

3-gVirtualXRay_vs_DR

September 14, 2022

```
[1]: from IPython.display import display
     from IPython.display import Image
```

```
[2]: from utils import * # Code shared across more than one notebook
```

```
[3]: output_path = "3-output_data/"

     if not os.path.exists(output_path):
         os.mkdir(output_path)
```

1 gVirtualXray vs DR

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Purpose: We aim to reproduce a real digital radiograph taken with a clinically utilised X-ray equipment.

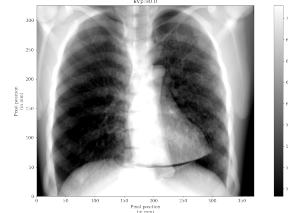
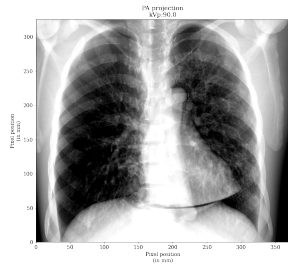
Material and Methods:

1. The CT of a chest phantom has been generated from a real scanner ahead of time.
2. Structures in the reference CT have been segmented and labelled.
3. The resultant surfaces from the segmentations form a virtual lungman model.
4. A digital radiograph was taken with a clinically utilised X-ray equipment.
5. We extract acquisition parameters from the DICOM file and initialise the X-ray simulation parameters.
6. Using a multi-objective optimisation algorithm, the virtual phantom is registered so that its simulated radiograph closely match the real digital radiograph.

Results: The **zero-mean normalised cross-correlation** is **98.92%**. The **Structural Similarity Index (SSIM)** is **0.94**. The **mean absolute percentage error (MAPE)** is **1.55%**. These results show that the two images are comparable.

Ground truth

Simulation



The calculations were performed on the following platform:

```
[4]: printSystemInfo()
```

OS:

Linux 5.14.21-150400.24.11-default
x86_64

CPU:

Intel(R) Core(TM) i9-9900K CPU @ 3.60GHz

RAM:

31 GB

GPU:

Name: NVIDIA GeForce RTX 2080 Ti
Drivers: 515.48.07
Video memory: 11 GB

1.1 Import packages

```
[5]: %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

# 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 sklearn.metrics import mean_absolute_error, mean_squared_error
from skimage.metrics import normalized_mutual_information
# from sklearn.metrics.cluster import normalized_mutual_info_score
from skimage.filters import gaussian # Implementing the image sharpening filter
from sklearn.metrics.cluster import normalized_mutual_info_score

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 random
import base64
from stl import mesh

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

import spekpy as sp # Generate a beam spectrum
from scipy import signal # Resampling the beam spectrum

import SimpleITK as sitk

from gvxrPython3 import gvxr # Simulate X-ray images
gvxr.useLogFile()
from gvxrPython3 import json2gvxr # Set gVirtualXRay and the simulation up

from scipy.spatial import distance # Euclidean distance

# Ignore some warnings
import warnings
warnings.filterwarnings("ignore", category=UserWarning)

# Pymoo
from pymoo.algorithms.moo.nsga3 import NSGA3
from pymoo.algorithms.soo.nonconvex.cmaes import CMAES

```

```

from pymoo.factory import get_reference_directions
from pymoo.factory import get_termination
from pymoo.factory import get_problem

# from pymoo.util.ref_dirs import get_reference_directions

from pymoo.core.problem import Problem

from pymoo.optimize import minimize

# from pymoo.termination.default import DefaultMultiObjectiveTermination
from pymoo.util.termination import collection
from pymoo.util.normalization import denormalize


# Visualisation

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 pymoo.visualization.scatter import Scatter
from pymoo.visualization.pcp import PCP

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

import k3d

```

SimpleGVXR 2.0.2 (2022-09-13T19:01:41) [Compiler: GNU g++] on Linux

gVirtualXRay core library (gvxr) 2.0.2 (2022-09-13T19:01:41) [Compiler: GNU g++]
on Linux

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

2 Preparation of the ground truth image

2.1 Read the real X-ray radiograph from a DICOM file

```
[7]: reader = sitk.ImageFileReader()  
reader.SetImageIO("GDCMImageIO")  
reader.SetFileName("lungman_data/CD3/DICOM/ST000000/SE000000/DX000000")  
reader.LoadPrivateTagsOn()  
reader.ReadImageInformation()  
volume = reader.Execute()  
raw_reference_before_cropping = sitk.GetArrayFromImage(volume)[0]  
raw_reference_before_cropping.shape = raw_reference_before_cropping.shape  
  
y_min_id = 200  
y_max_id = raw_reference_before_cropping.shape[0] - 170  
x_min_id = 50  
x_max_id = raw_reference_before_cropping.shape[1] - 100  
  
raw_reference = raw_reference_before_cropping[y_min_id:y_max_id, x_min_id:  
↪x_max_id]  
  
print("The shape was", raw_reference_before_cropping.shape, "| now it is",  
↪raw_reference.shape)
```

The shape was (1881, 1871) | now it is (1511, 1721)

```
[8]: imwrite(output_path + '/real_projection-lungman.tif', raw_reference.astype(np.  
↪single))
```

3 Extract information about the “sizes” of pixels from the DICOM file

The descriptions have been extracted from <https://dicom.innolitics.com>

3.1 Imager Pixel Spacing Attribute

Physical distance measured at the front plane of the Image Receptor housing between the center of each pixel. Specified by a numeric pair - row spacing value (delimiter) column spacing value - in mm.

In the case of CR, the front plane is defined to be the external surface of the CR plate closest to the patient and radiation source.

3.2 Detector Element Physical Size Attribute

Physical dimensions of each detector element that comprises the detector matrix, in mm.

Expressed as row dimension followed by column.

Note:

This may not be the same as Detector Element Spacing (0018,7022) due to the presence of spacing material between detector elements.

3.3 Detector Element Spacing Attribute

Physical distance between the center of each detector element, specified by a numeric pair - row spacing value(delimiter) column spacing value in mm. See Section 10.7.1.3 for further explanation of the value order.

Note:

This may not be the same as the Imager Pixel Spacing (0018,1164), and should not be assumed to describe the stored image.

```
[9]: imager_pixel_spacing = np.array(volume.GetMetaData("0018|1164").split("\\")).  
      ↪astype(np.single)  
detector_element_physical_size = np.array(volume.GetMetaData("0018|7020").  
      ↪split("\\")).astype(np.single)  
detector_element_spacing = np.array(volume.GetMetaData("0018|7022").  
      ↪split("\\")).astype(np.single)  
  
print("Imager Pixel Spacing (in mm): ", imager_pixel_spacing)  
print("Detector Element Physical Size (in mm): ",  
      ↪detector_element_physical_size)  
print("Detector Element Spacing (in mm): ", detector_element_spacing)
```

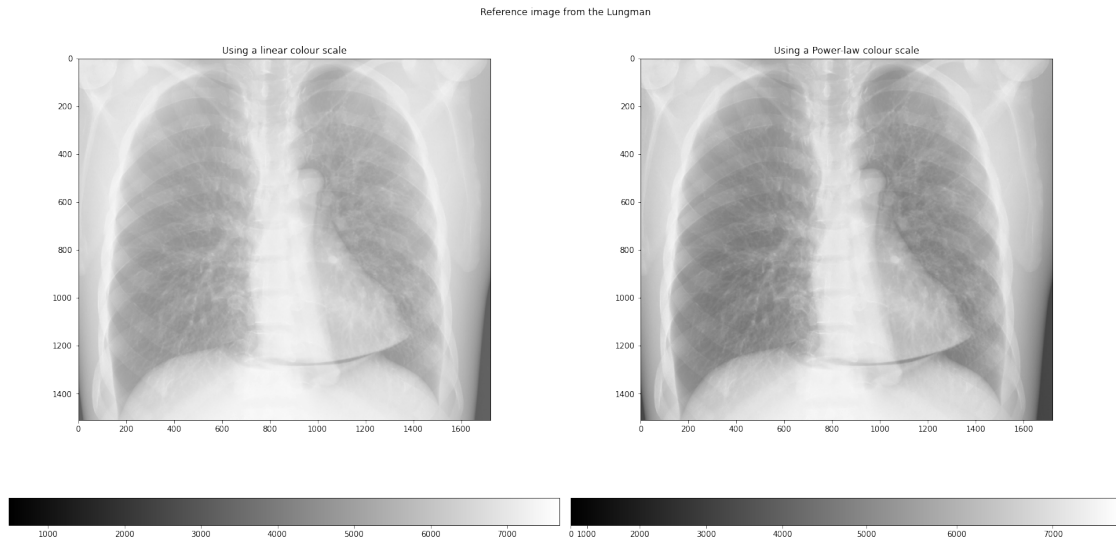
```
Imager Pixel Spacing (in mm): [0.194556 0.194556]
```

```
Detector Element Physical Size (in mm): [0.2 0.2]
```

```
Detector Element Spacing (in mm): [0.2 0.2]
```

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

```
[10]: displayLinearPowerScales(raw_reference,  
                                "Reference image from the Lungman",  
                                output_path + "/reference-lungman-proj",  
                                log=False,  
                                vmin=-93, vmax=89)
```



