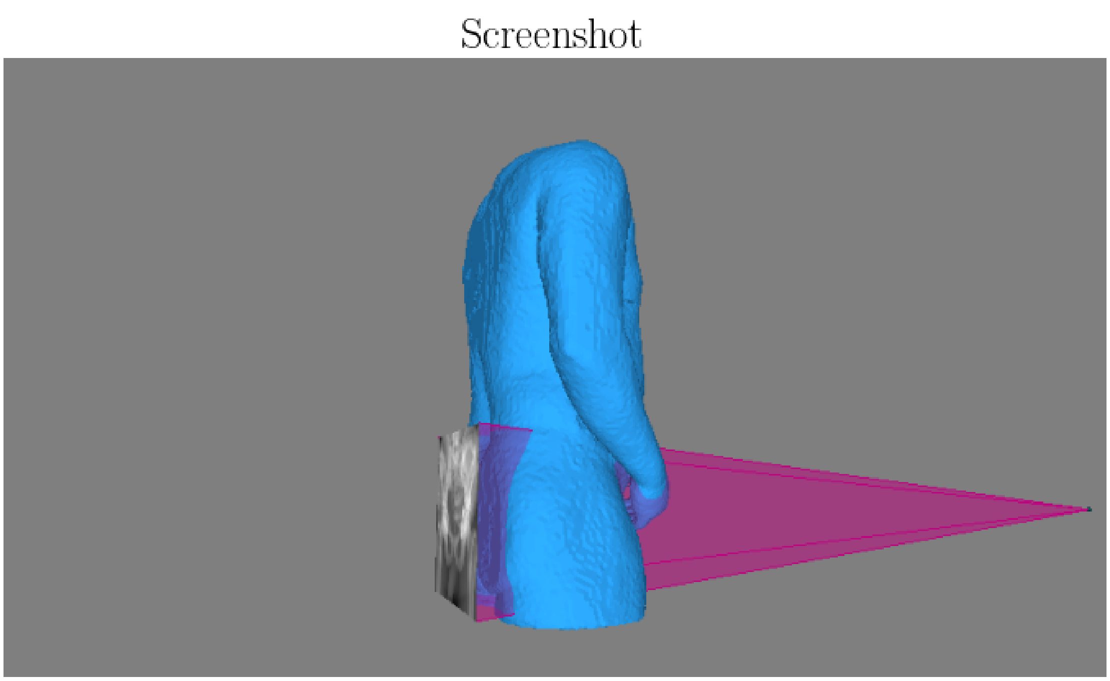
```
# gvxr.renderLoop()
```

[31]:
```
# print(gvxr.getZoom())
# print(gvxr.getSceneRotationMatrix())
```

[32]:
```
screenshot = (255 * np.array(gvxr.takeScreenshot())).astype(np.uint8)
```

[33]:
```
fname = 'VHP/default-screenshot.png'
if True:#not os.path.isfile(fname):

    plt.imsave(fname, screenshot)
```

[34]:
```
plt.figure(figsize= (10,10))
plt.title("Screenshot")
plt.imshow(screenshot)
plt.axis('off')

plt.tight_layout()

plt.savefig('plots/default-screenshot-beam-on-VHP.pdf')
plt.savefig('plots/default-screenshot-beam-on-VHP.png')
```

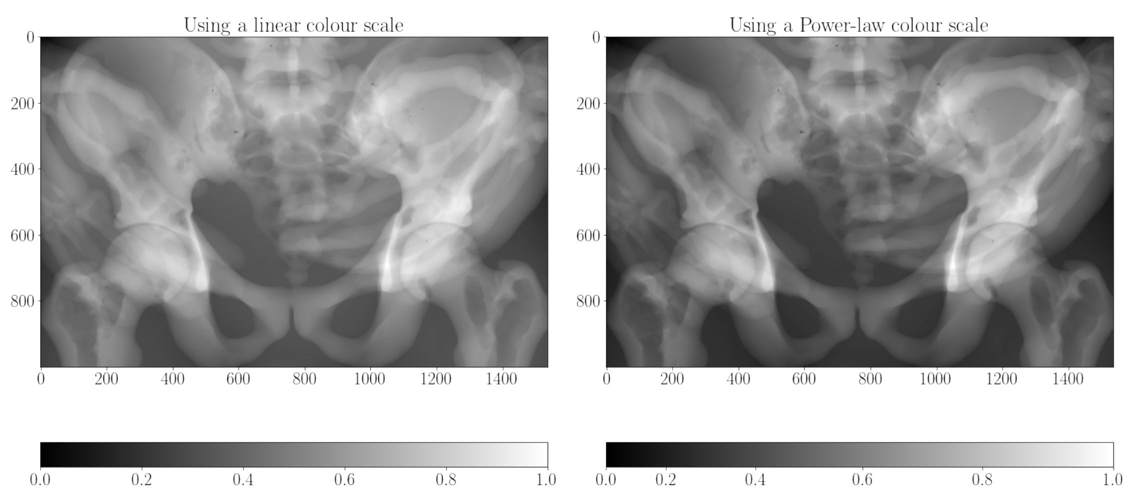


[35]:
```
def logImage(xray_image: np.array, min_val: float, max_val: float) -> np.array:

    log_epsilon = 1.0e-9

    shift_filter = -math.log(min_val + log_epsilon)
```

```
    if min_val != max_val:
        scale_filter = 1.0 / (math.log(max_val + log_epsilon) - math.
↪log(min_val + log_epsilon))
    else:
        scale_filter = 1.0

    corrected_image = np.log(xray_image + log_epsilon)

    return (corrected_image + shift_filter) * scale_filter
```

[36]:
```
displayLinearPowerScales(1 - logImage(xray_image, xray_image.min(), xray_image.
↪max()),
                         "Image simulated using gVirtualXRay before the␣
↪registration",
                         "plots/gVirtualXRay-before_registration-VHP",
                         log=False)
```

Image simulated using gVirtualXRay before the registration



4 Registration

4.1 Single-objective optimisation with CMA-ES

1st using CMA-ES with 5 different fitness functions, then using NSGA2 and NSGA3.

[37]:
```
roi_ground_truth_min = ground_truth.min()
roi_ground_truth_max = ground_truth.max()
standardised_roi_ground_truth = standardisation(ground_truth)
```

```
imsave('gVirtualXRay_output_data/standardised_roi_ground_truth-VHP.tif',␣
↪standardised_roi_ground_truth.astype(np.single))
```

```
/tmp/ipykernel_4067/1698494017.py:5: DeprecationWarning: <tifffile.imsave> is
deprecated. Use tifffile.imwrite
  imsave('gVirtualXRay_output_data/standardised_roi_ground_truth-VHP.tif',
standardised_roi_ground_truth.astype(np.single))
```

[38]:
```
source_position = gvxr.getSourcePosition("cm")
detector_position = gvxr.getDetectorPosition("cm")

x_init = [
    # Orientation of the sample
    0.0, 0.0,

    # Position of the source
    source_position[0],
    source_position[1],
    source_position[2],

    # Position of the detector
    detector_position[0],
    detector_position[1],
    detector_position[2]#,

    # Orientation of the detector
    #     det_rotation_angle1 = x[8]
    #     det_rotation_angle2 = x[9]

#         1.0 / 3.0, # c1
#         1.0, # gain1
#         0.0, # bias1

#         1.0 / 3.0, # c2
#         1.0, # gain2
#         0.0#, # bias2

#         1.0 / 3.0, # c3
#         1.0, # gain3
#         0.0, # bias3
#         2.0 # gamma
]
```

[39]:
```
pos_offset = 20
angle_offset = 5
```

```
xl = [
            -angle_offset, -angle_offset,
            source_position[0] - pos_offset, source_position[1] - pos_offset,␣
 ↪source_position[2] - pos_offset,
            detector_position[0] - pos_offset, detector_position[1] -␣
 ↪pos_offset, detector_position[2] - pos_offset#,
#              -90, -90,
#              -10.0,
#              -10.0,
#              -10.0,

#              -10.0,
#              0.0,
#              0.0#,

#              -10.0,
#              -10.0,
#              -10.0,
#              0.0
        ]

xu = [
            angle_offset, angle_offset,
            source_position[0] + pos_offset, source_position[1] + pos_offset,␣
 ↪source_position[2] + pos_offset,
            detector_position[0] + pos_offset, detector_position[1] +␣
 ↪pos_offset, detector_position[2] + pos_offset #,
#              90, 90,
#              10.0,
#              10.0,
#              10.0,

#              10.0,
#              10.0,
#              10.0#,

#              10.0,
#              10.0,
#              10.0,
#              100.0
        ]
```

[40]:
```
def setTransformations(x):
    # Orientation of the sample
    sample_rotation_angle1 = x[0]
    sample_rotation_angle2 = x[1]
```

```
    gvxr.rotateScene(sample_rotation_angle1, 1, 0, 0)
    gvxr.rotateScene(sample_rotation_angle2, 0, 1, 0)

    # Position of the source
    source_position_x = x[2]
    source_position_y = x[3]
    source_position_z = x[4]

    gvxr.setSourcePosition(
        source_position_x,
        source_position_y,
        source_position_z,
        "cm"
    )

    # Position of the detector
    det_position_x = x[5]
    det_position_y = x[6]
    det_position_z = x[7]

    gvxr.setDetectorPosition(
        det_position_x,
        det_position_y,
        det_position_z,
        "cm"
    )

    # Orientation of the detector
#     det_rotation_angle1 = x[8]
#     det_rotation_angle2 = x[9]
```

[41]:
```
def resetToDefaultParameters():
    json2gvxr.initDetector("notebook-8.json")
    json2gvxr.initSourceGeometry("notebook-8.json")
    source_position = gvxr.getSourcePosition("cm")
    detector_position = gvxr.getDetectorPosition("cm")

    # Restore the transformation matrix
    gvxr.setSceneTransformationMatrix(global_matrix_backup)
```

[42]:
```
def updateXRayImage(x):


    # Backup the transformation matrix
    matrix_backup = gvxr.getSceneTransformationMatrix()

    # Set the transformations
```

```
    setTransformations(x)

    # Compute the X-ray image
    xray_image = getXRayImage()

#     gvxr.displayScene()
#     screenshot = gvxr.takeScreenshot()

    # Restore the transformation matrix
    gvxr.setSceneTransformationMatrix(matrix_backup)

    return xray_image #, screenshot
```

[43]:
```
def applyLogScaleAndNegative(image: np.array) -> np.array:
    temp = logImage(image, image.min(), image.max())
    return 1.0 - temp
```

[44]:
```
timeout_in_sec = 20 * 60 # 20 minutes
```

4.2 Define an objective function

[45]:
```
def objectiveFunction(x):

    global objective_function_string

    global ground_truth, standardised_roi_ground_truth
    global best_fitness, best_fitness_id, fitness_function_call_id,␣
↪evolution_fitness, evolution_parameters


    xray_image = updateXRayImage(x)
    corrected_xray_image = applyLogScaleAndNegative(xray_image)
    standardised_corrected_xray_image = standardisation(corrected_xray_image)

    if objective_function_string == "zncc":
        zncc = np.mean(standardised_roi_ground_truth *␣
↪standardised_corrected_xray_image)
        dzncc = (1.0 - zncc) / 2.0
        objective = dzncc
    elif objective_function_string == "mae":
        mae = np.mean(np.abs(standardised_roi_ground_truth -␣
↪standardised_corrected_xray_image))
        objective = mae
    elif objective_function_string == "rmse":
```

```
        rmse = math.sqrt(np.mean(np.square(standardised_roi_ground_truth -␣
↪standardised_corrected_xray_image)))
        objective = rmse
    elif objective_function_string == "ssim":
        ssim_value = ssim(standardised_roi_ground_truth,␣
↪standardised_corrected_xray_image, data_range=standardised_roi_ground_truth.
↪max() - standardised_roi_ground_truth.min())
        dssim = (1.0 - ssim_value) / 2.0
        objective = dssim
    elif objective_function_string == "mape":
        # Avoid div by 0
        offset1 = min(standardised_roi_ground_truth.min(),␣
↪standardised_corrected_xray_image.min())
        offset2 = 0.01 * (standardised_roi_ground_truth.max() -␣
↪standardised_roi_ground_truth.min())
        offset = offset2 - offset1
        mape_value = mape(standardised_roi_ground_truth + offset,␣
↪standardised_corrected_xray_image + offset)
        objective = mape_value

    if best_fitness > objective:

        evolution_fitness.append([fitness_function_call_id, objective])

        row = [fitness_function_call_id]
        for i in x:
            row.append(i)
        evolution_parameters.append(row)

        best_fitness = objective

    fitness_function_call_id += 1

    return objective
```