Apply a zero-mean, unit-variance normalisation

```
[11]: ground_truth = raw_reference
      normalised_ground_truth = standardisation(ground_truth)
      imwrite(output_path + '/lungman-normalised_ground_truth.tif',
              ↪normalised_ground_truth.astype(np.single))
```

```
[12]: # meta_data_keys = volume.GetMetaDataKeys()

      # print("DICOM fields:")
      # for key in meta_data_keys:
      #     print(key, volume.GetMetaData(key))
```

```
[13]: # def cleanTags(raw_string):
      #     regular_expression = re.compile('<.*?>')
      #     clean_text = re.sub(regular_expression, '', raw_string)
      #     return clean_text
```

```
[14]: # field = volume.GetMetaData("0033|1022")

      # for item in field.split("\n"):
      #     if "KV" in item:
      #         kv = float(cleanTags(item))

      # print(kv)
```

3.4 Extract the image size and pixel spacing using SimpleITK

It will be useful to set the X-ray detector parameters for the simulation, and to display the images in millimetres. We can compare these values with the ones extracted above from the DICOM attributes.

```
[15]: sitk_pixel_spacing = volume.GetSpacing()[0:2]
      size = volume.GetSize()[0:2]

      print("SITK Pixel Spacing (in mm): ", sitk_pixel_spacing)
      print("Image size (in pixels): ", str(size[0]) + " x " + str(size[1]))
```

```
SITK Pixel Spacing (in mm): (0.194556, 0.194556)
Image size (in pixels): 1871 x 1881
```

3.5 Extract the kVp from the DICOM file

It will be useful to generate a realistic beam spectrum.

```
[16]: kVp = float(volume.GetMetaData("0018|0060"))
      print("Peak kilo voltage output of the x-ray generator used: ", kVp)
```

```
Peak kilo voltage output of the x-ray generator used: 90.0
```

4 Extract the mAs from the DICOM file

```
[17]: mAs = volume.GetMetaData("0018|1152")
      print("The exposure expressed in mAs, for example calculated from Exposure Time_
      and X-ray Tube Current:", mAs)
```

```
The exposure expressed in mAs, for example calculated from Exposure Time and
X-ray Tube Current: 1
```

5 Extract the time of X-Ray exposure from the DICOM file

```
[18]: exposure = volume.GetMetaData("0018|1150")
      print(" Time of X-Ray exposure in msec.:", exposure)
```

```
Time of X-Ray exposure in msec.: 5
```

6 Initialise gVirtualXRay

6.1 Set the experimental parameters (e.g. source and detector positions, etc.)

We use known parameters as much as possible, for example we know the size and composition of the sample. Some parameters are extracted from the DICOM file, such as detector size, pixel resolution, and voltage of the X-ray tube.


```
[19]: distance_source_to_detector = float(volume.GetMetaData("0018|1110"))
distance_source_to_patient = float(volume.GetMetaData("0018|1111"))

print("Distance Source to Detector: ", distance_source_to_detector, "mm")
print("Distance Source to Patient: ", distance_source_to_patient, "mm")

window_size = [800, 450]
# source_position = [0.0, 0.0, source_detector_distance_in_cm -
    ↪ block_thickness_in_cm / 2, "mm"]
# detector_position = [0.0, 0.0, - block_thickness_in_cm / 2, "cm"]
detector_up = [0, 1, 0]
```

Distance Source to Detector: 1800.0 mm
 Distance Source to Patient: 1751.0 mm

6.2 Initialise the simulation engine

```
[20]: # Create an OpenGL context
print("Create an OpenGL context:",
      str(window_size[0]) + "x" + str(window_size[1])
)

gvxr.createWindow(-1, True, "OPENGL")

gvxr.setWindowSize(
    window_size[0],
    window_size[1]
)
```

Create an OpenGL context: 800x450

6.3 Load the scanned object

```
[21]: json2gvxr.initSamples("notebook-3.json", verbose=0)
```

```
[22]: 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
```

```
[23]: skin_bbox = gvxr.getNodeOnlyBoundingBox("Skin", "mm")
print(skin_bbox)
```

(-159.375, -117.5, -148.40000915527344, 159.375, 107.5, 148.40000915527344)

6.4 Set the source position

```
[24]: # Set up the beam
print("Set up the beam")
print("\tSource position:", (skin_bbox[0] + skin_bbox[3]) / 2,
      ↪distance_source_to_detector + skin_bbox[1] + distance_source_to_patient -
      ↪distance_source_to_detector, (skin_bbox[2] + skin_bbox[5]) / 2, "mm")

gvxr.setSourcePosition((skin_bbox[0] + skin_bbox[3]) / 2,
      ↪distance_source_to_detector + skin_bbox[1] + distance_source_to_patient -
      ↪distance_source_to_detector, (skin_bbox[2] + skin_bbox[5]) / 2, "mm")

gvxr.usePointSource()
```

Set up the beam

Source position: 0.0 1633.5 0.0 mm

6.5 Get the spectrum from the DICOM file

```
[25]: spectrum = {};
# filter_material = "Al"      # See email Mon 05/07/2021 15:29
# filter_thickness_in_mm = 3  # See email Mon 05/07/2021 15:29

s = sp.Spek(kvp=kVp)
# s.filter(filter_material, filter_thickness_in_mm) # Filter by 3 mm of Al
unit = "keV"
k, f = s.get_spectrum(edges=True) # Get the spectrum

min_energy = sys.float_info.max
max_energy = -sys.float_info.max

for energy, count in zip(k, f):
    count = round(count)

    if count > 0:

        max_energy = max(max_energy, energy)
        min_energy = min(min_energy, energy)

        if energy in spectrum.keys():
            spectrum[energy] += count
        else:
            spectrum[energy] = count
```

Reformat the data

```
[26]: # get the integral nb of photons
nbphotons=0.
```

```

energy1 = -1.
energy2 = -1.

for energy in spectrum.keys():

    if energy1<0:
        energy1 = float(energy)
    elif energy2<0:
        energy2 = float(energy)
    nbphotons += float(spectrum[energy])
sampling = (energy2-energy1)

# get spectrum
data = []
for energy in spectrum.keys():
    source = [float(energy),float(spectrum[energy])/(nbphotons*sampling)]
    data.append(source)

data_array = np.array(data)

energies, counts = data_array.T

```

Resample the data to reduce the number of bins

```

[27]: temp_count_set = signal.decimate(counts, 6)
      number_of_energy_bins = temp_count_set.shape[0]
      temp_energy_set = np.linspace(energies.min(), energies.max(),
      ↪number_of_energy_bins, endpoint=True)

      test = temp_count_set > 0
      count_set = temp_count_set[test]
      energy_set = temp_energy_set[test]

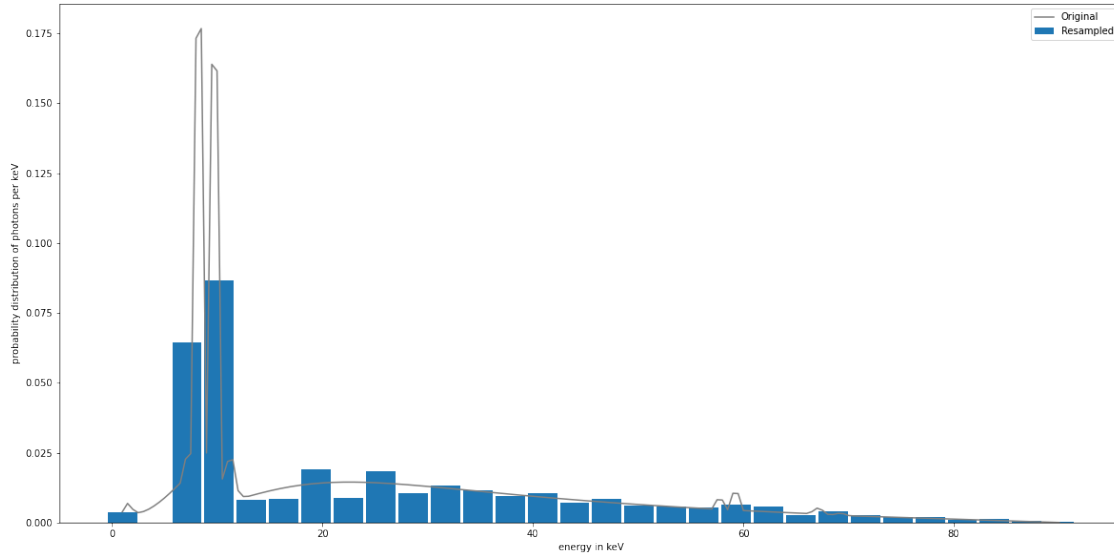
```

Plot the beam spectrum from spekpy and the resampled version

```

[28]: plt.figure(figsize= (20,10))
      plt.bar(energy_set, count_set, width=2.8, label="Resampled")
      plt.plot(energies, counts, label="Original", color="gray")
      plt.xlabel('energy in keV')
      plt.ylabel('probability distribution of photons per keV')
      plt.legend()
      plt.savefig(output_path + "/lungman-projection-spectrum.pdf")

```



6.6 Load the beam spectrum in the simulator

```
[29]: gvxr.resetBeamSpectrum() # To be on the safe side when debugging
for energy, count in zip(energy_set, count_set):
    gvxr.addEnergyBinToSpectrum(energy, unit, count);
```

6.7 Set the X-ray detector

```
[30]: # Set up the detector
print("Set up the detector");
print("\tDetector position:", (skin_bbox[0] + skin_bbox[3]) / 2, skin_bbox[1] +
    ↪distance_source_to_patient - distance_source_to_detector, (skin_bbox[2] +
    ↪skin_bbox[5]) / 2, "mm")
gvxr.setDetectorPosition((skin_bbox[0] + skin_bbox[3]) / 2, skin_bbox[1] +
    ↪distance_source_to_patient - distance_source_to_detector, (skin_bbox[2] +
    ↪skin_bbox[5]) / 2, "mm");

print("\tDetector up vector:", [0, 0, 1])
gvxr.setDetectorUpVector(0, 0, 1);
```

Set up the detector

Detector position: 0.0 -166.5 0.0 mm

Detector up vector: [0, 0, 1]

```
[31]: print("\tDetector number of pixels:", size)
gvxr.setDetectorNumberOfPixels(
    size[0],
    size[1])
```

```
);

print("\tPixel spacing:", imager_pixel_spacing)
gvxr.setDetectorPixelSize(
    imager_pixel_spacing[0],
    imager_pixel_spacing[1],
    "mm"
);
```

```
Detector number of pixels: (1871, 1881)
Pixel spacing: [0.194556 0.194556]
```

Load the detector response in energy

```
[32]: gvxr.clearDetectorEnergyResponse() # To be on the safe side
gvxr.loadDetectorEnergyResponse("Gate_data/responseDetector.txt",
                                "MeV")
```

6.8 Take a screenshot of the 3D environment

```
[33]: gvxr.displayScene()

gvxr.useNegative()
gvxr.useLighting()
gvxr.useWireframe()
gvxr.setSceneRotationMatrix([0.43813619017601013, 0.09238918125629425, -0.
↪8941444158554077, 0.0,
                                0.06627026945352554, 0.9886708855628967, 0.
↪13463231921195984, 0.0,
                                0.8964602947235107, -0.11824299395084381, 0.
↪4270564019680023, 0.0,
                                0.0, 0.0, 0.0, 1.0])
gvxr.setZoom(2639.6787109375)

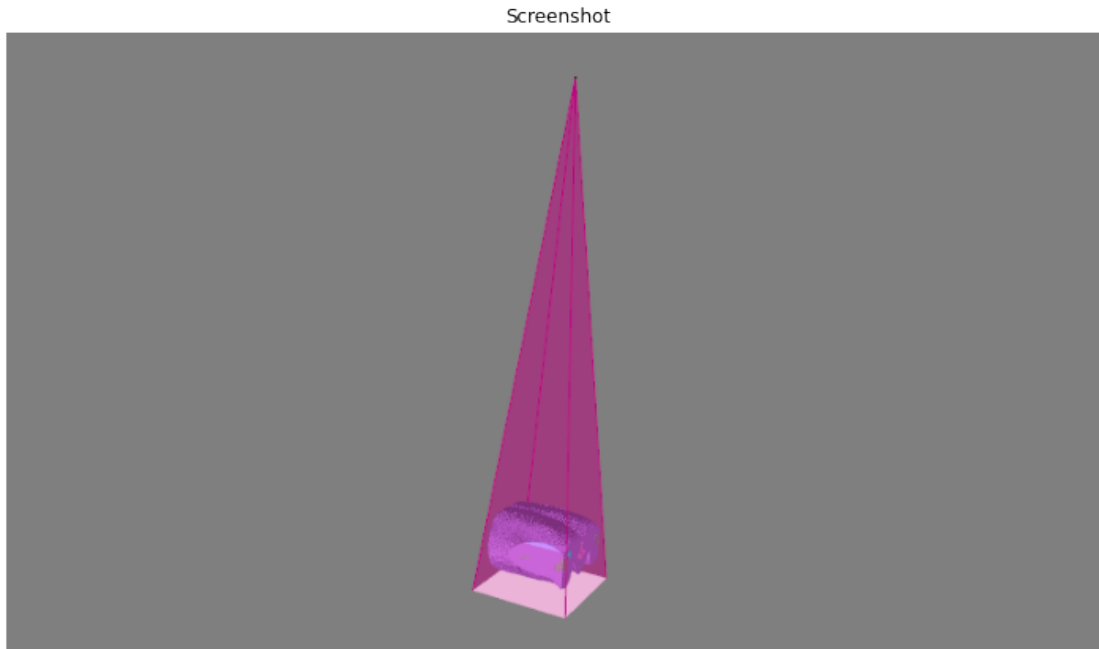
gvxr.displayScene()
```

```
[34]: screenshot = gvxr.takeScreenshot()
```

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

plt.tight_layout()

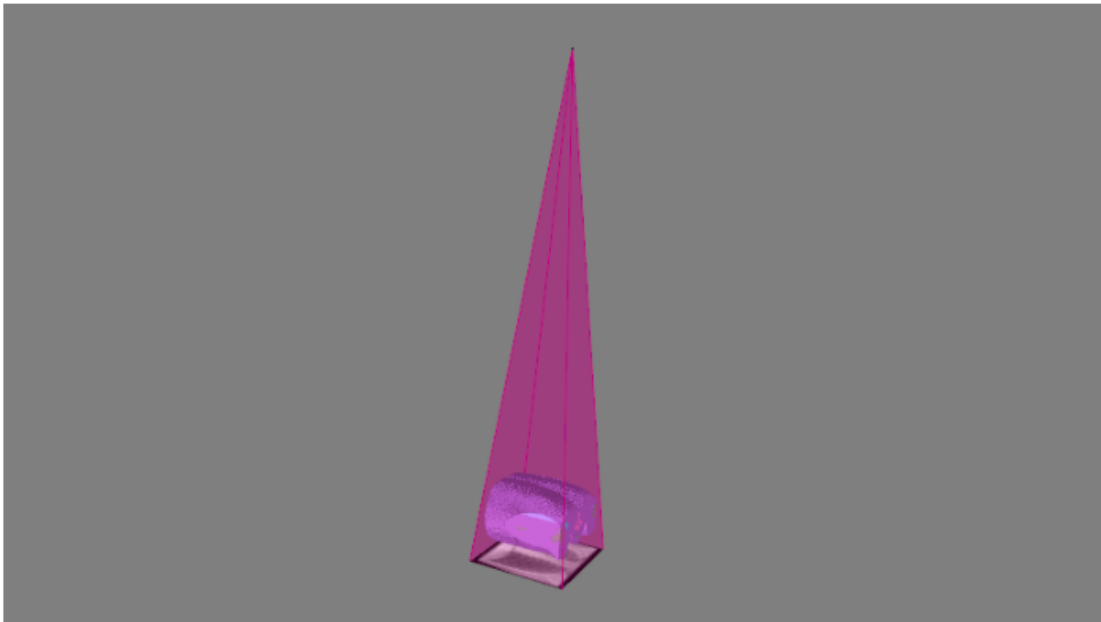
plt.savefig(output_path + '/lungman-projection-screenshot-beam-off.pdf')
plt.savefig(output_path + '/lungman-projection-screenshot-beam-off.png')
```



```
[36]: gvxr.computeXRayImage()  
      gvxr.displayScene()
```

```
[37]: screenshot = gvxr.takeScreenshot()  
  
plt.figure(figsize= (10,10))  
plt.title("Screenshot")  
plt.imshow(screenshot)  
plt.axis('off')  
  
plt.tight_layout()  
  
plt.savefig(output_path + '/lungman-projection-screenshot-beam-on.pdf')  
plt.savefig(output_path + '/lungman-projection-screenshot-beam-on.png')
```

Screenshot



7 Visualise the virtual patient

```
[38]: plot = k3d.plot()
      plot.background_color = 0xffffffff

      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
    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 = [458.4242199518181, -394.5268107574361, 59.58430140683608, 93.
↳26420522817403, -15.742963565665017, -45.88423611599179, -0.
↳08892603121323975, 0.11140808541436767, 0.9897880578573034]

```

Output()

```

[39]: fname = output_path + '/lungman_model.png'
    if not os.path.isfile(fname):

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

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

```

7.1 Simulation with the default values

```

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

```

```

[41]: def getXRayImage():
    global total_energy_in_MeV

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

    # Flat-field
    # xray_image /= total_energy_in_MeV

    # Negative

```



```

    # x_ray_image = 1.0 - x_ray_image
    return np.flip(xray_image) #np.ones(xray_image.shape).astype(np.single) -
    ↪xray_image

```