[46]:
```
def optimiseWithCMAES(objective_function_str: str):

    global objective_function_string
    global best_fitness
    global best_fitness_id
    global fitness_function_call_id
    global evolution_fitness
    global evolution_parameters

    resetToDefaultParameters()

    objective_function_string = objective_function_str
```

```
    source_position = [0.0, 0.0, 0.0]
    detector_position = [0.0, 0.0, 0.0]


    if os.path.exists("gVirtualXRay_output_data/HIPS-" +␣
↪objective_function_string + ".dat") and \
        os.path.exists("gVirtualXRay_output_data/HIPS_evolution-" +␣
↪objective_function_string + ".dat") and \
        os.path.exists("gVirtualXRay_output_data/HIPS_evolution_parameters-" +␣
↪objective_function_string + ".dat"):

        temp = np.loadtxt("gVirtualXRay_output_data/HIPS-" +␣
↪objective_function_string + ".dat")

        sample_rotation_angle1 = temp[0]
        sample_rotation_angle2 = temp[1]
        source_position[0] = temp[2]
        source_position[1] = temp[3]
        source_position[2] = temp[4]
        detector_position[0] = temp[5]
        detector_position[1] = temp[6]
        detector_position[2] = temp[7]

        evolution_fitness = np.loadtxt("gVirtualXRay_output_data/
↪HIPS_evolution-" + objective_function_string + ".dat")
        evolution_parameters = np.loadtxt("gVirtualXRay_output_data/
↪HIPS_evolution_parameters-" + objective_function_string + ".dat")

    # CMA-ES
    else:

        opts = cma.CMAOptions()
        opts.set('tolfun', 1e-5)
        opts['tolx'] = 1e-5
        opts['timeout'] = timeout_in_sec
        opts['bounds'] = [xl, xu]

        opts['CMA_stds'] = []

        for min_val, max_val in zip(opts['bounds'][0], opts['bounds'][1]):
            opts['CMA_stds'].append(abs(max_val - min_val) * 0.5)

        best_fitness = sys.float_info.max
        best_fitness_id = 0
        fitness_function_call_id = 0
```

```
        evolution_fitness = []
        evolution_parameters = []

        res = cma.fmin(objectiveFunction,
                    x_init,
                    0.5,
                    opts,
                    restarts=0)

        # Save the best individual
        sample_rotation_angle1 = res[0][0]
        sample_rotation_angle2 = res[0][1]
        source_position[0] = res[0][2]
        source_position[1] = res[0][3]
        source_position[2] = res[0][4]
        detector_position[0] = res[0][5]
        detector_position[1] = res[0][6]
        detector_position[2] = res[0][7]

        # Save best parameters from the optimiser
        answer = np.array([sample_rotation_angle1, sample_rotation_angle2,␣
↪source_position[0], source_position[1], source_position[2],␣
↪detector_position[0], detector_position[1], detector_position[2]])
        answer = answer.reshape(1, answer.shape[0])
        np.savetxt("gVirtualXRay_output_data/HIPS-" + objective_function_string␣
↪+ ".dat",
                      answer,
                      header='sample_rotation_angle1,␣
↪sample_rotation_angle2,source_pos_x,source_pos_y,source_pos_z,detector_pos_x,detector_pos_y

        # Save the list of zncc for plotting
        evolution_fitness = np.array(evolution_fitness)
        np.savetxt("gVirtualXRay_output_data/HIPS_evolution-" +␣
↪objective_function_string + ".dat",
                      evolution_fitness,
                      header='t,' + objective_function_string)

        # Save the list of parameters for plotting
        evolution_parameters = np.array(evolution_parameters)
        print(evolution_parameters.shape)

        np.savetxt("gVirtualXRay_output_data/HIPS_evolution_parameters-" +␣
↪objective_function_string + ".dat",
                      evolution_parameters,
                     ␣
↪header='t,sample_rotation_angle1,sample_rotation_angle2,source_pos_x,source_pos_y,source_po
```

```
    return [sample_rotation_angle1, sample_rotation_angle2, source_position[0],␣
↪source_position[1], source_position[2], detector_position[0],␣
↪detector_position[1], detector_position[2]], \
        evolution_fitness, \
        evolution_parameters
```

4.3 Run the optimisation for each image comparison method

[47]:
```
objective_function_string = "zncc"
x_zncc, evolution_fitness_zncc, evolution_parameters_zncc =␣
 ↪optimiseWithCMAES("zncc")

resetToDefaultParameters()
xray_image_zncc = applyLogScaleAndNegative(updateXRayImage(x_zncc))
```

```
Set up the detector
        Detector position: [0.0, -30.5, -20.5, 'cm']
        Detector up vector: [0, -1, 0]
        Detector number of pixels: [1536, 1248]
        Pixel spacing: [0.026347682927083334, 0.026347683, 'cm']
Set up the beam
        Source position: [0.0, -30.5, 150.0, 'cm']
        Source shape: PointSource
(5_w,10)-aCMA-ES (mu_w=3.2,w_1=45%) in dimension 8 (seed=382232, Wed Mar  2
18:08:38 2022)


Iterat #Fevals   function value  axis ratio  sigma  min&max std  t[m:s]
    1     10 2.836667776043340e-01 1.0e+00 4.51e-01  2e+00  9e+00 0:18.1
    2     20 2.722087167261154e-01 1.2e+00 4.44e-01  2e+00  9e+00 0:36.7
    3     30 2.825318498194490e-01 1.3e+00 5.21e-01  3e+00  1e+01 0:52.9
    4     40 2.719996984773466e-01 1.4e+00 5.79e-01  3e+00  1e+01 1:08.4
    5     50 2.800381193296418e-01 1.6e+00 6.06e-01  3e+00  1e+01 1:23.6
    6     60 2.808661065900667e-01 1.7e+00 6.02e-01  3e+00  1e+01 1:39.1
    7     70 3.005600636426897e-01 1.7e+00 6.39e-01  3e+00  1e+01 1:55.8
    8     80 2.773135675967033e-01 2.1e+00 6.01e-01  3e+00  1e+01 2:12.8
    9     90 2.704227129058216e-01 2.0e+00 5.97e-01  3e+00  1e+01 2:29.7
   10    100 2.714359221041655e-01 2.0e+00 5.62e-01  3e+00  1e+01 2:47.1
   11    110 2.835956018054445e-01 2.1e+00 4.98e-01  2e+00  1e+01 3:03.2
   12    120 2.574088704231697e-01 2.0e+00 4.92e-01  2e+00  1e+01 3:20.2
   13    130 2.987913854635590e-01 2.0e+00 4.72e-01  2e+00  1e+01 3:35.1
   14    140 2.676740956546922e-01 2.1e+00 4.37e-01  2e+00  9e+00 3:51.4
   15    150 2.618080654248216e-01 2.3e+00 4.61e-01  2e+00  1e+01 4:07.9
   16    160 2.649801904035337e-01 2.3e+00 4.77e-01  2e+00  1e+01 4:24.5
   17    170 2.575614208480665e-01 2.4e+00 5.20e-01  3e+00  1e+01 4:41.1
```

```
   18    180 2.814030043501947e-01 2.4e+00 5.24e-01  3e+00  1e+01 4:58.9
   20    200 2.658724226229408e-01 2.6e+00 5.49e-01  3e+00  1e+01 5:31.7
   22    220 2.745628081679110e-01 3.0e+00 7.94e-01  4e+00  2e+01 6:02.3
   24    240 2.676654116068145e-01 3.7e+00 6.93e-01  4e+00  2e+01 6:33.3
   26    260 2.737988566435164e-01 4.1e+00 5.90e-01  3e+00  2e+01 7:04.7
   28    280 2.772947262489623e-01 4.3e+00 4.78e-01  3e+00  1e+01 7:36.3
   30    300 2.724686531311194e-01 4.6e+00 4.96e-01  3e+00  1e+01 8:07.3
   32    320 2.641144598709793e-01 4.8e+00 5.43e-01  3e+00  1e+01 8:37.9
   34    340 2.825039717235119e-01 5.7e+00 5.61e-01  3e+00  2e+01 9:10.4
   36    360 2.558374316503360e-01 6.3e+00 5.39e-01  3e+00  1e+01 9:42.0
   38    380 2.457924097011788e-01 6.9e+00 4.22e-01  2e+00  1e+01 10:12.7
   40    400 2.646676729741324e-01 7.5e+00 4.20e-01  2e+00  1e+01 10:44.6
   42    420 2.552710927929039e-01 7.5e+00 4.31e-01  2e+00  1e+01 11:17.7
   44    440 2.458358462016098e-01 7.1e+00 3.67e-01  2e+00  1e+01 11:49.6
   46    460 2.494288692243756e-01 7.7e+00 3.14e-01  1e+00  8e+00 12:23.3
   48    480 2.430770829941931e-01 7.6e+00 2.97e-01  1e+00  9e+00 12:57.2
   50    500 2.397169370325826e-01 8.7e+00 2.47e-01  1e+00  7e+00 13:30.3
   52    520 2.366954223780613e-01 8.2e+00 2.27e-01  1e+00  6e+00 14:05.0
   55    550 2.384403543771392e-01 8.5e+00 2.08e-01  9e-01  6e+00 14:56.2
   58    580 2.332567001804368e-01 9.1e+00 1.78e-01  7e-01  5e+00 15:47.5
   61    610 2.338315444681189e-01 9.7e+00 1.31e-01  5e-01  4e+00 16:38.8
   64    640 2.326434289546733e-01 1.0e+01 1.03e-01  4e-01  3e+00 17:30.5
   67    670 2.320865751263594e-01 9.7e+00 7.92e-02  3e-01  2e+00 18:22.2
   70    700 2.328671018196897e-01 1.3e+01 1.01e-01  4e-01  3e+00 19:13.9
   73    730 2.312060178391220e-01 1.2e+01 8.10e-02  3e-01  2e+00 20:05.8
termination on timeout=1200 (Wed Mar  2 18:28:46 2022)
final/bestever f-value = 2.315344e-01 2.312060e-01
incumbent solution: [-4.998974026500497, 1.5361909985068536,
-17.954644162151165, -16.361522895194494, 130.0302130073531, 18.04905943500427,
-49.77185991997291, -40.43485264564243]
std deviation: [0.28847917564298414, 0.3516951239955791, 1.1619195331734589,
1.2410411341672563, 2.37537962232658, 0.3354009083950652, 0.7628757971677332,
0.8877460844392998]
(17, 9)
Set up the detector
        Detector position: [0.0, -30.5, -20.5, 'cm']
        Detector up vector: [0, -1, 0]
        Detector number of pixels: [1536, 1248]
        Pixel spacing: [0.026347682927083334, 0.026347683, 'cm']
Set up the beam
        Source position: [0.0, -30.5, 150.0, 'cm']
        Source shape: PointSource
```

[48]:
```
objective_function_string = "mae"
x_mae, evolution_fitness_mae, evolution_parameters_mae =␣
 ↪optimiseWithCMAES("mae")
```

```
resetToDefaultParameters()
xray_image_mae = applyLogScaleAndNegative(updateXRayImage(x_mae))
```

```
Set up the detector
        Detector position: [0.0, -30.5, -20.5, 'cm']
        Detector up vector: [0, -1, 0]
        Detector number of pixels: [1536, 1248]
        Pixel spacing: [0.026347682927083334, 0.026347683, 'cm']
Set up the beam
        Source position: [0.0, -30.5, 150.0, 'cm']
        Source shape: PointSource
(5_w,10)-aCMA-ES (mu_w=3.2,w_1=45%) in dimension 8 (seed=358857, Wed Mar  2
18:28:52 2022)


Iterat #Fevals   function value  axis ratio  sigma  min&max std  t[m:s]
    1     10 9.374713948502835e-01 1.0e+00 4.78e-01  2e+00  1e+01 0:19.5
    2     20 9.244753957781333e-01 1.2e+00 4.45e-01  2e+00  9e+00 0:39.8
    3     30 8.644369894435934e-01 1.2e+00 4.69e-01  2e+00  1e+01 0:59.0
    4     40 9.341010149739571e-01 1.4e+00 4.67e-01  2e+00  1e+01 1:16.6
    5     50 8.582970215359739e-01 1.5e+00 5.08e-01  3e+00  1e+01 1:34.6
    6     60 9.363346712354921e-01 1.6e+00 5.01e-01  2e+00  1e+01 1:50.9
    7     70 8.387521979183704e-01 1.7e+00 4.77e-01  2e+00  1e+01 2:07.7
    8     80 8.679412798312346e-01 1.8e+00 4.42e-01  2e+00  1e+01 2:24.2
    9     90 8.098846380278579e-01 1.9e+00 4.02e-01  2e+00  9e+00 2:40.9
   10    100 8.191157486673785e-01 1.9e+00 3.71e-01  2e+00  8e+00 2:57.0
   11    110 8.199907170333630e-01 1.8e+00 3.32e-01  2e+00  7e+00 3:13.0
   12    120 8.427676329563809e-01 1.8e+00 3.46e-01  2e+00  7e+00 3:28.3
   13    130 8.083769665536453e-01 2.1e+00 3.48e-01  2e+00  7e+00 3:44.3
   14    140 8.314204206906822e-01 2.1e+00 3.87e-01  2e+00  9e+00 3:59.9
   15    150 8.484425503313813e-01 2.2e+00 3.84e-01  2e+00  8e+00 4:16.5
   16    160 8.548708695807727e-01 2.4e+00 3.81e-01  2e+00  8e+00 4:31.6
   18    180 8.242633712970828e-01 2.5e+00 3.22e-01  1e+00  7e+00 5:03.7
   20    200 8.343519742251926e-01 2.6e+00 2.96e-01  1e+00  7e+00 5:34.9
   22    220 8.159062107154144e-01 2.6e+00 2.96e-01  1e+00  7e+00 6:07.7
   24    240 8.129762671017163e-01 3.0e+00 3.35e-01  2e+00  8e+00 6:41.2
   26    260 8.170566396196074e-01 3.4e+00 3.02e-01  2e+00  7e+00 7:13.8
   28    280 8.111340006076992e-01 3.3e+00 2.62e-01  1e+00  6e+00 7:47.6
   30    300 8.080933420759249e-01 3.5e+00 2.27e-01  1e+00  5e+00 8:20.6
   32    320 8.076399410471513e-01 3.7e+00 1.87e-01  9e-01  4e+00 8:52.6
   34    340 8.073962516122402e-01 4.1e+00 1.53e-01  7e-01  3e+00 9:24.6
   36    360 8.091919232260351e-01 4.2e+00 1.36e-01  6e-01  3e+00 9:57.2
   38    380 8.084128684207648e-01 4.8e+00 1.34e-01  6e-01  3e+00 10:30.0
   40    400 8.082349362911319e-01 5.5e+00 1.30e-01  6e-01  3e+00 11:02.7
   42    420 8.073838832956641e-01 5.9e+00 1.20e-01  6e-01  3e+00 11:35.0
   44    440 8.069406064858179e-01 6.3e+00 1.18e-01  5e-01  3e+00 12:07.4
```

```
   46    460 8.066772788076430e-01 6.9e+00 1.09e-01  5e-01  3e+00 12:39.6
   48    480 8.071120533230370e-01 7.5e+00 1.03e-01  4e-01  2e+00 13:11.8
   50    500 8.066893976767069e-01 7.6e+00 8.45e-02  4e-01  2e+00 13:43.9
   53    530 8.068212760901602e-01 7.4e+00 9.75e-02  4e-01  2e+00 14:32.1
   56    560 8.071700053006147e-01 7.6e+00 7.69e-02  3e-01  2e+00 15:20.2
   59    590 8.066788075294536e-01 8.2e+00 6.62e-02  3e-01  1e+00 16:08.3
   62    620 8.065592926635288e-01 9.4e+00 5.11e-02  2e-01  1e+00 16:56.3
   65    650 8.066046689229931e-01 9.7e+00 4.39e-02  2e-01  1e+00 17:44.4
   68    680 8.065313277566502e-01 1.1e+01 3.88e-02  1e-01  8e-01 18:32.4
   71    710 8.065342900929388e-01 1.2e+01 2.99e-02  1e-01  7e-01 19:20.4
   74    740 8.064679169267140e-01 1.5e+01 3.32e-02  1e-01  8e-01 20:08.4
termination on timeout=1200 (Wed Mar  2 18:49:02 2022)
final/bestever f-value = 8.064615e-01 8.064615e-01
incumbent solution: [4.649051604407845, 4.998379452144532, 9.078956046824455,
-12.151074192798289, 154.58878048434738, 11.128765898262738, -50.49893176206971,
-40.48815781125466]
std deviation: [0.12722817863434444, 0.12787826509925934, 0.764858393793311,
0.33581051213284474, 0.6906416131935139, 0.1675610596066584, 0.2318367261386447,
0.4900987474179509]
(24, 9)
Set up the detector
        Detector position: [0.0, -30.5, -20.5, 'cm']
        Detector up vector: [0, -1, 0]
        Detector number of pixels: [1536, 1248]
        Pixel spacing: [0.026347682927083334, 0.026347683, 'cm']
Set up the beam
        Source position: [0.0, -30.5, 150.0, 'cm']
        Source shape: PointSource
```

[49]:
```
objective_function_string = "rmse"
x_rmse, evolution_fitness_rmse, evolution_parameters_rmse =␣
 ↪optimiseWithCMAES("rmse")

resetToDefaultParameters()
xray_image_rmse = applyLogScaleAndNegative(updateXRayImage(x_rmse))
```

```
Set up the detector
        Detector position: [0.0, -30.5, -20.5, 'cm']
        Detector up vector: [0, -1, 0]
        Detector number of pixels: [1536, 1248]
        Pixel spacing: [0.026347682927083334, 0.026347683, 'cm']
Set up the beam
        Source position: [0.0, -30.5, 150.0, 'cm']
        Source shape: PointSource
(5_w,10)-aCMA-ES (mu_w=3.2,w_1=45%) in dimension 8 (seed=366574, Wed Mar  2
18:49:07 2022)
```

```
Iterat #Fevals   function value  axis ratio  sigma  min&max std  t[m:s]
    1     10 1.032840372146427e+00 1.0e+00 4.92e-01  2e+00  1e+01 0:19.6
    2     20 1.095233695382328e+00 1.2e+00 4.87e-01  2e+00  1e+01 0:39.9
    3     30 1.074671618044777e+00 1.4e+00 5.26e-01  2e+00  1e+01 0:59.2
    4     40 1.088976626924912e+00 1.5e+00 5.27e-01  2e+00  1e+01 1:16.9
    5     50 1.066972571035801e+00 1.4e+00 5.25e-01  2e+00  1e+01 1:34.7
    6     60 9.745079521465659e-01 1.6e+00 5.17e-01  2e+00  1e+01 1:51.2
    7     70 1.092085603846369e+00 1.7e+00 4.78e-01  2e+00  1e+01 2:08.6
    8     80 1.092252146941009e+00 1.8e+00 5.44e-01  2e+00  1e+01 2:26.6
    9     90 1.039822997874571e+00 2.0e+00 6.39e-01  3e+00  2e+01 2:42.9
   10    100 1.052534907141260e+00 2.1e+00 6.69e-01  3e+00  2e+01 2:59.9
   11    110 1.109753164059375e+00 2.2e+00 6.80e-01  3e+00  2e+01 3:19.1
   12    120 1.145083520371625e+00 2.2e+00 6.78e-01  3e+00  2e+01 3:38.0
   13    130 1.038235843580670e+00 2.3e+00 6.14e-01  3e+00  1e+01 3:55.7
   14    140 1.091230501631045e+00 2.3e+00 5.56e-01  2e+00  1e+01 4:12.0
   15    150 1.063951933507061e+00 2.4e+00 5.73e-01  2e+00  1e+01 4:29.2
   16    160 1.103840720971852e+00 2.4e+00 5.54e-01  2e+00  1e+01 4:45.6
   18    180 1.100183948383566e+00 2.5e+00 5.92e-01  2e+00  1e+01 5:16.7
   20    200 1.083831896959563e+00 2.5e+00 4.71e-01  2e+00  1e+01 5:46.6
   22    220 1.062028749802367e+00 2.8e+00 4.17e-01  2e+00  1e+01 6:17.6
   24    240 1.044306658415071e+00 3.1e+00 3.71e-01  1e+00  9e+00 6:49.1
   26    260 1.036523255692632e+00 3.2e+00 3.49e-01  1e+00  8e+00 7:21.1
   28    280 1.045028345145760e+00 3.2e+00 3.48e-01  1e+00  8e+00 7:57.8
   30    300 1.028677459160844e+00 3.0e+00 2.70e-01  1e+00  6e+00 8:33.0
   32    320 1.015645204946805e+00 3.5e+00 2.35e-01  9e-01  5e+00 9:07.3
   34    340 1.021366561949353e+00 3.7e+00 2.49e-01  9e-01  6e+00 9:40.7
   36    360 1.010541453434931e+00 3.8e+00 2.35e-01  9e-01  6e+00 10:15.1
   38    380 1.011371525959475e+00 4.5e+00 1.99e-01  7e-01  5e+00 10:48.7
   40    400 1.012685769198383e+00 5.0e+00 2.07e-01  8e-01  5e+00 11:22.5
   42    420 1.014215472954336e+00 5.5e+00 1.91e-01  8e-01  5e+00 11:57.2
   44    440 1.018690874801621e+00 5.5e+00 1.95e-01  8e-01  5e+00 12:31.1
   46    460 1.007922261674527e+00 6.1e+00 1.86e-01  7e-01  4e+00 13:05.8
   48    480 1.012622899170703e+00 6.0e+00 1.70e-01  7e-01  4e+00 13:40.5
   50    500 1.006411172630391e+00 6.4e+00 1.74e-01  8e-01  4e+00 14:15.4
   52    520 1.009432454263561e+00 6.6e+00 1.65e-01  8e-01  4e+00 14:50.0
   54    540 1.004823942467403e+00 7.7e+00 1.46e-01  7e-01  3e+00 15:24.5
   57    570 1.003630455236759e+00 8.5e+00 1.28e-01  6e-01  3e+00 16:15.9
   60    600 9.982178234042608e-01 9.4e+00 1.57e-01  7e-01  4e+00 17:07.4
   63    630 9.894072160047258e-01 1.0e+01 1.62e-01  7e-01  5e+00 17:59.0
   66    660 9.957627546373636e-01 1.1e+01 1.65e-01  7e-01  5e+00 18:51.1
   69    690 9.858491690433482e-01 1.3e+01 1.54e-01  6e-01  5e+00 19:42.3
   71    710 9.827240279271210e-01 1.6e+01 1.59e-01  6e-01  6e+00 20:17.0
termination on timeout=1200 (Wed Mar  2 19:09:26 2022)
final/bestever f-value = 9.813209e-01 9.745080e-01
incumbent solution: [-4.935383791711773, 0.40461794739839535,
-11.101145729620598, -49.20865860649451, 130.5800788972686, 15.03108966130817,
```

```
-37.203045893530295, -40.45940152480975]
std deviation: [0.6546314147851089, 0.7742335356007642, 3.1949970375537697,
2.334135271707133, 5.534209479538157, 0.9464236231916329, 0.6249732537507022,
2.4991623010526176]
(4, 9)
Set up the detector
        Detector position: [0.0, -30.5, -20.5, 'cm']
        Detector up vector: [0, -1, 0]
        Detector number of pixels: [1536, 1248]
        Pixel spacing: [0.026347682927083334, 0.026347683, 'cm']
Set up the beam
        Source position: [0.0, -30.5, 150.0, 'cm']
        Source shape: PointSource
```

[50]:

```
objective_function_string = "ssim"
x_ssim, evolution_fitness_ssim, evolution_parameters_ssim =␣
 ↪optimiseWithCMAES("ssim")

resetToDefaultParameters()
xray_image_ssim = applyLogScaleAndNegative(updateXRayImage(x_ssim))
```

```
Set up the detector
        Detector position: [0.0, -30.5, -20.5, 'cm']
        Detector up vector: [0, -1, 0]
        Detector number of pixels: [1536, 1248]
        Pixel spacing: [0.026347682927083334, 0.026347683, 'cm']
Set up the beam
        Source position: [0.0, -30.5, 150.0, 'cm']
        Source shape: PointSource
(5_w,10)-aCMA-ES (mu_w=3.2,w_1=45%) in dimension 8 (seed=377591, Wed Mar  2
19:09:32 2022)


Iterat #Fevals   function value  axis ratio  sigma  min&max std  t[m:s]
    1     10 4.179254522462432e-01 1.0e+00 4.53e-01  2e+00  9e+00 0:19.8
    2     20 4.299147699535565e-01 1.2e+00 4.69e-01  2e+00  9e+00 0:37.9
    3     30 4.471636208509718e-01 1.4e+00 4.32e-01  2e+00  9e+00 0:56.4
    4     40 3.888435899945630e-01 1.5e+00 4.07e-01  2e+00  8e+00 1:15.1
    5     50 3.911052525143428e-01 1.5e+00 4.20e-01  2e+00  9e+00 1:32.8
    6     60 3.880606771210888e-01 1.6e+00 4.39e-01  2e+00  9e+00 1:50.2
    7     70 4.225425229731761e-01 1.6e+00 4.30e-01  2e+00  9e+00 2:06.3
    8     80 4.011443700303535e-01 1.8e+00 4.05e-01  2e+00  8e+00 2:21.6
    9     90 3.879102810946111e-01 1.8e+00 3.54e-01  2e+00  7e+00 2:37.0
   10    100 3.956002631469493e-01 1.9e+00 3.34e-01  1e+00  7e+00 2:52.5
   11    110 3.883144030623428e-01 1.9e+00 3.69e-01  2e+00  8e+00 3:06.9
   12    120 3.869382478612545e-01 2.1e+00 3.87e-01  2e+00  8e+00 3:22.2
```

```
   13    130 3.917323290089218e-01 2.2e+00 4.26e-01  2e+00  9e+00 3:37.2
   14    140 3.901219111250442e-01 2.2e+00 4.87e-01  2e+00  1e+01 3:52.0
   15    150 4.139692108474560e-01 2.3e+00 5.15e-01  2e+00  1e+01 4:07.5
   16    160 4.126521278419440e-01 2.3e+00 5.12e-01  2e+00  1e+01 4:22.9
   18    180 4.107568136702358e-01 2.4e+00 5.44e-01  3e+00  1e+01 4:53.6
   20    200 3.987671898408569e-01 2.5e+00 5.37e-01  3e+00  1e+01 5:25.3
   22    220 3.999767828642312e-01 2.7e+00 4.89e-01  2e+00  1e+01 5:55.4
   24    240 4.009892402140991e-01 2.6e+00 5.28e-01  2e+00  1e+01 6:24.8
   26    260 3.869626190832802e-01 3.0e+00 4.94e-01  2e+00  1e+01 6:54.5
   28    280 3.918741854984211e-01 3.2e+00 4.43e-01  2e+00  1e+01 7:24.0
   30    300 4.103060603988922e-01 3.5e+00 4.37e-01  2e+00  1e+01 7:53.3
   32    320 3.879837742684350e-01 4.0e+00 3.89e-01  2e+00  9e+00 8:23.4
   34    340 4.021019577607592e-01 4.0e+00 4.17e-01  2e+00  1e+01 8:52.7
   36    360 3.901321868588720e-01 4.4e+00 4.33e-01  2e+00  1e+01 9:21.9
   38    380 3.893233594040005e-01 4.6e+00 3.83e-01  2e+00  9e+00 9:52.4
   40    400 3.866702370797415e-01 4.6e+00 3.18e-01  2e+00  8e+00 10:21.8
   42    420 3.908273470752084e-01 5.1e+00 3.24e-01  2e+00  9e+00 10:50.2
   44    440 3.865401645113431e-01 5.8e+00 3.42e-01  2e+00  1e+01 11:19.4
   47    470 3.850375409806059e-01 6.7e+00 2.47e-01  1e+00  7e+00 12:02.7
   50    500 3.843198000231869e-01 6.8e+00 2.01e-01  1e+00  5e+00 12:46.1
   53    530 3.830666038317918e-01 6.9e+00 1.76e-01  9e-01  5e+00 13:29.6
   56    560 3.827612131291541e-01 7.4e+00 1.39e-01  7e-01  3e+00 14:12.9
   59    590 3.816675003593483e-01 8.2e+00 1.10e-01  6e-01  2e+00 14:56.3
   62    620 3.815395055325337e-01 9.2e+00 9.30e-02  4e-01  2e+00 15:39.4
   65    650 3.813651314665338e-01 1.0e+01 1.14e-01  5e-01  2e+00 16:22.5
   68    680 3.816100829987861e-01 9.6e+00 9.54e-02  4e-01  2e+00 17:05.7
   71    710 3.814022148135247e-01 1.1e+01 1.14e-01  5e-01  2e+00 17:48.9
   74    740 3.810439892693131e-01 1.3e+01 1.17e-01  4e-01  3e+00 18:32.0
   77    770 3.805115297023780e-01 1.7e+01 1.16e-01  4e-01  3e+00 19:15.3
   80    800 3.801987480003062e-01 1.9e+01 1.25e-01  4e-01  3e+00 19:58.7
   81    810 3.802493454377647e-01 2.0e+01 1.20e-01  4e-01  3e+00 20:12.9
termination on timeout=1200 (Wed Mar  2 19:29:47 2022)
final/bestever f-value = 3.801953e-01 3.801953e-01
incumbent solution: [4.905210191659805, 4.90763455379317, -17.140402264330053,
-50.47892834383879, 145.38525136216327, 12.226240016145116, -50.49920395165418,
-9.327431849743975]
std deviation: [0.8435623715669692, 0.6699869315645265, 1.7250420434041391,
1.7473090932387167, 2.9784290945465997, 0.7672704677704162, 0.3895910030601276,
2.242740853190941]
(27, 9)
Set up the detector
        Detector position: [0.0, -30.5, -20.5, 'cm']
        Detector up vector: [0, -1, 0]
        Detector number of pixels: [1536, 1248]


        Pixel spacing: [0.026347682927083334, 0.026347683, 'cm']
Set up the beam
```

```
        Source position: [0.0, -30.5, 150.0, 'cm']
        Source shape: PointSource
```