```

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

```

```

[43]: xray_image = getXRayImage()

```

```

[44]: # 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()

```

```

[45]: gvxr.displayScene()
gvxr.useNegative()

gvxr.setZoom(1339.6787109375)
gvxr.setSceneRotationMatrix([0.8227577805519104, 0.1368587613105774, -0.
    ↪5516625642776489, 0.0, -0.5680444240570068, 0.23148967325687408, -0.
    ↪7897683382034302, 0.0, 0.01961756870150566, 0.9631487131118774, 0.
    ↪26820749044418335, 0.0, 0.0, 0.0, 0.0, 1.0])

gvxr.setWindowBackGroundColour(0.5, 0.5, 0.5)

gvxr.displayScene()

```

```

[46]: # gvxr.renderLoop()

```

```

[47]: # print(gvxr.getZoom())
# print(gvxr.setSceneRotationMatrix())

```

```

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

```

```

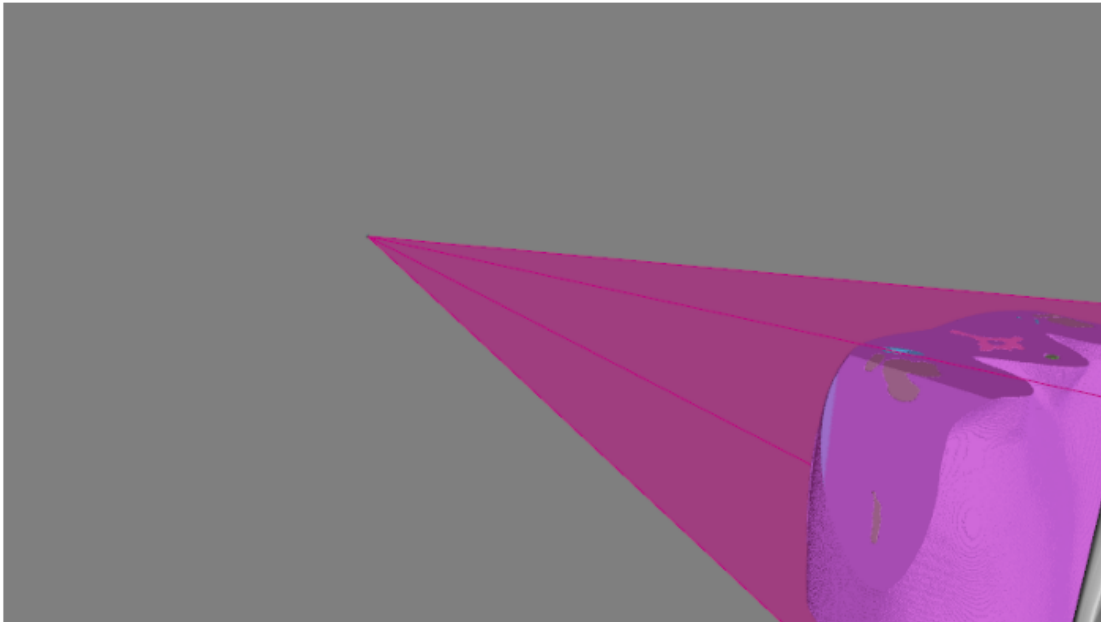
[49]: plt.figure(figsize= (10,10))
plt.title("Screenshot")
plt.imshow(screenshot)
plt.axis('off')

plt.tight_layout()

```

```
plt.savefig(output_path + '/default-screenshot-beam-on-lungman.pdf')
plt.savefig(output_path + '/default-screenshot-beam-on-lungman.png')
```

Screenshot



```
[50]: 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
```

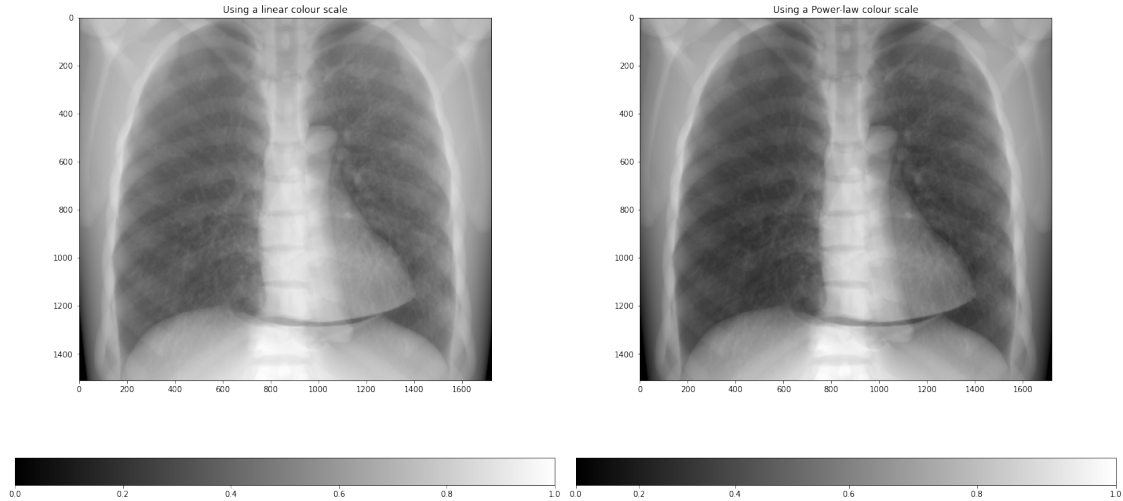
```
[51]: xray_image_cropped = xray_image[y_min_id:y_max_id, x_min_id:x_max_id]
displayLinearPowerScales(1 - logImage(xray_image_cropped, xray_image_cropped.
↪min(), xray_image_cropped.max()),
                                "Image simulated using gVirtualXRay before the
↪registration",
```

```

        output_path + "/"
↪gVirtualXRay-before_registration-lungman",
        log=False)

```

Image simulated using gVirtualXRay before the registration



7.2 Registration

```

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

      imwrite(output_path + '/standardised_roi_ground_truth-lungman.tif',
↪standardised_roi_ground_truth.astype(np.single))

```

```

[53]: source_position_bak = gvxr.getSourcePosition("cm")
      detector_position_bak = gvxr.getDetectorPosition("cm")

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

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

          # Position of the detector
          detector_position_bak[0],
          detector_position_bak[1],

```

```

detector_position_bak[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
]

```

```

[54]: pos_offset = 30
angle_offset = 10

x1 = [
    -angle_offset, -angle_offset, -angle_offset,
    source_position_bak[0] - pos_offset, source_position_bak[1] -
    ↪pos_offset, source_position_bak[2] - pos_offset,
    detector_position_bak[0] - pos_offset, detector_position_bak[1] -
    ↪pos_offset, detector_position_bak[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, angle_offset,

```

```

        source_position_bak[0] + pos_offset, source_position_bak[1] +
↪pos_offset, source_position_bak[2] + pos_offset,
        detector_position_bak[0] + pos_offset, detector_position_bak[1] +
↪pos_offset, detector_position_bak[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
    ]

```

```

[55]: def setTransformations(x):
    # Orientation of the sample
    sample_rotation_angle1 = x[0]
    sample_rotation_angle2 = x[1]
    sample_rotation_angle3 = x[2]

    gvxr.rotateScene(sample_rotation_angle1, 1, 0, 0)
    gvxr.rotateScene(sample_rotation_angle2, 0, 1, 0)
    gvxr.rotateScene(sample_rotation_angle3, 0, 0, 1)

    # Position of the source
    source_position_x = x[3]
    source_position_y = x[4]
    source_position_z = x[5]

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

    # Position of the detector
    det_position_x = x[6]
    det_position_y = x[7]
    det_position_z = x[8]

    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]

```

```

[56]: def resetToDefaultParameters():
        gvxr.setSourcePosition(source_position_bak[0], source_position_bak[1],
↪source_position_bak[2], "cm")
        gvxr.setDetectorPosition(detector_position_bak[0],
↪detector_position_bak[1], detector_position_bak[2], "cm")

        # Restore the transformation matrix
        gvxr.setSceneTransformationMatrix(global_matrix_backup)

```

```

[57]: def updateXRayImage(x, restore_transformation=True):

        # Backup the transformation matrix
        if restore_transformation:
            matrix_backup = gvxr.setSceneTransformationMatrix()

        # Set the transformations
        setTransformations(x)

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

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

        # Restore the transformation matrix
        if restore_transformation:
            gvxr.setSceneTransformationMatrix(matrix_backup)

        return xray_image #, screenshot

```

```

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

```

```

[59]: timeout_in_sec = 30 * 60 # 20 minutes

```

7.3 NSGA-III

```
[60]: standardised_roi_ground_truth = standardised_roi_ground_truth.astype(np.single)
gX = cv2.Sobel(standardised_roi_ground_truth, ddepth=cv2.CV_32F, dx=1, dy=0)
gY = cv2.Sobel(standardised_roi_ground_truth, ddepth=cv2.CV_32F, dx=0, dy=1)
gX = cv2.convertScaleAbs(gX)
gY = cv2.convertScaleAbs(gY)
ref_grad_magn = cv2.addWeighted(gX, 0.5, gY, 0.5, 0)
ref_grad_magn = standardisation(ref_grad_magn)

def objectiveFunctions(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

    objectives = []

    for ind in x:
        xray_image = updateXRayImage(ind)
        corrected_xray_image = applyLogScaleAndNegative(xray_image[y_min_id:
    ↪ y_max_id, x_min_id:x_max_id])
        corrected_xray_image = corrected_xray_image.astype(np.single)

        if corrected_xray_image.min() != corrected_xray_image.max():
            standardised_corrected_xray_image =
    ↪ standardisation(corrected_xray_image)
        else:
            standardised_corrected_xray_image = corrected_xray_image

        # gX = cv2.Sobel(corrected_xray_image, ddepth=cv2.CV_32F, dx=1, dy=0)
        # gY = cv2.Sobel(corrected_xray_image, ddepth=cv2.CV_32F, dx=0, dy=1)
        # gX = cv2.convertScaleAbs(gX)
        # gY = cv2.convertScaleAbs(gY)
        # test_grad_magn = cv2.addWeighted(gX, 0.5, gY, 0.5, 0)

    ref_image = standardised_roi_ground_truth
    test_image = standardised_corrected_xray_image

    # ref_image = ref_grad_magn
    # if test_grad_magn.min() != test_grad_magn.max():
    #     test_grad_magn = standardisation(test_grad_magn)
    # else:
    #     test_image = test_grad_magn
```