[51]:
```
objective_function_string = "mape"
x_mape, evolution_fitness_mape, evolution_parameters_mape =␣
 ↪optimiseWithCMAES("mape")

resetToDefaultParameters()
xray_image_mape = applyLogScaleAndNegative(updateXRayImage(x_mape))
```

```
Set up the detector
        Detector position: [0.0, -30.5, -20.5, 'cm']
        Detector up vector: [0, -1, 0]
        Detector number of pixels: [1536, 1248]


        Pixel spacing: [0.026347682927083334, 0.026347683, 'cm']
Set up the beam
        Source position: [0.0, -30.5, 150.0, 'cm']
        Source shape: PointSource
(5_w,10)-aCMA-ES (mu_w=3.2,w_1=45%) in dimension 8 (seed=350882, Wed Mar  2
19:29:49 2022)
Iterat #Fevals   function value  axis ratio  sigma  min&max std  t[m:s]
    1     10 2.822432608784872e-01 1.0e+00 4.63e-01  2e+00  1e+01 0:03.6
    2     20 1.928680541588584e-01 1.3e+00 4.19e-01  2e+00  9e+00 0:07.4
    3     30 1.800003967256550e-01 1.3e+00 3.92e-01  2e+00  8e+00 0:11.2
    4     40 2.239860816545852e-01 1.4e+00 3.88e-01  2e+00  8e+00 0:15.0
    6     60 1.868328783947753e-01 1.6e+00 3.91e-01  2e+00  9e+00 0:22.7
    8     80 1.683223790839860e-01 1.8e+00 3.71e-01  2e+00  8e+00 0:30.0
   10    100 1.668113770861747e-01 2.0e+00 3.73e-01  2e+00  9e+00 0:37.3
   12    120 1.779967188057863e-01 2.2e+00 3.76e-01  2e+00  9e+00 0:44.9
   15    150 1.778587877357825e-01 2.4e+00 4.56e-01  2e+00  1e+01 0:56.2
   18    180 1.647347568735913e-01 2.6e+00 4.42e-01  2e+00  1e+01 1:07.1
   21    210 1.490774207953159e-01 3.4e+00 5.86e-01  3e+00  2e+01 1:18.4
   24    240 1.568900274733861e-01 4.0e+00 5.89e-01  3e+00  2e+01 1:29.7
   28    280 1.480455389021865e-01 5.0e+00 8.79e-01  5e+00  2e+01 1:44.7
   32    320 2.432421092404949e-01 6.2e+00 8.94e-01  5e+00  2e+01 1:59.5
   36    360 1.775774376043622e-01 7.7e+00 6.93e-01  4e+00  2e+01 2:14.4
   40    400 1.712144789815952e-01 9.1e+00 7.63e-01  4e+00  3e+01 2:29.7
   45    450 1.752972401322352e-01 1.4e+01 8.75e-01  3e+00  3e+01 2:48.6
   50    500 1.564687996174600e-01 1.6e+01 7.98e-01  3e+00  3e+01 3:07.1
   55    550 1.710752834914694e-01 2.1e+01 7.00e-01  2e+00  3e+01 3:25.9
   60    600 1.461606749090995e-01 2.4e+01 4.51e-01  1e+00  2e+01 3:45.0
   66    660 1.418574884332416e-01 3.0e+01 3.57e-01  8e-01  1e+01 4:08.0
   72    720 1.239100335187807e-01 2.7e+01 2.23e-01  5e-01  8e+00 4:31.0
   78    780 1.232941892044355e-01 2.6e+01 1.84e-01  4e-01  5e+00 4:54.0
   84    840 1.200844647948416e-01 3.2e+01 1.44e-01  3e-01  4e+00 5:17.3
   91    910 1.169911154676578e-01 3.9e+01 1.12e-01  3e-01  3e+00 5:44.2
```

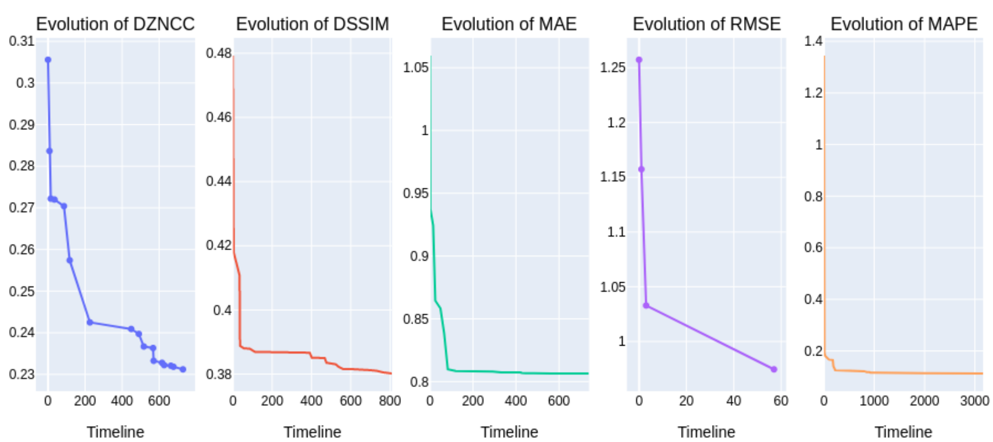
```
   98    980 1.172306258578437e-01 4.9e+01 7.93e-02  2e-01  2e+00 6:10.5
  100   1000 1.174478879842586e-01 4.8e+01 7.29e-02  2e-01  2e+00 6:17.9
  108   1080 1.159196772847974e-01 6.3e+01 1.13e-01  2e-01  3e+00 6:48.4
  116   1160 1.155973202931897e-01 6.6e+01 7.43e-02  2e-01  2e+00 7:19.0
  124   1240 1.152560612540994e-01 7.3e+01 5.54e-02  1e-01  2e+00 7:48.9
  132   1320 1.151838458147787e-01 9.4e+01 5.42e-02  9e-02  2e+00 8:19.1
  141   1410 1.151974648868865e-01 1.1e+02 4.62e-02  8e-02  1e+00 8:52.7
  150   1500 1.147378996736192e-01 1.2e+02 6.08e-02  1e-01  2e+00 9:26.4
  159   1590 1.145277371469342e-01 1.3e+02 6.09e-02  1e-01  2e+00 10:00.2
  168   1680 1.140735025022039e-01 1.4e+02 5.54e-02  1e-01  1e+00 10:34.3
  178   1780 1.139363818259420e-01 1.4e+02 4.87e-02  7e-02  1e+00 11:12.5
  188   1880 1.138684871359428e-01 1.8e+02 3.46e-02  5e-02  9e-01 11:50.0
  198   1980 1.138596102583210e-01 2.0e+02 2.65e-02  4e-02  6e-01 12:27.9
  200   2000 1.138082472231399e-01 2.1e+02 2.57e-02  4e-02  5e-01 12:35.5
  211   2110 1.137490508270514e-01 3.1e+02 1.58e-02  2e-02  3e-01 13:16.7
  222   2220 1.137402820200659e-01 3.2e+02 1.78e-02  2e-02  3e-01 13:58.0
  233   2330 1.136779386077626e-01 3.5e+02 2.69e-02  4e-02  5e-01 14:39.5
  245   2450 1.136151472638742e-01 4.6e+02 2.78e-02  3e-02  5e-01 15:24.7
  257   2570 1.135436020629846e-01 4.7e+02 3.06e-02  2e-02  5e-01 16:09.7
  269   2690 1.134069453405901e-01 4.7e+02 5.23e-02  4e-02  8e-01 16:55.6
  281   2810 1.133486669523867e-01 5.3e+02 3.45e-02  2e-02  5e-01 17:40.8
  294   2940 1.131459020917214e-01 6.3e+02 5.74e-02  3e-02  8e-01 18:29.2
  300   3000 1.132245354665068e-01 6.3e+02 1.02e-01  5e-02  1e+00 18:51.8
  313   3130 1.129569193977482e-01 6.4e+02 7.02e-02  3e-02  8e-01 19:41.7
  318   3180 1.128123228566415e-01 6.3e+02 9.53e-02  4e-02  1e+00 20:00.6
termination on timeout=1200 (Wed Mar  2 19:49:50 2022)
final/bestever f-value = 1.127765e-01 1.127756e-01
incumbent solution: [-4.999194164531257, -3.7848203044373943,
-7.249186151953962, -49.26651430701722, 130.01000957213384, 7.114029295120312,
-13.069905113570401, -40.474302085490905]
std deviation: [0.16344167120121497, 0.3956462036769397, 0.8342789850065333,
0.35215375415971345, 0.9589360255231316, 0.2738374257028348,
0.038690615892085486, 0.17991742116547535]
(114, 9)
Set up the detector
        Detector position: [0.0, -30.5, -20.5, 'cm']
        Detector up vector: [0, -1, 0]
        Detector number of pixels: [1536, 1248]
        Pixel spacing: [0.026347682927083334, 0.026347683, 'cm']
Set up the beam
        Source position: [0.0, -30.5, 150.0, 'cm']
        Source shape: PointSource
```

[52]:

```
fig = make_subplots(rows=1, cols=5, start_cell="bottom-left",
                    subplot_titles=("Evolution of DZNCC", "Evolution of DSSIM",␣
 ↪"Evolution of MAE", "Evolution of RMSE", "Evolution of MAPE"))
```

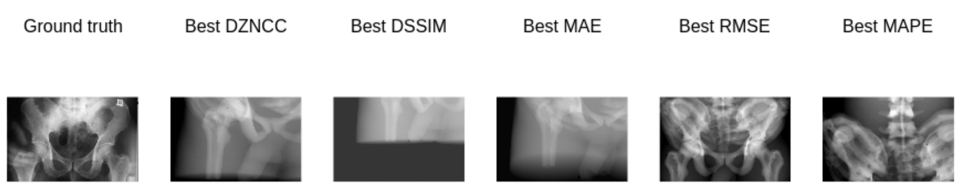
```python
# fig.add_trace(go.Scatter(x=evolution_fitness_zncc[:,0], y=1.0 - (2.0 *␣
↪evolution_fitness_zncc[:,1])),
fig.add_trace(go.Scatter(x=evolution_fitness_zncc[:,0],␣
↪y=evolution_fitness_zncc[:,1]),
              row=1, col=1)

# fig.add_trace(go.Scatter(x=evolution_fitness_ssim[:,0], y=1.0 - (2.0 *␣
↪evolution_fitness_ssim[:,1])),
fig.add_trace(go.Scatter(x=evolution_fitness_ssim[:,0],␣
↪y=evolution_fitness_ssim[:,1]),
              row=1, col=2)

fig.add_trace(go.Scatter(x=evolution_fitness_mae[:,0], y=evolution_fitness_mae[:
↪,1]),
              row=1, col=3)

fig.add_trace(go.Scatter(x=evolution_fitness_rmse[:,0],␣
↪y=evolution_fitness_rmse[:,1]),
              row=1, col=4)

fig.add_trace(go.Scatter(x=evolution_fitness_mape[:,0],␣
↪y=evolution_fitness_mape[:,1]),
              row=1, col=5)

# Update xaxis properties
fig.update_xaxes(title_text="Timeline", row=1, col=1)
fig.update_xaxes(title_text="Timeline", row=1, col=2)
fig.update_xaxes(title_text="Timeline", row=1, col=3)
fig.update_xaxes(title_text="Timeline", row=1, col=4)
fig.update_xaxes(title_text="Timeline", row=1, col=5)

# Update yaxis properties
# fig.update_yaxes(title_text="Ojective function: ZNCC", row=1, col=1)
# fig.update_yaxes(title_text="Ojective function: MAE", row=1, col=2)
# fig.update_yaxes(title_text="Ojective function: RMSE", row=1, col=3)
# fig.update_yaxes(title_text="Ojective function: SSIM", row=1, col=4)
# fig.update_yaxes(title_text="Ojective function: MAPE", row=1, col=5)

# fig.update_yaxes(title_text="yaxis 2 title", range=[40, 80], row=1, col=2)
# fig.update_yaxes(title_text="yaxis 3 title", showgrid=False, row=2, col=1)
# fig.update_yaxes(title_text="yaxis 4 title", row=2, col=2)

fig.update_layout(showlegend=False)

fig.update_layout(
```

```
    font_family="Arial",
    font_color="black",
    title_font_family="Arial",
    title_font_color="black",
    legend_title_font_color="black"
)

fig.update_layout(
    height=500,
    width=1000
)

fig.write_image("plots/HIPS_evolution-objectives.pdf", engine="kaleido")
fig.write_image("plots/HIPS_evolution-objectives.png", engine="kaleido")

fig.show()
```



[53]:
```
fig = make_subplots(rows=1, cols=6,
                    start_cell="bottom-left",
                    subplot_titles=("Ground truth", "Best DZNCC", "Best DSSIM",␣
 ↪"Best MAE", "Best RMSE", "Best MAPE"))

cmaes_img_set = [standardised_roi_ground_truth,
                 standardisation(xray_image_zncc),
                 standardisation(xray_image_ssim),
                 standardisation(xray_image_mae),
                 standardisation(xray_image_rmse),
                 standardisation(xray_image_mape)]
```

```python
for n, image in enumerate(cmaes_img_set):

    im = px.imshow(image, aspect="equal", binary_string=True, zmin=standardised_roi_ground_truth.min(), zmax=standardised_roi_ground_truth.max())
    fig.add_trace(im.data[0], 1, n + 1)

fig.update_xaxes(showticklabels=False) # hide all the xticks
fig.update_yaxes(showticklabels=False) # hide all the yticks
fig.update_layout(coloraxis_showscale=False)

fig.update_layout(
    font_family="Arial",
    font_color="black",
    title_font_family="Arial",
    title_font_color="black",
    legend_title_font_color="black"
)

fig.update_layout(
    height=300,
    width=1200
)

fig.write_image("plots/HIPS_cmaes-objectives.pdf", engine="kaleido")
fig.write_image("plots/HIPS_cmaes-objectives.png", engine="kaleido")

fig.show()
```



[54]:
```python
cmaes_x_set   =  [x_zncc, x_mae, x_rmse, x_ssim, x_mape]
cmaes_img_set = [xray_image_zncc, xray_image_mae, xray_image_rmse, xray_image_ssim, xray_image_mape]
```

```
temp_res_cmaes = []

for n, [x, image] in enumerate(zip(cmaes_x_set, cmaes_img_set)):

    row = copy.deepcopy(x)

    xray_image = updateXRayImage(x)
    corrected_xray_image = applyLogScaleAndNegative(xray_image)
    standardised_corrected_xray_image = standardisation(corrected_xray_image)

    zncc = np.mean(standardised_roi_ground_truth *␣
 ↪standardised_corrected_xray_image)
    row.append((1.0 - zncc) / 2.0)

    mae = np.mean(np.abs(standardised_roi_ground_truth -␣
 ↪standardised_corrected_xray_image))
    row.append(mae)

    rmse = math.sqrt(np.mean(np.square(standardised_roi_ground_truth -␣
 ↪standardised_corrected_xray_image)))
    row.append(rmse)

    ssim_value = ssim(standardised_roi_ground_truth,␣
 ↪standardised_corrected_xray_image, data_range=standardised_roi_ground_truth.
 ↪max() - standardised_roi_ground_truth.min())
    row.append((1.0 - ssim_value) / 2.0)

    # Avoid div by 0
    offset1 = min(standardised_roi_ground_truth.min(),␣
 ↪standardised_corrected_xray_image.min())
    offset2 = 0.01 * (standardised_roi_ground_truth.max() -␣
 ↪standardised_roi_ground_truth.min())
    offset = offset2 - offset1
    mape_value = mape(standardised_roi_ground_truth + offset,␣
 ↪standardised_corrected_xray_image + offset)
    row.append(mape_value)

    temp_res_cmaes.append(row)
```

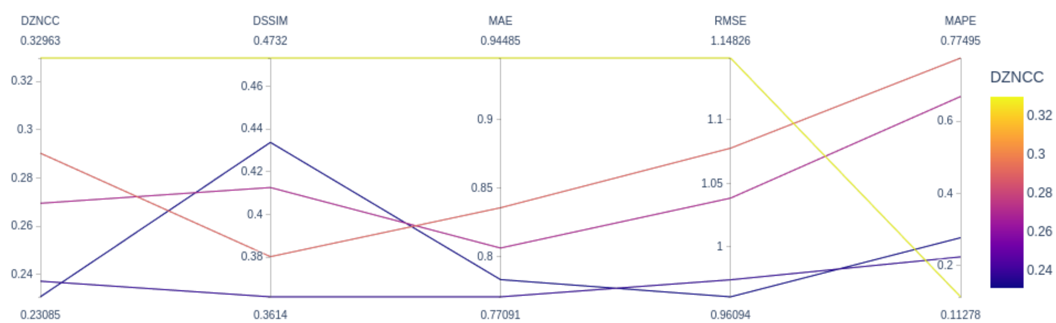
[55]:
```
df_cmaes = pd.DataFrame(data=temp_res_cmaes,
                  columns=["sample_rotation_angle1", "sample_rotation_angle2",␣
 ↪"src_pos_x", "src_pos_y", "src_pos_z", "det_pos_x", "det_pos_y",␣
 ↪"det_pos_z", "DZNCC", "MAE", "RMSE", "DSSIM", "MAPE"])

df_cmaes["Optimiser"] = "CMA-ES"
```

```
df_cmaes["Optimiser_code"] = 1
df_cmaes.to_csv("gVirtualXRay_output_data/hips-optimiser-cmaes.csv")
```

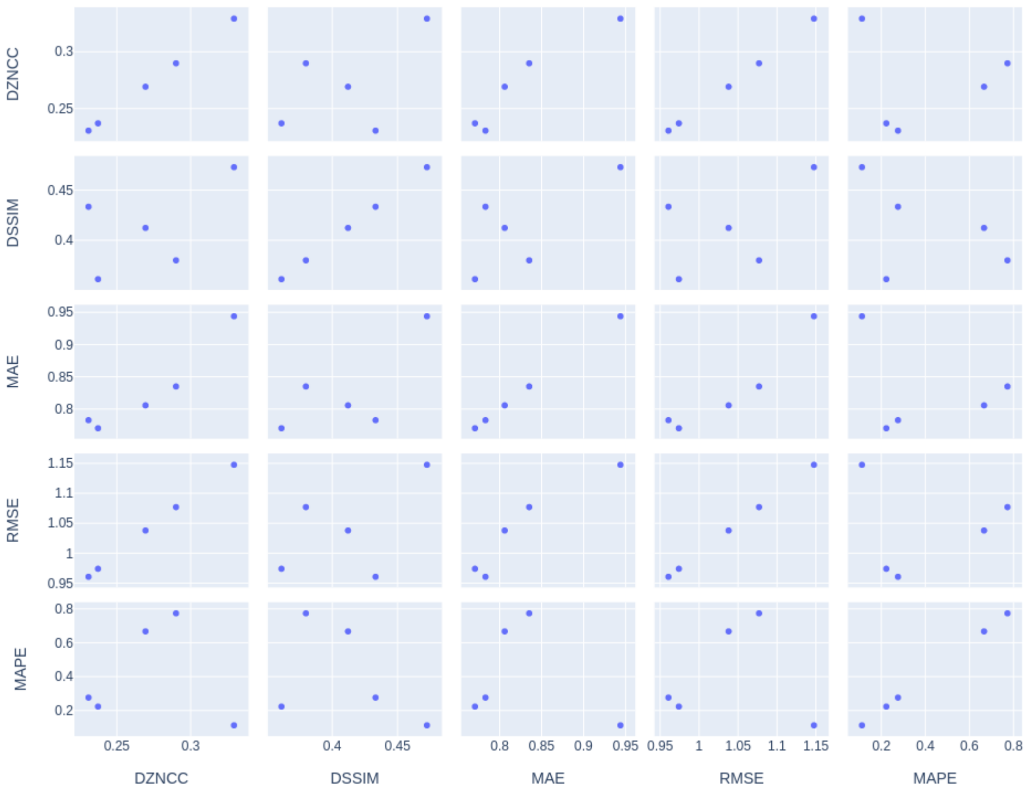
[56]:
```
display(df_cmaes)
```

```
   sample_rotation_angle1  sample_rotation_angle2  src_pos_x  src_pos_y  \
0               -4.991866                1.353755 -18.613038 -17.393354
1                4.649052                4.998379   9.078956 -12.151074
2               -1.889165                1.161676  12.320442 -43.726923
3                4.905210                4.907635 -17.140402 -50.478928
4               -4.999746               -4.085573  -8.004148 -49.225494

    src_pos_z  det_pos_x  det_pos_y  det_pos_z     DZNCC       MAE      RMSE  \
0  130.217666  18.218264 -49.387763 -40.499971  0.230849  0.783463  0.960936
1  154.588780  11.128766 -50.498932 -40.488158  0.269551  0.806452  1.038367
2  168.519270  -0.359930 -31.929943  -2.716826  0.237318  0.770913  0.974306
3  145.385251  12.226240 -50.499204  -9.327432  0.290274  0.835789  1.077541
4  130.016563   7.358184 -13.090978 -40.443481  0.329628  0.944848  1.148264

      DSSIM      MAPE Optimiser  Optimiser_code
0  0.433716  0.276732    CMA-ES               1
1  0.412572  0.668308    CMA-ES               1
2  0.361399  0.223484    CMA-ES               1
3  0.380203  0.774947    CMA-ES               1
4  0.473198  0.112777    CMA-ES               1
```

[57]:
```
fig = px.parallel_coordinates(df_cmaes[["DZNCC", "DSSIM", "MAE", "RMSE",␣
↪"MAPE"]], color="DZNCC")
fig.show()

fig.write_image("plots/HIPS-cmaes-parallel_coordinates.pdf", engine="kaleido")
fig.write_image("plots/HIPS-cmaes-parallel_coordinates.png", engine="kaleido")
```



[58]:
```
fig = px.scatter_matrix(df_cmaes[["DZNCC", "DSSIM", "MAE", "RMSE", "MAPE"]])

fig.update_layout(
    height=800,
    width=800
)

fig.show()

fig.write_image("plots/HIPS-cmaes-scatter_matrix.pdf", engine="kaleido")
fig.write_image("plots/HIPS-cmaes-scatter_matrix.png", engine="kaleido")
```



4.4 Multi-objective optimisation with NSGA-II

[59]:
```
def objectiveFunctions(x):

    global objective_function_string
```

```python
    global ground_truth, standardised_roi_ground_truth
    global best_fitness, best_fitness_id, fitness_function_call_id,␣
↪evolution_fitness, evolution_parameters

    objectives = []

    for ind in x:
        xray_image = updateXRayImage(ind)
        corrected_xray_image = applyLogScaleAndNegative(xray_image)
        standardised_corrected_xray_image =␣
↪standardisation(corrected_xray_image)

        row = []

        zncc = np.mean(standardised_roi_ground_truth *␣
↪standardised_corrected_xray_image)
        dzncc = (1.0 - zncc) / 2.0
        row.append(dzncc)

        mae = np.mean(np.abs(standardised_roi_ground_truth -␣
↪standardised_corrected_xray_image))
        row.append(mae)

        rmse = math.sqrt(np.mean(np.square(standardised_roi_ground_truth -␣
↪standardised_corrected_xray_image)))
        row.append(rmse)

        ssim_value = ssim(standardised_roi_ground_truth,␣
↪standardised_corrected_xray_image, data_range=standardised_roi_ground_truth.
↪max() - standardised_roi_ground_truth.min())
        dssim = (1.0 - ssim_value) / 2.0
        row.append(dssim)

        # Avoid div by 0
        offset1 = min(standardised_roi_ground_truth.min(),␣
↪standardised_corrected_xray_image.min())
        offset2 = 0.01 * (standardised_roi_ground_truth.max() -␣
↪standardised_roi_ground_truth.min())
        offset = offset2 - offset1
        mape_value = mape(standardised_roi_ground_truth + offset,␣
↪standardised_corrected_xray_image + offset)
        row.append(mape_value)

        objectives.append(row)

    return objectives
```

[60]:
```python
from pymoo.core.problem import Problem

class MyMultiObjectiveProblem(Problem):

    def __init__(self):
        super().__init__(n_var=len(x_init),
                         n_obj=5,
                         n_constr=0,
                         xl=xl,
                         xu=xu)

    def _evaluate(self, x, out, *args, **kwargs):
        out["F"] = objectiveFunctions(x)
```

[61]:
```python
from pymoo.algorithms.moo.nsga2 import NSGA2
from pymoo.optimize import minimize
from pymoo.factory import get_termination
from pymoo.util.termination import collection

resetToDefaultParameters()

problem = MyMultiObjectiveProblem()

pop_size = 210

x_tol_termination = get_termination("x_tol", 1e-5)
f_tol_termination = get_termination("f_tol", 1e-5)
time_termination = get_termination("time", "00:20:00")

termination = collection.TerminationCollection(x_tol_termination,␣
 ↪f_tol_termination, time_termination)

if os.path.exists("gVirtualXRay_output_data/VHP-res-nsga2-X.dat") and os.path.
 ↪exists("gVirtualXRay_output_data/VHP-res-nsga2-F.dat"):

    res_nsga2_X = np.loadtxt("gVirtualXRay_output_data/VHP-res-nsga2-X.dat")
    res_nsga2_F = np.loadtxt("gVirtualXRay_output_data/VHP-res-nsga2-F.dat")

else:

    algorithm = NSGA2(
        pop_size=pop_size,
#         n_offsprings=int(pop_size*0.05),
        eliminate_duplicates=True
    )

    res_nsga2 = minimize(problem,
```

```
                  algorithm,
                  termination,
                  seed=1,
                  save_history=True,
                  verbose=True)

    res_nsga2_X = res_nsga2.X
    res_nsga2_F = res_nsga2.F

    np.savetxt("gVirtualXRay_output_data/VHP-res-nsga2-X.dat", res_nsga2_X)
    np.savetxt("gVirtualXRay_output_data/VHP-res-nsga2-F.dat", res_nsga2_F)
```

```
Set up the detector
        Detector position: [0.0, -30.5, -20.5, 'cm']
        Detector up vector: [0, -1, 0]
        Detector number of pixels: [1536, 1248]
        Pixel spacing: [0.026347682927083334, 0.026347683, 'cm']
Set up the beam
        Source position: [0.0, -30.5, 150.0, 'cm']
        Source shape: PointSource


=======================================================
n_gen  |  n_eval  |  n_nds  |      eps      |  indicator
=======================================================
     1 |      210 |       6 |             - |          -
     2 |      420 |       7 |  0.154055622 |      ideal
     3 |      630 |       5 |  0.207845299 |      ideal
     4 |      840 |       8 |  0.127065447 |      ideal
     5 |     1050 |       7 |  0.158647150 |      ideal
     6 |     1260 |      13 |  0.172631859 |      ideal
     7 |     1470 |      17 |  0.060337139 |      ideal
     8 |     1680 |      27 |  0.016166080 |      ideal
     9 |     1890 |      31 |  0.093798221 |      ideal
    10 |     2100 |      22 |  0.043846917 |      ideal
    11 |     2310 |      15 |  0.199342023 |      ideal
```

[62]:
```
best_dzncc_id = np.argmin(res_nsga2_F[:,0])
best_mae_id = np.argmin(res_nsga2_F[:,1])
best_rmse_id = np.argmin(res_nsga2_F[:,2])
best_dssim_id = np.argmin(res_nsga2_F[:,3])
best_mape_id = np.argmin(res_nsga2_F[:,4])

print("Lowest DZNCC:", res_nsga2_F[:,0].min(), best_dzncc_id,␣
 ↪res_nsga2_X[best_dzncc_id])
print("Lowest DSSIM:", res_nsga2_F[:,3].min(), best_dssim_id,␣
 ↪res_nsga2_X[best_dssim_id])
```