```

        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)

        mi = normalized_mutual_information(standardised_roi_ground_truth,
↪standardised_corrected_xray_image)
        dmi = (1.0 - mi) / 2.0
        row.append(dmi)

        objectives.append(row)

    return objectives

```

```

[61]: class MyMultiObjectiveProblem(Problem):

        def __init__(self):
            super().__init__(n_var=len(x_init),

```



```

        n_obj=6,
        n_constr=0,
        xl=xl,
        xu=xu)

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

```

```

[62]: 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", "00:30:00")

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

# termination = DefaultMultiObjectiveTermination(
#     xtol=1e-8,
#     cvtol=1e-6,
#     ftol=0.0025,
#     period=30,
#     n_max_gen=1000,
#     n_max_evals=100000
# )

if os.path.exists(output_path + "/lungman-res-nsga3-X.dat") and os.path.
↪exists(output_path + "/lungman-res-nsga3-F.dat"):

    res_nsga3_X = np.loadtxt(output_path + "/lungman-res-nsga3-X.dat")
    res_nsga3_F = np.loadtxt(output_path + "/lungman-res-nsga3-F.dat")

else:

    n_objs = 6
    n_partitions = 6

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

    problem = MyMultiObjectiveProblem()
    # print(2 * ref_dirs.shape[0])

```

```

#     pop_size = 462 #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(output_path + "/lungman-res-nsga3-X.dat", res_nsga3_X)
np.savetxt(output_path + "/lungman-res-nsga3-F.dat", res_nsga3_F)

```

```

[63]: # font = {'family' : 'serif',
#           #'weight' : 'bold',
#           'size' : 12.5
#       }
# matplotlib.rc('font', **font)

```

```

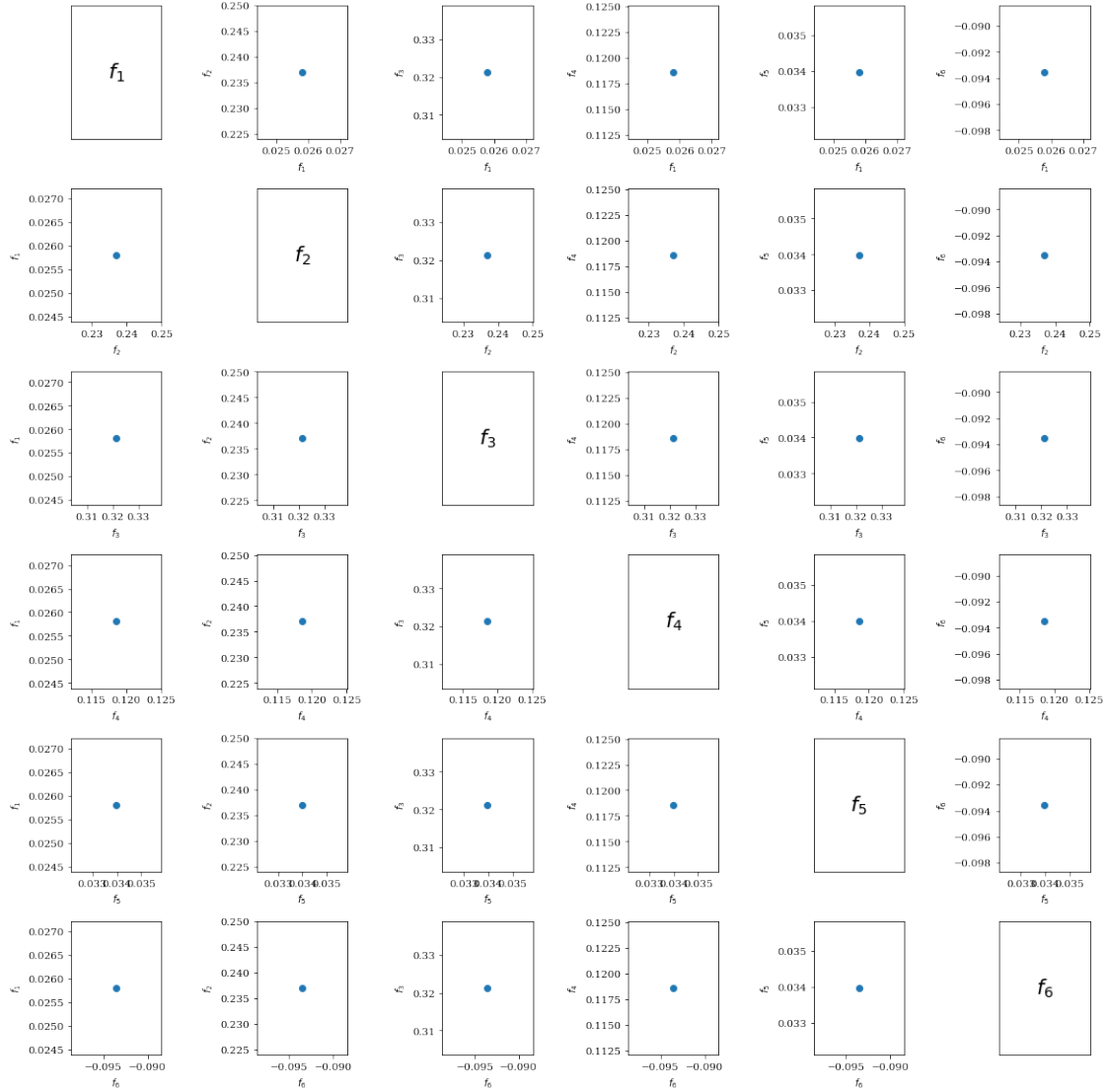
[64]: plot = Scatter(tight_layout=True, figsize=(15,15))
plot.add(res_nsga3_F)
# plot.add(res_nsga3_F[10], s=30, color="red")
plot.show()

```

```

[64]: <pymoo.visualization.scatter.Scatter at 0x7f001b2fa040>

```

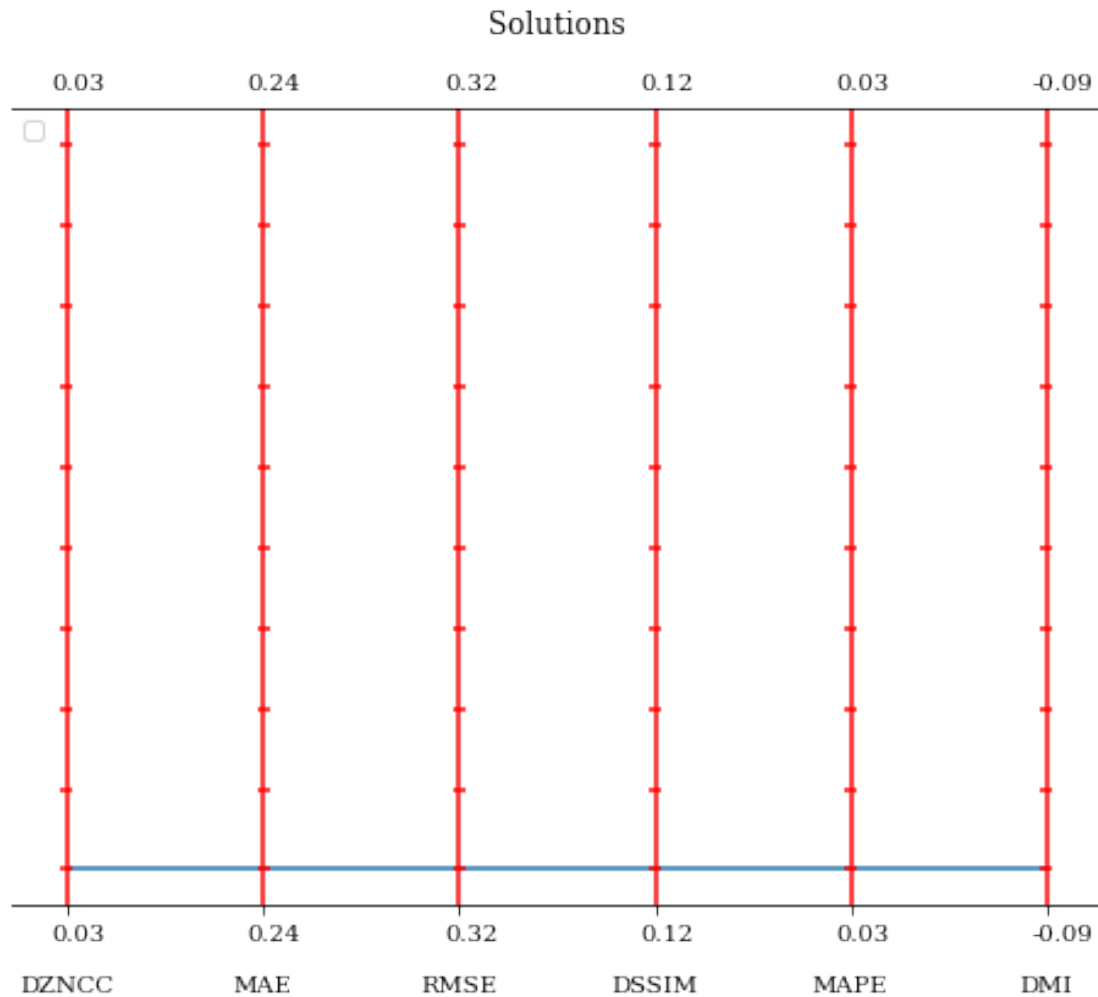


```
[65]: plot = PCP(title=("Solutions", {'pad': 30}),
    n_ticks=10,
    legend=(True, {'loc': "upper left"}),
    labels=["DZNCC", "MAE", "RMSE", "DSSIM", "MAPE", "DMI"]
)