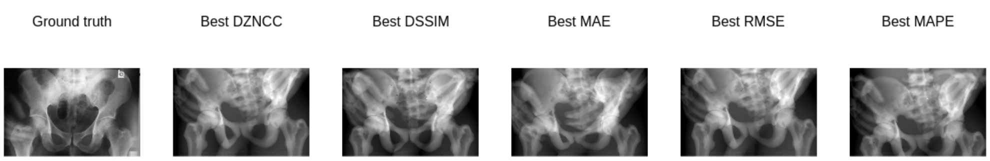
```
print("Lowest MAE:",   res_nsga2_F[:,1].min(), best_mae_id,  ␣
 ↪res_nsga2_X[best_mae_id])
print("Lowest RMSE:",  res_nsga2_F[:,2].min(), best_rmse_id, ␣
 ↪res_nsga2_X[best_rmse_id])
print("Lowest MAPE:",  res_nsga2_F[:,4].min(), best_mape_id, ␣
 ↪res_nsga2_X[best_mape_id])
```

```
Lowest DZNCC: 0.2056734187678198 13 [ -4.80017831   2.02236986 -19.38453686
-40.78936236 135.0337335
   1.72300748 -32.71928014  -5.74874761]
Lowest DSSIM: 0.3464964634449592 10 [ -3.4237942    4.2729067    3.51200803
-37.13736563 143.07105177
  -0.29108234 -31.46022789  -3.77390637]
Lowest MAE: 0.7346392266657226 12 [ -2.04779024   3.4534029  -17.62389519
-15.37767021 157.64983682
  -0.44383489 -31.94142827  -3.26032314]
Lowest RMSE: 0.9070246275990965 13 [ -4.80017831   2.02236986 -19.38453686
-40.78936236 135.0337335
   1.72300748 -32.71928014  -5.74874761]
Lowest MAPE: 0.12242530000040054 14 [ -4.80119866   2.25448126 -19.31016859
-42.14669936 130.9075416
   1.76844189 -28.77783655  -6.70479739]
```

[63]:
```
xray_image_dzncc_nsga2 =␣
 ↪applyLogScaleAndNegative(updateXRayImage(res_nsga2_X[best_dzncc_id]))
xray_image_mae_nsga2   =␣
 ↪applyLogScaleAndNegative(updateXRayImage(res_nsga2_X[best_mae_id]))
xray_image_rmse_nsga2  =␣
 ↪applyLogScaleAndNegative(updateXRayImage(res_nsga2_X[best_rmse_id]))
xray_image_dssim_nsga2 =␣
 ↪applyLogScaleAndNegative(updateXRayImage(res_nsga2_X[best_dssim_id]))
xray_image_mape_nsga2  =␣
 ↪applyLogScaleAndNegative(updateXRayImage(res_nsga2_X[best_mape_id]))
```

[64]:
```
fig = make_subplots(rows=1, cols=6,
                    start_cell="bottom-left",
                    subplot_titles=("Ground truth", "Best DZNCC", "Best DSSIM",␣
 ↪"Best MAE", "Best RMSE", "Best MAPE"))

nsga2_img_set = [standardised_roi_ground_truth,
                 standardisation(xray_image_dzncc_nsga2),
                 standardisation(xray_image_dssim_nsga2),
                 standardisation(xray_image_mae_nsga2),
                 standardisation(xray_image_rmse_nsga2),
                 standardisation(xray_image_mape_nsga2)]

for n, image in enumerate(nsga2_img_set):
```

```python
    im = px.imshow(image, aspect="equal", binary_string=True, zmin=standardised_roi_ground_truth.min(), zmax=standardised_roi_ground_truth.max())
    fig.add_trace(im.data[0], 1, n + 1)

fig.update_xaxes(showticklabels=False) # hide all the xticks
fig.update_yaxes(showticklabels=False) # hide all the yticks
fig.update_layout(coloraxis_showscale=False)

fig.update_layout(
    font_family="Arial",
    font_color="black",
    title_font_family="Arial",
    title_font_color="black",
    legend_title_font_color="black"
)

fig.update_layout(
    height=300,
    width=1200
)

fig.write_image("plots/HIPS-NSGA2-objectives.pdf", engine="kaleido")
fig.write_image("plots/HIPS-NSGA2-objectives.png", engine="kaleido")

fig.show()
```



[65]:

```python
df_nsga2 = pd.DataFrame(data=np.append(res_nsga2_X, res_nsga2_F, axis=1),
                  columns=["sample_rotation_angle1", "sample_rotation_angle2", "src_pos_x", "src_pos_y", "src_pos_z", "det_pos_x", "det_pos_y", "det_pos_z", "DZNCC", "MAE", "RMSE", "DSSIM", "MAPE"])

df_nsga2["Optimiser"] = "NSGA-II"
df_nsga2["Optimiser_code"] = 2
```

```python
df_nsga2.to_csv("gVirtualXRay_output_data/hips-optimiser-nsga2.csv")
```

[66]:

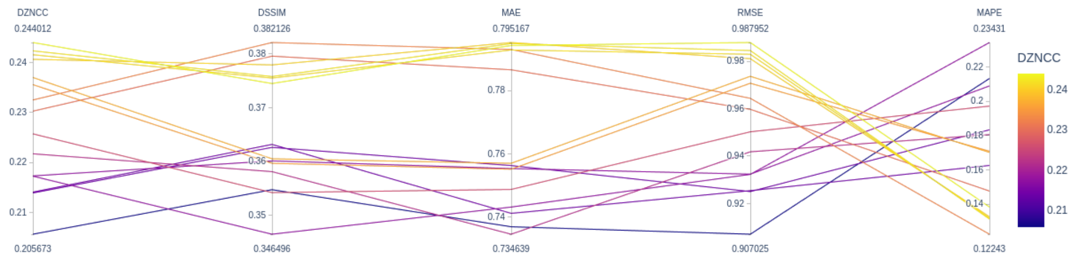
```python
display(df_nsga2)
```

```
    sample_rotation_angle1  sample_rotation_angle2  src_pos_x  src_pos_y  \
0                -4.801199                3.523439 -18.989922 -40.609397
1                 4.750313                4.546072   4.558581 -12.444532
2                 2.716301                4.667951 -17.652187 -27.843845
3                 4.743385                4.542779   4.558581 -12.444532
4                -0.259423                2.217000 -18.498818 -42.144576
5                -0.265537                2.216896 -17.879057 -40.296790
6                 0.381326                2.216033 -17.879057 -44.193307
7                 0.860375                4.839917 -15.675989 -20.824581
8                 0.381326                2.216033 -17.879057 -48.215224
9                 0.783735                1.997034 -10.238915 -33.544945
10               -3.423794                4.272907   3.512008 -37.137366
11                0.381326                2.216033 -18.856332 -44.193307
12               -2.047790                3.453403 -17.623895 -15.377670
13               -4.800178                2.022370 -19.384537 -40.789362
14               -4.801199                2.254481 -19.310169 -42.146699

     src_pos_z  det_pos_x  det_pos_y  det_pos_z     DZNCC       MAE      RMSE  \
0   164.568174   1.503564 -30.160007  -6.779000  0.213919  0.756316  0.925027
1   133.202439  -0.341241 -31.181381 -13.663767  0.237022  0.757029  0.973698
2   165.238728   1.767666 -31.933806 -19.616895  0.217337  0.755366  0.932388
3   133.202439  -0.352418 -31.257200 -13.663767  0.235594  0.755161  0.970761
4   130.848758   1.495441 -29.741233  -5.987344  0.230283  0.786561  0.959756
5   133.436956   0.199370 -29.089868  -5.988549  0.244012  0.794209  0.987952
6   133.753225   0.199370 -29.089868  -4.042146  0.242344  0.794814  0.984569
7   136.966274   0.720353 -31.925211  -8.374534  0.214098  0.741227  0.925415
8   131.941508   0.199370 -29.089868  -2.730746  0.240653  0.795167  0.981128
9   136.761226  -0.336469 -31.926204  -6.391126  0.225749  0.748777  0.950262
10  143.071052  -0.291082 -31.460228  -3.773906  0.217291  0.743214  0.932290
11  133.992531   0.218121 -29.089868  -4.042146  0.241567  0.792814  0.982990
12  157.649837  -0.443835 -31.941428  -3.260323  0.221757  0.734639  0.941822
13  135.033733   1.723007 -32.719280  -5.748748  0.205673  0.737000  0.907025
14  130.907542   1.768442 -28.777837  -6.704797  0.232516  0.792968  0.964398

       DSSIM      MAPE Optimiser  Optimiser_code
0   0.362638  0.183362   NSGA-II               2
1   0.360512  0.170156   NSGA-II               2
2   0.360125  0.208975   NSGA-II               2
3   0.359677  0.170872   NSGA-II               2
4   0.379593  0.147615   NSGA-II               2
5   0.374502  0.138283   NSGA-II               2
6   0.375801  0.131265   NSGA-II               2
7   0.363188  0.162560   NSGA-II               2
```

8	0.377964	0.132616	NSGA-II	2
9	0.354234	0.197201	NSGA-II	2
10	0.346496	0.234312	NSGA-II	2
11	0.375515	0.131783	NSGA-II	2
12	0.358131	0.180548	NSGA-II	2
13	0.354772	0.213318	NSGA-II	2
14	0.382126	0.122425	NSGA-II	2

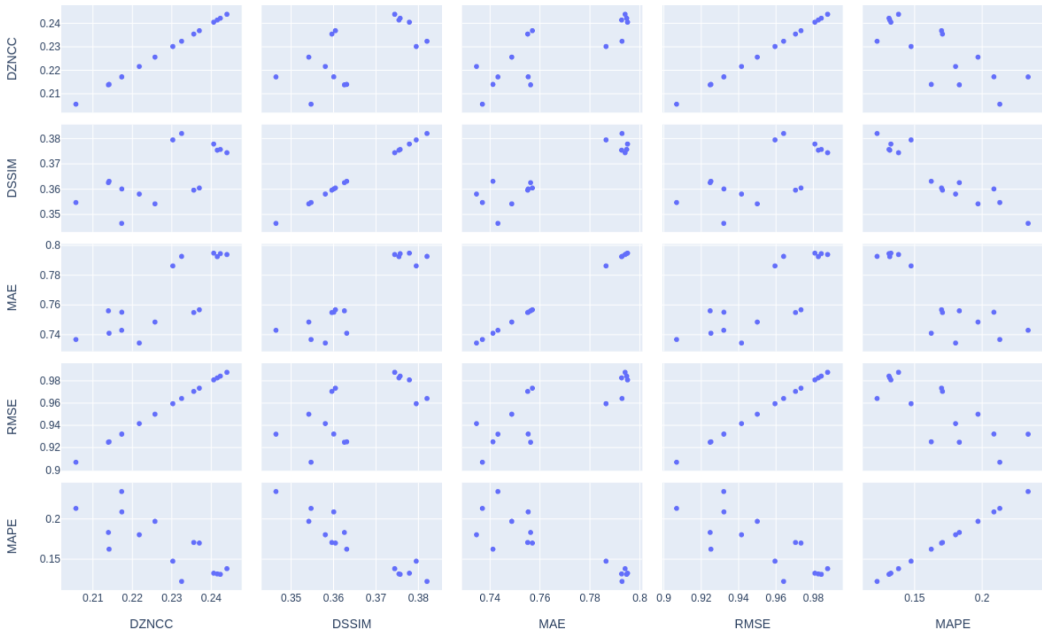
[67]:

```
fig = px.parallel_coordinates(df_nsga2[["DZNCC", "DSSIM", "MAE", "RMSE", "MAPE"]], color="DZNCC")
fig.show()

fig.write_image("plots/HIPS-NSGA2-parallel_coordinates.pdf", engine="kaleido")
fig.write_image("plots/HIPS-NSGA2-parallel_coordinates.png", engine="kaleido")
```



[68]:

```
fig = px.scatter_matrix(df_nsga2[["DZNCC", "DSSIM", "MAE", "RMSE", "MAPE"]])

fig.update_layout(
    height=800,
    width=800
)

fig.show()

fig.write_image("plots/HIPS-NSGA2-scatter_matrix.pdf", engine="kaleido")
fig.write_image("plots/HIPS-NSGA2-scatter_matrix.png", engine="kaleido")
```



[69]:
```
runtimes = []

resetToDefaultParameters()
setTransformations(res_nsga2_X[best_dzncc_id])

for i in range(25):
    start_time = datetime.datetime.now()

    raw_x_ray_image = gvxr.computeXRayImage()

    end_time = datetime.datetime.now()
    delta_time = end_time - start_time
    runtimes.append(delta_time.total_seconds() * 1000)
```

```
Set up the detector
        Detector position: [0.0, -30.5, -20.5, 'cm']
        Detector up vector: [0, -1, 0]
        Detector number of pixels: [1536, 1248]
        Pixel spacing: [0.026347682927083334, 0.026347683, 'cm']
Set up the beam
        Source position: [0.0, -30.5, 150.0, 'cm']
        Source shape: PointSource
```

[70]:
```
runtime_avg = round(np.mean(runtimes))
runtime_std = round(np.std(runtimes))

raw_x_ray_image = np.array(raw_x_ray_image)
```

[71]:
```
ZNCC = 1.0 - (2.0 * res_nsga2_F[:,0].min())
SSIM = 1.0 - (2.0 * res_nsga2_F[:,3].min())
MAPE = res_nsga2_F[:,4].min()

print("Registration VHP & Real image & " +
      "{0:0.2f}".format(100 * MAPE) + "\\%    &    " +
      "{0:0.2f}".format(100 * ZNCC) + "\\%    &    " +
      "{0:0.2f}".format(SSIM) + "    &    $" +
      str(raw_x_ray_image.shape[1]) + " \\times " + str(raw_x_ray_image.
 ↪shape[0]) + "$    &    " +
      str(number_of_triangles) + "    &    " +
      "$" + str(runtime_avg) + " \\pm " + str(runtime_std) + "$ \\\\")
```

```
Registration VHP & Real image & 12.24\%    &    58.87\%    &    0.31    &
$1536 \times 1248$    &    1273438    &    $273 \pm 9$ \\
```

4.5 Single-objective optimisation with NSGA-3

[72]:
```
from pymoo.algorithms.moo.nsga3 import NSGA3
from pymoo.factory import get_reference_directions

resetToDefaultParameters()

if os.path.exists("gVirtualXRay_output_data/VHP-res-nsga3-X.dat") and os.path.
 ↪exists("gVirtualXRay_output_data/VHP-res-nsga3-F.dat"):

    res_nsga3_X = np.loadtxt("gVirtualXRay_output_data/VHP-res-nsga3-X.dat")
    res_nsga3_F = np.loadtxt("gVirtualXRay_output_data/VHP-res-nsga3-F.dat")

else:
    n_objs = 5
    n_partitions = 6

    ref_dirs = get_reference_directions("das-dennis", n_objs,␣
 ↪n_partitions=n_partitions)

    problem = MyMultiObjectiveProblem()

    pop_size = 210 #2 * ref_dirs.shape[0]

    algorithm = NSGA3(
```

```
        pop_size=pop_size,
#         n_offsprings=int(pop_size*0.05),
        eliminate_duplicates=True,
        ref_dirs=ref_dirs
    )

    res_nsga3 = minimize(problem,
                   algorithm,
                   termination,
                   seed=1,
                   save_history=True,
                   verbose=True)

    res_nsga3_X = res_nsga3.X
    res_nsga3_F = res_nsga3.F

    np.savetxt("gVirtualXRay_output_data/VHP-res-nsga3-X.dat", res_nsga3_X)
    np.savetxt("gVirtualXRay_output_data/VHP-res-nsga3-F.dat", res_nsga3_F)
```

```
Set up the detector
        Detector position: [0.0, -30.5, -20.5, 'cm']
        Detector up vector: [0, -1, 0]
        Detector number of pixels: [1536, 1248]
        Pixel spacing: [0.026347682927083334, 0.026347683, 'cm']
Set up the beam
        Source position: [0.0, -30.5, 150.0, 'cm']
        Source shape: PointSource


=======================================================
n_gen |  n_eval |  n_nds  |     eps      |  indicator
=======================================================
    1 |     210 |       4 |            - |            -
    2 |     420 |       6 |  0.336456514 |        nadir
    3 |     630 |       4 |  0.587138721 |        ideal
    4 |     840 |       5 |  0.210446306 |        ideal
    5 |    1050 |       4 |  0.215471051 |        ideal
    6 |    1260 |       3 |  1.000000000 |        ideal
    7 |    1470 |       3 |  0.00000E+00 |            f
    8 |    1680 |       6 |  0.182129207 |        ideal
    9 |    1890 |       5 |  0.512255814 |        ideal
   10 |    2100 |       8 |  0.070854951 |        ideal
   11 |    2310 |       9 |  0.017436343 |        ideal
```

[73]:
```
best_dzncc_id = np.argmin(res_nsga3_F[:,0])
best_mae_id = np.argmin(res_nsga3_F[:,1])
best_rmse_id = np.argmin(res_nsga3_F[:,2])
```

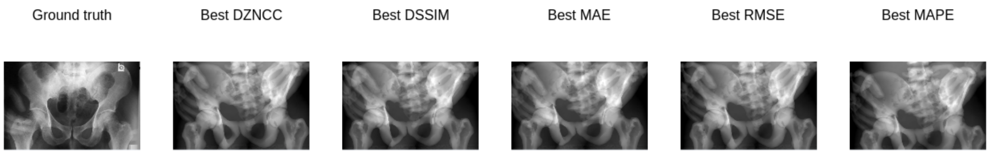
```
best_dssim_id = np.argmin(res_nsga3_F[:,3])
best_mape_id = np.argmin(res_nsga3_F[:,4])

print("Lowest DZNCC:", res_nsga3_F[:,0].min(), best_dzncc_id,␣
↪res_nsga3_X[best_dzncc_id])
print("Lowest DSSIM:", res_nsga3_F[:,3].min(), best_dssim_id,␣
↪res_nsga3_X[best_dssim_id])
print("Lowest MAE:",   res_nsga3_F[:,1].min(), best_mae_id,  ␣
↪res_nsga3_X[best_mae_id])
print("Lowest RMSE:",  res_nsga3_F[:,2].min(), best_rmse_id, ␣
↪res_nsga3_X[best_rmse_id])
print("Lowest MAPE:",  res_nsga3_F[:,4].min(), best_mape_id, ␣
↪res_nsga3_X[best_mape_id])
```

```
Lowest DZNCC: 0.20215343159590854 2 [ -4.71361951   1.46285025 -18.50315949
-45.34973518 136.32730054
   1.53609435 -30.54058222  -6.83045612]
Lowest DSSIM: 0.34552555335462154 8 [ -3.61910225  -0.69126174 -18.16922549
-40.28953476 143.90974679
   0.29253839 -31.31304627  -4.15908267]
Lowest MAE: 0.7267045616387656 4 [ -4.88084394   0.57293031 -18.27452312
-29.99267438 139.99645013
   0.47330137 -31.87617784  -4.5229943 ]
Lowest RMSE: 0.8992295181896753 2 [ -4.71361951   1.46285025 -18.50315949
-45.34973518 136.32730054
   1.53609435 -30.54058222  -6.83045612]
Lowest MAPE: 0.12654639634134934 7 [ -4.87311646   4.16833171 -18.45080919
-43.65581438 143.38028609
   1.50464372 -28.43888343  -6.82439597]
```

[74]:
```
xray_image_dzncc_nsga3 =␣
↪applyLogScaleAndNegative(updateXRayImage(res_nsga3_X[best_dzncc_id]))
xray_image_mae_nsga3   =␣
↪applyLogScaleAndNegative(updateXRayImage(res_nsga3_X[best_mae_id]))
xray_image_rmse_nsga3  =␣
↪applyLogScaleAndNegative(updateXRayImage(res_nsga3_X[best_rmse_id]))
xray_image_dssim_nsga3 =␣
↪applyLogScaleAndNegative(updateXRayImage(res_nsga3_X[best_dssim_id]))
xray_image_mape_nsga3  =␣
↪applyLogScaleAndNegative(updateXRayImage(res_nsga3_X[best_mape_id]))
```

[75]:
```
import plotly.express as px

fig = make_subplots(rows=1, cols=6,
                    start_cell="bottom-left",
```

```
                    subplot_titles=("Ground truth", "Best DZNCC", "Best DSSIM",␣
↪"Best MAE", "Best RMSE", "Best MAPE"))

nsga3_img_set = [standardised_roi_ground_truth,
                 standardisation(xray_image_dzncc_nsga3),
                 standardisation(xray_image_dssim_nsga3),
                 standardisation(xray_image_mae_nsga3),
                 standardisation(xray_image_rmse_nsga3),
                 standardisation(xray_image_mape_nsga3)]

for n, image in enumerate(nsga3_img_set):

    im = px.imshow(image, aspect="equal", binary_string=True,␣
↪zmin=standardised_roi_ground_truth.min(), zmax=standardised_roi_ground_truth.
↪max())
    fig.add_trace(im.data[0], 1, n + 1)

fig.update_xaxes(showticklabels=False) # hide all the xticks
fig.update_yaxes(showticklabels=False) # hide all the yticks
fig.update_layout(coloraxis_showscale=False)

fig.update_layout(
    font_family="Arial",
    font_color="black",
    title_font_family="Arial",
    title_font_color="black",
    legend_title_font_color="black"
)

fig.update_layout(
    height=300,
    width=1200
)

fig.write_image("plots/HIPS-NSGA3-objectives.pdf", engine="kaleido")
fig.write_image("plots/HIPS-NSGA3-objectives.png", engine="kaleido")

fig.show()
```



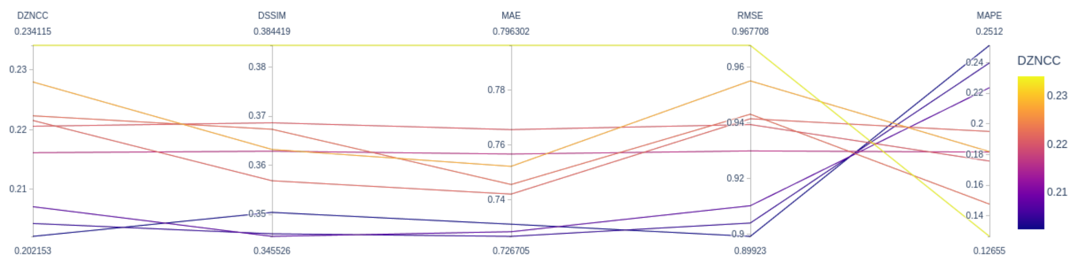
[76]:
```
df_nsga3 = pd.DataFrame(data=np.append(res_nsga3_X, res_nsga3_F, axis=1),
                        columns=["sample_rotation_angle1", "sample_rotation_angle2",␣
 ↪"src_pos_x", "src_pos_y", "src_pos_z", "det_pos_x", "det_pos_y",␣
 ↪"det_pos_z", "DZNCC", "MAE", "RMSE", "DSSIM", "MAPE"])

df_nsga3["Optimiser"] = "NSGA3"
df_nsga3["Optimiser_code"] = 3
df_nsga3.to_csv("gVirtualXRay_output_data/hips-optimiser-nsga3.csv")
```

[77]:
```
display(df_nsga3)
```

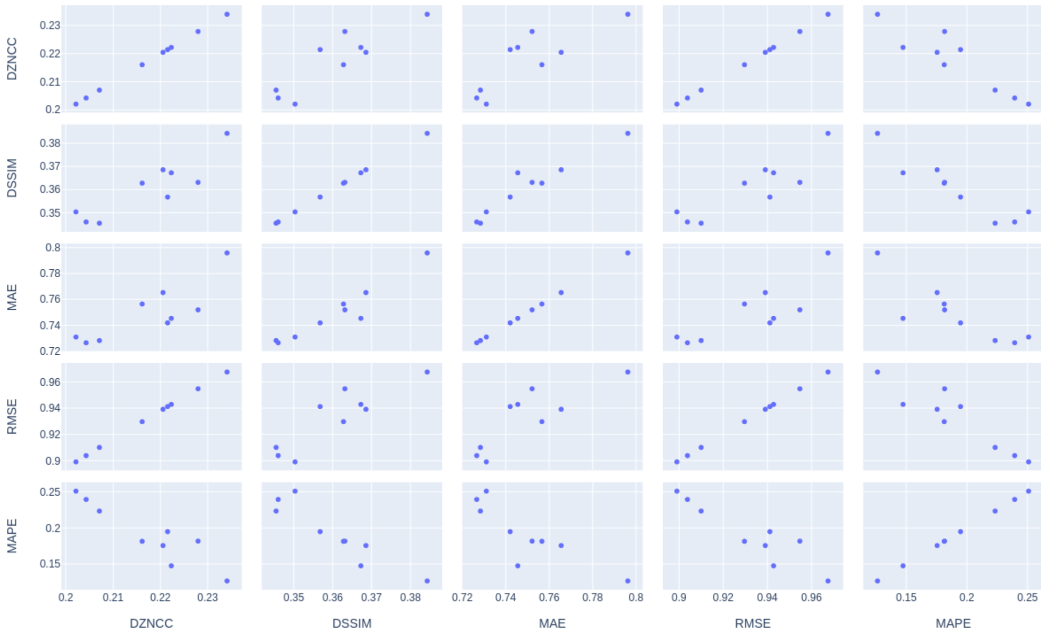
```
   sample_rotation_angle1  sample_rotation_angle2  src_pos_x  src_pos_y  \
0                4.710833               -4.915385  12.073449 -20.548692
1               -3.259530                1.510502 -18.504058 -25.705307
2               -4.713620                1.462850 -18.503159 -45.349735
3                3.257878               -4.307683  12.238064 -31.360337
4               -4.880844                0.572930 -18.274523 -29.992674
5                4.666708               -4.915385 -18.278564 -20.134696
6               -3.259530                1.483115 -18.472732 -29.011183
7               -4.873116                4.168332 -18.450809 -43.655814
8               -3.619102               -0.691262 -18.169225 -40.289535

    src_pos_z  det_pos_x  det_pos_y  det_pos_z     DZNCC       MAE      RMSE  \
0  133.221320   0.433057 -30.870648  -6.397939  0.222325  0.745606  0.943027
1  136.327301   1.754844 -31.678266  -6.830456  0.220576  0.765604  0.939311
2  136.327301   1.536094 -30.540582  -6.830456  0.202153  0.731139  0.899230
3  143.829392   0.432507 -30.757385  -4.411907  0.227990  0.752215  0.954967
4  139.996450   0.473301 -31.876178  -4.522994  0.204311  0.726705  0.904015
5  155.251040   0.466725 -30.870170  -6.426592  0.221552  0.742108  0.941385
6  150.982444   1.441053 -31.681522  -6.833707  0.216158  0.756712  0.929856
7  143.380286   1.504644 -28.438883  -6.824396  0.234115  0.796302  0.967708
8  143.909747   0.292538 -31.313046  -4.159083  0.207121  0.728398  0.910212

      DSSIM      MAPE Optimiser  Optimiser_code
0  0.367337  0.147590     NSGA3               3
```

```
1  0.368655  0.175708     NSGA3                3
2  0.350409  0.251203     NSGA3                3
3  0.363222  0.181863     NSGA3                3
4  0.346052  0.239707     NSGA3                3
5  0.356851  0.195013     NSGA3                3
6  0.362866  0.181575     NSGA3                3
7  0.384419  0.126546     NSGA3                3
8  0.345526  0.223553     NSGA3                3
```

[78]:
```
fig = px.parallel_coordinates(df_nsga3[["DZNCC", "DSSIM", "MAE", "RMSE",␣
  ↪"MAPE"]], color="DZNCC")
fig.show()

fig.write_image("plots/HIPS-NSGA3-parallel_coordinates.pdf", engine="kaleido")
fig.write_image("plots/HIPS-NSGA3-parallel_coordinates.png", engine="kaleido")
```



[79]:
```
fig = px.scatter_matrix(df_nsga3[["DZNCC", "DSSIM", "MAE", "RMSE", "MAPE"]])

fig.update_layout(
    height=800,
    width=800
)

fig.show()

fig.write_image("plots/HIPS-NSGA3-scatter_matrix.pdf", engine="kaleido")
fig.write_image("plots/HIPS-NSGA3-scatter_matrix.png", engine="kaleido")
```



5 Compare the results obtained with the 3 different optimisation algorithms

[80]:
```
df = pd.concat([df_cmaes, df_nsga2, df_nsga3])
df = df.reindex(columns=["Optimiser", "Optimiser_code",␣
↪"sample_rotation_angle1", "sample_rotation_angle2", "src_pos_x",␣
↪"src_pos_y", "src_pos_z", "det_pos_x", "det_pos_y", "det_pos_z", "DZNCC",␣
↪"MAE", "RMSE", "DSSIM", "MAPE"])

df.to_csv("gVirtualXRay_output_data/hips-optimiser.csv")
```