# plot.set_axis_style(color="grey", alpha=1)
# plot.add(res_nsga3_F, color="grey", alpha=0.3)
plot.add(res_nsga3_F)
# plot.add(res_nsga3_F[50], linewidth=5, color="red", label="Solution A")
# plot.add(res_nsga3_F[75], linewidth=5, color="blue", label="Solution B")
plot.show()
```

No artists with labels found to put in legend. Note that artists whose label start with an underscore are ignored when legend() is called with no argument.

[65]: <pymoo.visualization.pcp.PCP at 0x7f0021d39b20>



```
[66]: if len(res_nsga3_F.shape) == 1:
        res_nsga3_F.shape = [1,6]

    if len(res_nsga3_X.shape) == 1:
        res_nsga3_X.shape = [1,9]

    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])
```

```

best_dmi_id = np.argmin(res_nsga3_F[:,5])

best_dzncc_X = res_nsga3_X[best_dzncc_id]
best_mae_X = res_nsga3_X[best_mae_id]
best_rmse_X = res_nsga3_X[best_rmse_id]
best_dssim_X = res_nsga3_X[best_dssim_id]
best_mape_X = res_nsga3_X[best_mape_id]
best_dmi_X = res_nsga3_X[best_dmi_id]

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])
print("Lowest DMI:", res_nsga3_F[:,5].min(), best_dmi_id, ↵
      ↵res_nsga3_X[best_dmi_id])

```

```

Lowest DZNCC: 0.02580389380455017 0 [ -4.01995493  -0.86080154   1.70087074
23.06071983 138.40363669
-11.65987045 -1.07546136 -13.54020345   1.22049772]
Lowest DSSIM: 0.11858216205471156 0 [ -4.01995493  -0.86080154   1.70087074
23.06071983 138.40363669
-11.65987045 -1.07546136 -13.54020345   1.22049772]
Lowest MAE: 0.23700767755508423 0 [ -4.01995493  -0.86080154   1.70087074
23.06071983 138.40363669
-11.65987045 -1.07546136 -13.54020345   1.22049772]
Lowest RMSE: 0.32127187851052924 0 [ -4.01995493  -0.86080154   1.70087074
23.06071983 138.40363669
-11.65987045 -1.07546136 -13.54020345   1.22049772]
Lowest MAPE: 0.033977095037698746 0 [ -4.01995493  -0.86080154   1.70087074
23.06071983 138.40363669
-11.65987045 -1.07546136 -13.54020345   1.22049772]
Lowest DMI: -0.09353725199608232 0 [ -4.01995493  -0.86080154   1.70087074
23.06071983 138.40363669
-11.65987045 -1.07546136 -13.54020345   1.22049772]

```

```

[67]: xray_image_dzncc_nsga3 = applyLogScaleAndNegative(updateXRayImage(best_dzncc_X))
xray_image_mae_nsga3     = applyLogScaleAndNegative(updateXRayImage(best_mae_X))
xray_image_rmse_nsga3    = applyLogScaleAndNegative(updateXRayImage(best_rmse_X))
xray_image_dssim_nsga3   = applyLogScaleAndNegative(updateXRayImage(best_dssim_X))
xray_image_mape_nsga3    = applyLogScaleAndNegative(updateXRayImage(best_mape_X))
xray_image_dmi_nsga3     = applyLogScaleAndNegative(updateXRayImage(best_dmi_X))

```

```

[68]: fig = make_subplots(rows=1, cols=7,
                        start_cell="bottom-left",
                        subplot_titles=("Ground truth", "Best ZNCC", "Best SSIM",
↪ "Best MAE", "Best RMSE", "Best MAPE", "Best MI"))

nsga3_img_set = [standardised_roi_ground_truth,
                standardisation(xray_image_dzncc_nsga3[y_min_id:y_max_id,
↪ x_min_id:x_max_id]),
                standardisation(xray_image_dssim_nsga3[y_min_id:y_max_id,
↪ x_min_id:x_max_id]),
                standardisation(xray_image_mae_nsga3[y_min_id:y_max_id,
↪ x_min_id:x_max_id]),
                standardisation(xray_image_rmse_nsga3[y_min_id:y_max_id,
↪ x_min_id:x_max_id]),
                standardisation(xray_image_mape_nsga3[y_min_id:y_max_id,
↪ x_min_id:x_max_id]),
                standardisation(xray_image_dmi_nsga3[y_min_id:y_max_id,
↪ x_min_id:x_max_id])]

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=800
)

fig.write_image(output_path + "/lungman-NSGA3-objectives-cropped.pdf",
↪ engine="kaleido")

```

```
fig.write_image(output_path + "/lungman-NSGA3-objectives-cropped.png",
    ↪engine="kaleido")

fig.show()
```



```
[69]: fig = make_subplots(rows=1, cols=7,
    start_cell="bottom-left",
    subplot_titles=("Ground truth", "Best ZNCC", "Best SSIM",
    ↪"Best MAE", "Best RMSE", "Best MAPE", "Best MI"))

standardised_ground_truth = standardisation(raw_reference_before_cropping)
nsga3_img_set = [standardised_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),
    standardisation(xray_image_dmi_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",
```

```

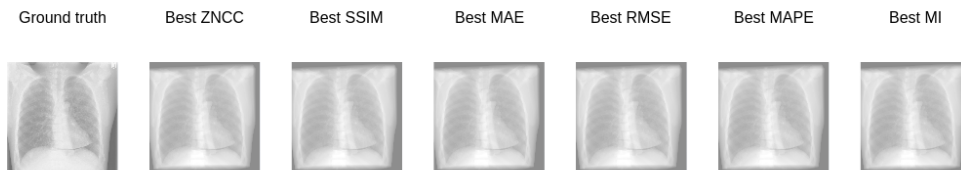
        title_font_color="black",
        legend_title_font_color="black"
    )

    fig.update_layout(
        height=300,
        width=800
    )

    fig.write_image(output_path + "/lungman-NSGA3-objectives.pdf", engine="kaleido")
    fig.write_image(output_path + "/lungman-NSGA3-objectives.png", engine="kaleido")

    fig.show()

```



```

[70]: temp_res_nsga3_F = np.copy(res_nsga3_F[:, [0, 3, 5]])
temp_res_nsga3_F[:,0] = 1.0 - (2.0 * temp_res_nsga3_F[:,0])
temp_res_nsga3_F[:,1] = 1.0 - (2.0 * temp_res_nsga3_F[:,1])
temp_res_nsga3_F[:,2] = 1.0 - (2.0 * temp_res_nsga3_F[:,2])

```

```

[71]: new_array = np.append(res_nsga3_X, res_nsga3_F, axis=1)
new_array = np.append(new_array, temp_res_nsga3_F, axis=1)

columns=["sample_rotation_angle1", "sample_rotation_angle2",
↪ "sample_rotation_angle3", "src_pos_x", "src_pos_y", "src_pos_z",
↪ "det_pos_x", "det_pos_y", "det_pos_z", "DZNCC", "MAE", "RMSE", "DSSIM",
↪ "MAPE", "DMI", "ZNCC", "SSIM", "MI"]
# 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", "DMI", "ZNCC", "SSIM", "MI"]

print(new_array.shape)
print(len(columns))

df_nsga3 = pd.DataFrame(data=new_array,

```



```

columns=columns)

df_nsga3["Optimiser"] = "NSGA-III"
df_nsga3["Optimiser_code"] = 2
df_nsga3.to_csv(output_path + "/lungman-optimiser-nsga3.csv")

```

```

(1, 18)
18

```

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

```

sample_rotation_angle1 sample_rotation_angle2 sample_rotation_angle3 \
0          -4.019955          -0.860802          1.700871

src_pos_x  src_pos_y  src_pos_z  det_pos_x  det_pos_y  det_pos_z  \
0   23.06072  138.403637 -11.65987 -1.075461 -13.540203   1.220498

DZNCC      MAE      RMSE      DSSIM      MAPE      DMI      ZNCC  \
0  0.025804  0.237008  0.321272  0.118582  0.033977 -0.093537  0.948392

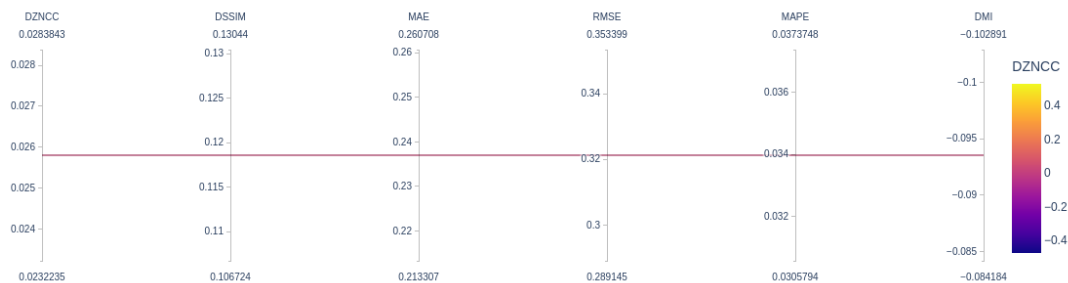
SSIM      MI Optimiser  Optimiser_code
0  0.762836  1.187075  NSGA-III          2

```

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

fig.write_image(output_path + "/lungman-nsga3-parallel_coordinates.pdf", engine="kaleido")
fig.write_image(output_path + "/lungman-nsga3-parallel_coordinates.png", engine="kaleido")