[81]:
```
display(df)
```

```
  Optimiser  Optimiser_code  sample_rotation_angle1  sample_rotation_angle2  \
0    CMA-ES               1               -4.991866                1.353755
1    CMA-ES               1                4.649052                4.998379
2    CMA-ES               1               -1.889165                1.161676
3    CMA-ES               1                4.905210                4.907635
4    CMA-ES               1               -4.999746               -4.085573
0   NSGA-II               2               -4.801199                3.523439
1   NSGA-II               2                4.750313                4.546072
2   NSGA-II               2                2.716301                4.667951
```

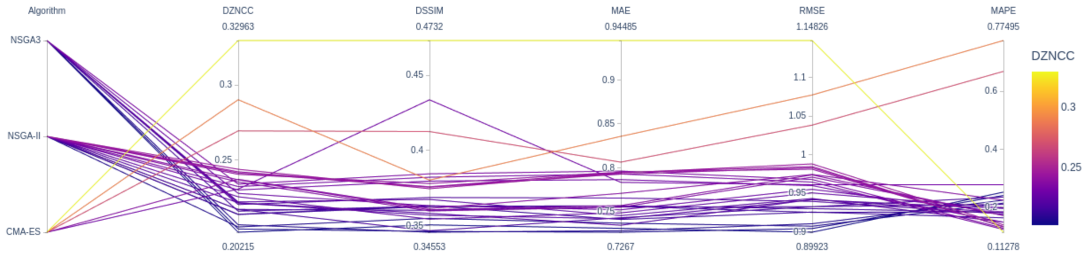
3	NSGA-II	2	4.743385	4.542779
4	NSGA-II	2	-0.259423	2.217000
5	NSGA-II	2	-0.265537	2.216896
6	NSGA-II	2	0.381326	2.216033
7	NSGA-II	2	0.860375	4.839917
8	NSGA-II	2	0.381326	2.216033
9	NSGA-II	2	0.783735	1.997034
10	NSGA-II	2	-3.423794	4.272907
11	NSGA-II	2	0.381326	2.216033
12	NSGA-II	2	-2.047790	3.453403
13	NSGA-II	2	-4.800178	2.022370
14	NSGA-II	2	-4.801199	2.254481
0	NSGA3	3	4.710833	-4.915385
1	NSGA3	3	-3.259530	1.510502
2	NSGA3	3	-4.713620	1.462850
3	NSGA3	3	3.257878	-4.307683
4	NSGA3	3	-4.880844	0.572930
5	NSGA3	3	4.666708	-4.915385
6	NSGA3	3	-3.259530	1.483115
7	NSGA3	3	-4.873116	4.168332
8	NSGA3	3	-3.619102	-0.691262

	src_pos_x	src_pos_y	src_pos_z	det_pos_x	det_pos_y	det_pos_z \
0	-18.613038	-17.393354	130.217666	18.218264	-49.387763	-40.499971
1	9.078956	-12.151074	154.588780	11.128766	-50.498932	-40.488158
2	12.320442	-43.726923	168.519270	-0.359930	-31.929943	-2.716826
3	-17.140402	-50.478928	145.385251	12.226240	-50.499204	-9.327432
4	-8.004148	-49.225494	130.016563	7.358184	-13.090978	-40.443481
0	-18.989922	-40.609397	164.568174	1.503564	-30.160007	-6.779000
1	4.558581	-12.444532	133.202439	-0.341241	-31.181381	-13.663767
2	-17.652187	-27.843845	165.238728	1.767666	-31.933806	-19.616895
3	4.558581	-12.444532	133.202439	-0.352418	-31.257200	-13.663767
4	-18.498818	-42.144576	130.848758	1.495441	-29.741233	-5.987344
5	-17.879057	-40.296790	133.436956	0.199370	-29.089868	-5.988549
6	-17.879057	-44.193307	133.753225	0.199370	-29.089868	-4.042146
7	-15.675989	-20.824581	136.966274	0.720353	-31.925211	-8.374534
8	-17.879057	-48.215224	131.941508	0.199370	-29.089868	-2.730746
9	-10.238915	-33.544945	136.761226	-0.336469	-31.926204	-6.391126
10	3.512008	-37.137366	143.071052	-0.291082	-31.460228	-3.773906
11	-18.856332	-44.193307	133.992531	0.218121	-29.089868	-4.042146
12	-17.623895	-15.377670	157.649837	-0.443835	-31.941428	-3.260323
13	-19.384537	-40.789362	135.033733	1.723007	-32.719280	-5.748748
14	-19.310169	-42.146699	130.907542	1.768442	-28.777837	-6.704797
0	12.073449	-20.548692	133.221320	0.433057	-30.870648	-6.397939
1	-18.504058	-25.705307	136.327301	1.754844	-31.678266	-6.830456
2	-18.503159	-45.349735	136.327301	1.536094	-30.540582	-6.830456
3	12.238064	-31.360337	143.829392	0.432507	-30.757385	-4.411907
4	-18.274523	-29.992674	139.996450	0.473301	-31.876178	-4.522994

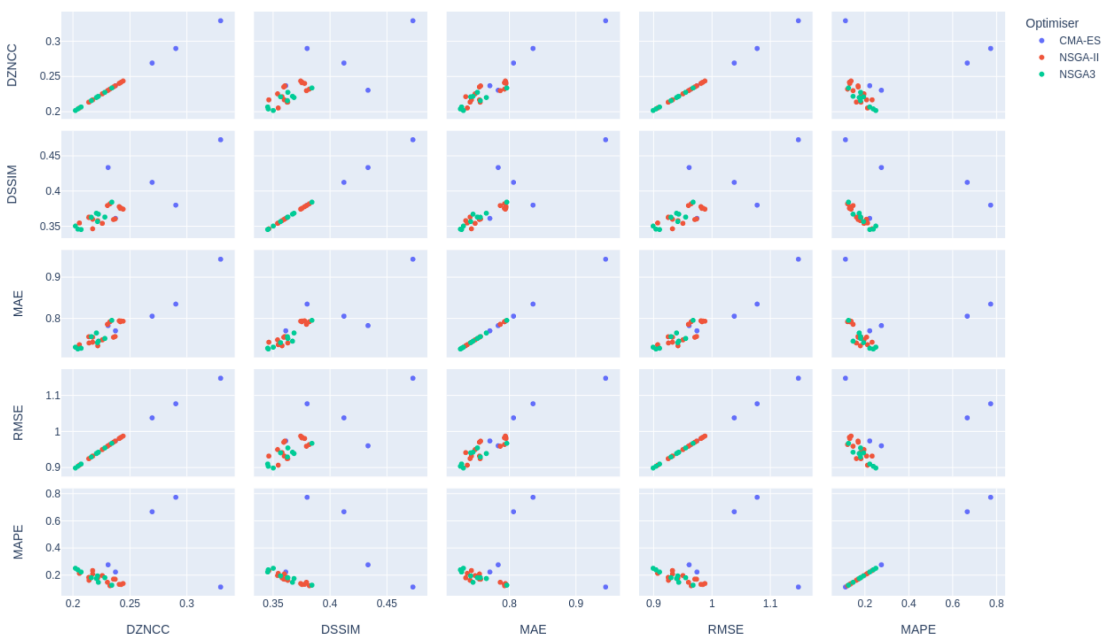
```
5   -18.278564 -20.134696  155.251040   0.466725 -30.870170   -6.426592
6   -18.472732 -29.011183  150.982444   1.441053 -31.681522   -6.833707
7   -18.450809 -43.655814  143.380286   1.504644 -28.438883   -6.824396
8   -18.169225 -40.289535  143.909747   0.292538 -31.313046   -4.159083

       DZNCC       MAE      RMSE     DSSIM      MAPE
0   0.230849  0.783463  0.960936  0.433716  0.276732
1   0.269551  0.806452  1.038367  0.412572  0.668308
2   0.237318  0.770913  0.974306  0.361399  0.223484
3   0.290274  0.835789  1.077541  0.380203  0.774947
4   0.329628  0.944848  1.148264  0.473198  0.112777
0   0.213919  0.756316  0.925027  0.362638  0.183362
1   0.237022  0.757029  0.973698  0.360512  0.170156
2   0.217337  0.755366  0.932388  0.360125  0.208975
3   0.235594  0.755161  0.970761  0.359677  0.170872
4   0.230283  0.786561  0.959756  0.379593  0.147615
5   0.244012  0.794209  0.987952  0.374502  0.138283
6   0.242344  0.794814  0.984569  0.375801  0.131265
7   0.214098  0.741227  0.925415  0.363188  0.162560
8   0.240653  0.795167  0.981128  0.377964  0.132616
9   0.225749  0.748777  0.950262  0.354234  0.197201
10  0.217291  0.743214  0.932290  0.346496  0.234312
11  0.241567  0.792814  0.982990  0.375515  0.131783
12  0.221757  0.734639  0.941822  0.358131  0.180548
13  0.205673  0.737000  0.907025  0.354772  0.213318
14  0.232516  0.792968  0.964398  0.382126  0.122425
0   0.222325  0.745606  0.943027  0.367337  0.147590
1   0.220576  0.765604  0.939311  0.368655  0.175708
2   0.202153  0.731139  0.899230  0.350409  0.251203
3   0.227990  0.752215  0.954967  0.363222  0.181863
4   0.204311  0.726705  0.904015  0.346052  0.239707
5   0.221552  0.742108  0.941385  0.356851  0.195013
6   0.216158  0.756712  0.929856  0.362866  0.181575
7   0.234115  0.796302  0.967708  0.384419  0.126546
8   0.207121  0.728398  0.910212  0.345526  0.223553
```

[82]:

```python
fig = px.parallel_coordinates(df, dimensions=['Optimiser_code', 'DZNCC',␣
↪'DSSIM', 'MAE', 'RMSE', 'MAPE'], color="DZNCC")
fig.data[0]["dimensions"][0]["label"] = "Algorithm"
fig.data[0]["dimensions"][0]["ticktext"] = ["CMA-ES", "NSGA-II", "NSGA3"]
fig.data[0]["dimensions"][0]["tickvals"] = [1, 2, 3]
fig.show()

fig.write_image("plots/HIPS-ALL-parallel_coordinates.pdf", engine="kaleido")
fig.write_image("plots/HIPS-ALL-parallel_coordinates.png", engine="kaleido")
```



[83]:
```python
fig = px.scatter_matrix(df,
    dimensions=["DZNCC", "DSSIM", "MAE", "RMSE", "MAPE"],
    color="Optimiser")

fig.update_layout(
    height=800,
    width=800
)

fig.show()

fig.write_image("plots/HIPS-ALL-scatter_matrix.pdf", engine="kaleido")
fig.write_image("plots/HIPS-ALL-scatter_matrix.png", engine="kaleido")
```



6 Performance analysis

[84]:
```
runtimes = []

resetToDefaultParameters()
setTransformations(res_nsga3_X[best_dzncc_id])

for i in range(25):
    start_time = datetime.datetime.now()

    raw_x_ray_image = gvxr.computeXRayImage()

    end_time = datetime.datetime.now()
    delta_time = end_time - start_time
    runtimes.append(delta_time.total_seconds() * 1000)
```

```
Set up the detector
        Detector position: [0.0, -30.5, -20.5, 'cm']
        Detector up vector: [0, -1, 0]
        Detector number of pixels: [1536, 1248]
        Pixel spacing: [0.026347682927083334, 0.026347683, 'cm']
Set up the beam
        Source position: [0.0, -30.5, 150.0, 'cm']
        Source shape: PointSource
```

[85]:
```
runtime_avg = round(np.mean(runtimes))
runtime_std = round(np.std(runtimes))

raw_x_ray_image = np.array(raw_x_ray_image)
```

[86]:
```
ZNCC = 1.0 - (2.0 * res_nsga3_F[:,0].min())
SSIM = 1.0 - (2.0 * res_nsga3_F[:,3].min())
MAPE = res_nsga3_F[:,4].min()

print("Registration VHP & Real image & " +
      "{0:0.2f}".format(100 * MAPE) + "\\%    &    " +
      "{0:0.2f}".format(100 * ZNCC) + "\\%    &    " +
      "{0:0.2f}".format(SSIM) + "    &    $" +
      str(raw_x_ray_image.shape[1]) + " \\times " + str(raw_x_ray_image.
 ↪shape[0]) + "$    &    " +
      str(number_of_triangles) + "    &    " +
      "$" + str(runtime_avg) + " \\pm " + str(runtime_std) + "$ \\\\")
```

```
Registration VHP & Real image & 12.65\%    &    59.57\%    &    0.31    &
$1536 \times 1248$    &    1273438    &    $276 \pm 9$ \\
```

7 Comparison of the analytic simulation with the real radiograph

[87]:
```python
data = [
    [
        "CMA-ES",
        np.max(1.0 - (2.0 * evolution_fitness_zncc[:,1])),
        np.max(1.0 - (2.0 * evolution_fitness_ssim[:,1])),
        np.min(evolution_fitness_mae[:,1]),
        np.min(evolution_fitness_rmse[:,1]),
        np.min(evolution_fitness_mape[:,1])
    ],

    [
        "NSGA-II",
        np.max(1.0 - (2.0 * res_nsga2_F[:,0])),
        np.max(1.0 - (2.0 * res_nsga2_F[:,3])),
        np.min(res_nsga2_F[:,1]),
        np.min(res_nsga2_F[:,2]),
        np.min(res_nsga2_F[:,4])
    ],

    [
        "NSGA-3",
        np.max(1.0 - (2.0 * res_nsga3_F[:,0])),
        np.max(1.0 - (2.0 * res_nsga3_F[:,3])),
        np.min(res_nsga3_F[:,1]),
        np.min(res_nsga3_F[:,2]),
        np.min(res_nsga3_F[:,4])
    ]
]

df = pd.DataFrame(data=data,
                  columns=["Optimisation algorithm", "ZNCC", "SSIM", "MAE",␣
 ↪"RMSE", "MAPE"])

df.to_csv("gVirtualXRay_output_data/hips-results.csv")

print(df)
```

```
  Optimisation algorithm      ZNCC      SSIM       MAE      RMSE      MAPE
0                 CMA-ES  0.537588  0.239609  0.806462  0.974508  0.112776
1                NSGA-II  0.588653  0.307007  0.734639  0.907025  0.122425
2                 NSGA-3  0.595693  0.308949  0.726705  0.899230  0.126546
```

8 All done

Destroy the window

[88]:
```
gvxr.destroyAllWindows()
```

```
0(0x556de111e0b0)
```