```



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

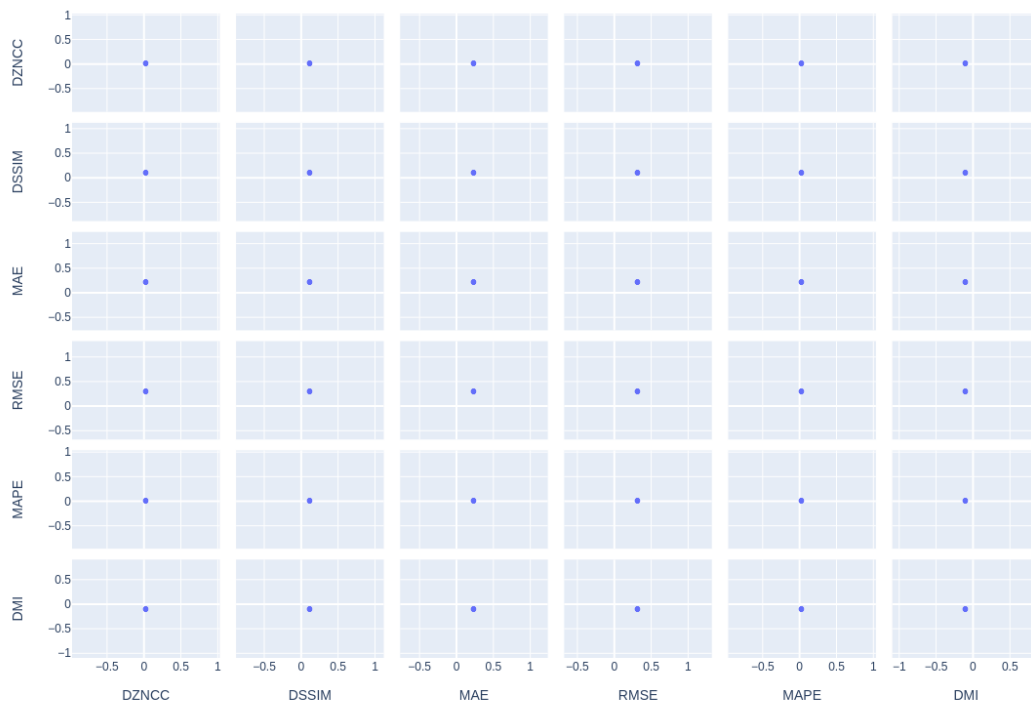
```

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

fig.show()

fig.write_image(output_path + "/lungman-nsga3-scatter_matrix.pdf",
    ↪engine="kaleido")
fig.write_image(output_path + "/lungman-nsga3-scatter_matrix.png",
    ↪engine="kaleido")

```



8 Refine the results with CMA-ES

```

[75]: def objectiveFunctionGeometry(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

```

```

objectives = []

for ind in x:
    xray_image = updateXRayImage(ind)
    corrected_xray_image = applyLogScaleAndNegative(xray_image[y_min_id:
↪y_max_id, x_min_id:x_max_id])
    corrected_xray_image = corrected_xray_image.astype(np.single)

    if corrected_xray_image.min() != corrected_xray_image.max():
        standardised_corrected_xray_image = □
↪standardisation(corrected_xray_image)
    else:
        standardised_corrected_xray_image = corrected_xray_image

    # gX = cv2.Sobel(corrected_xray_image, ddepth=cv2.CV_32F, dx=1, dy=0)
    # gY = cv2.Sobel(corrected_xray_image, ddepth=cv2.CV_32F, dx=0, dy=1)
    # gX = cv2.convertScaleAbs(gX)
    # gY = cv2.convertScaleAbs(gY)
    # test_grad_magn = cv2.addWeighted(gX, 0.5, gY, 0.5, 0)

    ref_image = standardised_roi_ground_truth
    test_image = standardised_corrected_xray_image

    # ref_image = ref_grad_magn
    # if test_grad_magn.min() != test_grad_magn.max():
    #     test_grad_magn = standardisation(test_grad_magn)
    # else:
    #     test_image = test_grad_magn

    # znc = np.mean(standardised_roi_ground_truth * □
↪standardised_corrected_xray_image)
    # dznc = (1.0 - znc) / 2.0
    # objective = dznc

    # mae = np.mean(np.abs(standardised_roi_ground_truth - □
↪standardised_corrected_xray_image))
    # objective = mae

    rmse = math.sqrt(np.mean(np.square(standardised_roi_ground_truth - □
↪standardised_corrected_xray_image)))
    objective = 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
#         objective = 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)
#         objective = mape_value

#         mi = normalized_mutual_information(standardised_roi_ground_truth,
↳ standardised_corrected_xray_image)
#         dmi = (1.0 - mi) / 2.0
#         objective = dmi

        objectives.append(objective)

    return objectives

```

```

[76]: class SingleObjectiveProblem(Problem):

    def __init__(self):
        super().__init__(n_var=len(x_init), n_obj=1, n_constr=0,
↳ n_ineq_constr=0, xl=xl, xu=xu, vtype=float)

    def _evaluate(self, x, out, *args, **kwargs):

        out["F"] = np.array(objectiveFunctionGeometry(x))
        out["F"].shape = [len(x), 1]

```

```

[77]: resetToDefaultParameters()

if os.path.exists(output_path + "/lungman-res-cmaes-X.dat") and os.path.
↳ exists(output_path + "/lungman-res-cmaes-F.dat"):
    res_cmaes_X = np.loadtxt(output_path + "/lungman-res-cmaes-X.dat")
    res_cmaes_F = np.loadtxt(output_path + "/lungman-res-cmaes-F.dat")
else:

    problem = SingleObjectiveProblem()
    algorithm = CMAES(x0=res_nsga3_X[best_dzncc_id])

    res = minimize(problem,
                    algorithm,

```

```

        ('n_iter', 100),
        # seed=1,
        save_history=True,
        verbose=True)

res_cmaes_X = res.X
res_cmaes_F = res.F

np.savetxt(output_path + "/lungman-res-cmaes-X.dat", res_cmaes_X)
np.savetxt(output_path + "/lungman-res-cmaes-F.dat", res_cmaes_F)

```

```
[78]: xray_image_rmse_cmaes = applyLogScaleAndNegative(updateXRayImage(res_cmaes_X))
```

```
[79]: fig = make_subplots(rows=1, cols=7,
                        start_cell="bottom-left",
                        subplot_titles=("Ground truth", "Best RMSE (NSGA-III)",
↪ "Best RMSE (CMA-ES)"))

standardised_ground_truth = standardisation(raw_reference_before_cropping)
rmse_img_set = [standardised_ground_truth,
                standardisation(xray_image_rmse_nsga3),
                standardisation(xray_image_rmse_cmaes)]

for n, image in enumerate(rmse_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"
)

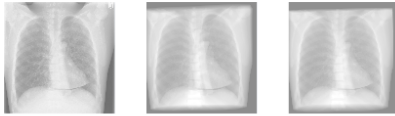
fig.update_layout(
    height=300,
    width=800
)

```

```
fig.write_image(output_path + "/lungman-CMAES-objectives.pdf", engine="kaleido")
fig.write_image(output_path + "/lungman-CMAES-objectives.png", engine="kaleido")

fig.show()
```

Ground truth Best RMSE (NSGA-IB) Best RMSE (CMA-ES)



```
[80]: # Apply the transformation
xray_image_rmse_cmaes = applyLogScaleAndNegative(updateXRayImage(res_cmaes_X,
↪restore_transformation=False));
```

```
[81]: standardised_corrected_xray_image =
↪standardisation(xray_image_rmse_cmaes[y_min_id:y_max_id, x_min_id:x_max_id])

imwrite(output_path + "/standardised_corrected_xray_image.tif",
↪standardised_corrected_xray_image.astype(np.single))
hist_ref = np.histogram(standardised_roi_ground_truth, 100)[0]

standardised_roi_ground_truth = standardised_roi_ground_truth.astype(np.single)
gX = cv2.Sobel(standardised_roi_ground_truth, ddepth=cv2.CV_32F, dx=1, dy=0)
gY = cv2.Sobel(standardised_roi_ground_truth, ddepth=cv2.CV_32F, dx=0, dy=1)
gX = cv2.convertScaleAbs(gX)
gY = cv2.convertScaleAbs(gY)
ref_grad_magn = cv2.addWeighted(gX, 0.5, gY, 0.5, 0)

hist_ref = np.histogram(ref_grad_magn, 100)[0]
```

```
[82]: gvxr.displayScene()
gvxr.useNegative()

gvxr.setZoom(1339.6787109375)
gvxr.setSceneRotationMatrix([0.8227577805519104, 0.1368587613105774, -0.
↪5516625642776489, 0.0, -0.5680444240570068, 0.23148967325687408, -0.
↪7897683382034302, 0.0, 0.01961756870150566, 0.9631487131118774, 0.
↪26820749044418335, 0.0, 0.0, 0.0, 0.0, 1.0])
```

```
gvxr.setWindowBackGroundColour(0.5, 0.5, 0.5)
```

```
gvxr.displayScene()
```

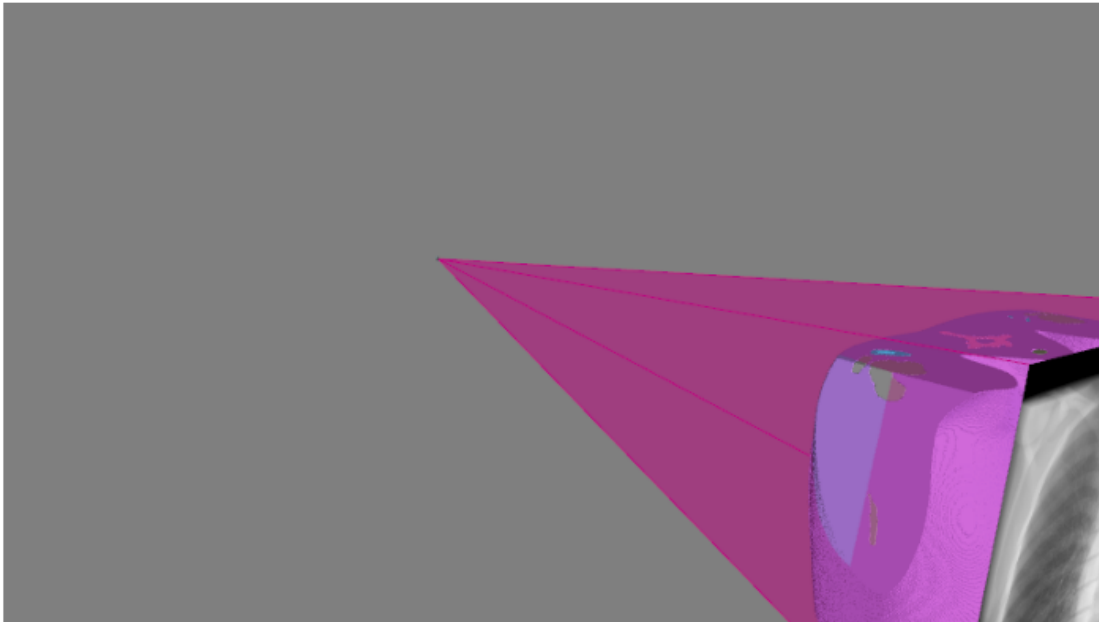
```
[83]: # gvxr.renderLoop()
```

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

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

```
[86]: plt.figure(figsize= (10,10))  
plt.title("Screenshot")  
plt.imshow(screenshot)  
plt.axis('off')  
  
plt.tight_layout()  
  
plt.savefig(output_path + '/lungman-optimised-screenshot-beam-on.pdf')  
plt.savefig(output_path + '/lungman-optimised-screenshot-beam-on.png')
```

Screenshot



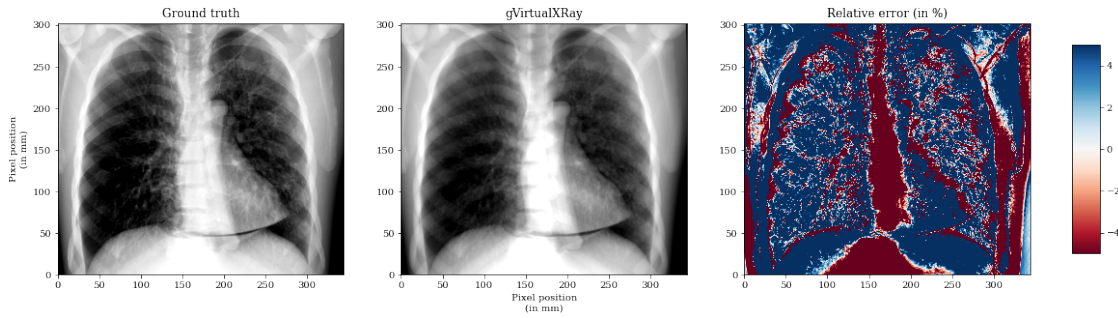
```
[87]: fullCompareImages(standardised_roi_ground_truth,  
                        standardised_corrected_xray_image,  
                        "gVirtualXRay",
```

```

# output_path + "/lungman-projection-rmse-cmaes",
↪vmin=standardised_roi_ground_truth.min(), vmax=standardised_roi_ground_truth.
↪max(),

output_path + "/lungman-projection-rmse-cmaes",
↪detector_element_spacing, vmin=-1.5, vmax=1.5)

```



```

[88]: ref_diag = np.diag(standardised_roi_ground_truth)
test_diag = np.diag(standardised_corrected_xray_image)

plt.figure(figsize=(15, 7))

ax = plt.subplot(111)

ax.set_title("Diagonal profiles")

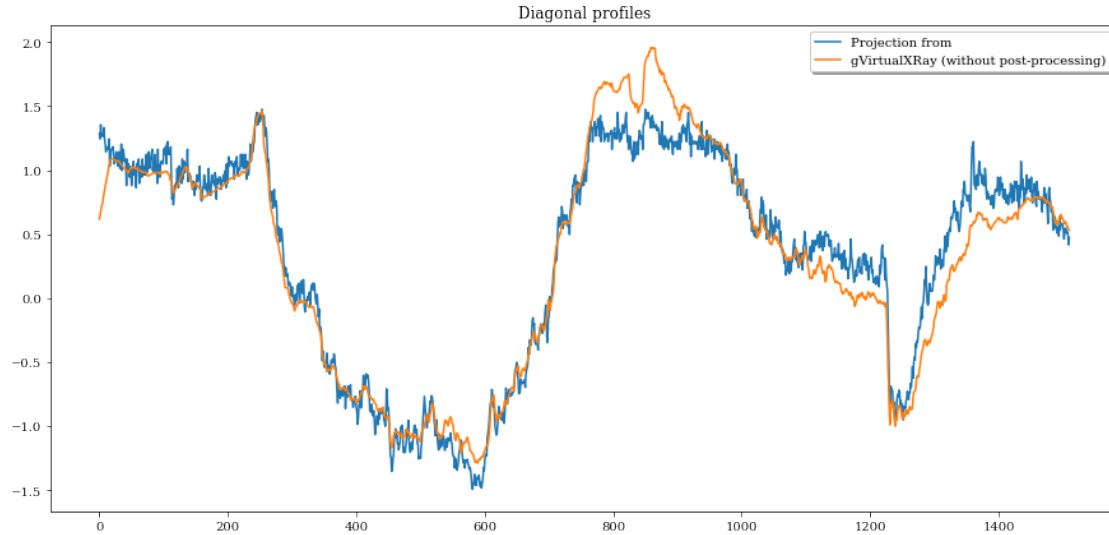
ax.plot(ref_diag, label="Projection from ")
ax.plot(test_diag, label="gVirtualXRay (without post-processing)")

ax.legend(loc='best',
          ncol=1, fancybox=True, shadow=True)

# plt.legend()

plt.savefig(output_path + '/lungman-profiles-projection-rmse-cmaes.pdf')
plt.savefig(output_path + '/lungman-profiles-projection-rmse-cmaes.png')

```

9 Compute the magnification

$magnification = \frac{SID}{SOD}$ with SID the source to imager distance and SOD the source to object distance.

```
[89]: source_position = gvxr.getSourcePosition("mm")
detector_position = gvxr.getDetectorPosition("mm")

object_bbox = gvxr.getNodeAndChildrenBoundingBox("root", "mm")
object_position = [(object_bbox[0] + object_bbox[3]) / 2,
                   (object_bbox[1] + object_bbox[4]) / 2,
                   (object_bbox[2] + object_bbox[5]) / 2
                  ]

source_imager_distance = distance.euclidean(source_position, detector_position)
source_object_distance = distance.euclidean(source_position, object_position)

magnification = source_imager_distance / source_object_distance

[90]: print("SID:", source_imager_distance, "mm")
print("SOD:", source_object_distance, "mm")
print("magnification:", magnification)
```

```
SID: 1662.6100648426484 mm
SOD: 1541.0320332447461 mm
magnification: 1.0788939029008446
```

10 Compute the pixel size in the object plane

```
[91]: spacing = source_imager_distance * detector_element_spacing /  
        ↪source_object_distance  
  
print("spacing in the object plane (in mm):", spacing)
```

```
spacing in the object plane (in mm): [0.2157788 0.2157788]
```

11 Post-processing using image sharpening

We can see from the real image that an image sharpening filter was applied. We will implement one and optimise its parameters.

```
[92]: def sharpen(image, ksize, shift, scale):  
        details = image - gaussian(image, ksize)  
  
        return (details + shift) * scale
```

11.1 Define an objective function

```
[93]: # Compute the X-ray image  
xray_image = np.flip(gvvr.computeXRayImage())  
  
# Flat-field  
xray_image_flat = xray_image[y_min_id:y_max_id, x_min_id:x_max_id] /  
        ↪total_energy_in_MeV
```

```
[94]: def objectiveFunctionSharpen(x):  
  
    global xray_image_flat  
    global standardised_roi_ground_truth  
  
    objectives = []  
  
    for parameters in x:  
  
        # Retrieve the parameters  
        shift1, scale1, sigma1, sigma2, shift2, scale2 = parameters  
  
        # Process the image  
        contrast = (xray_image_flat + shift1) * scale1  
        details = sharpen(xray_image_flat, (sigma1, sigma2), shift2, scale2)  
        sharpened = contrast + details  
        sharpened[sharpened < 1e-9] = 1e-9  
        log_image = np.log(contrast + details)  
        negative = log_image * -1
```

```

        normalised = standardisation(negative)

        # Return the objective
        objective = math.sqrt(mean_squared_error(standardised_roi_ground_truth,
↪normalised))
        # objective = math.sqrt(mean_squared_error(ref_grad_magn,
↪test_grad_magn))
        # objective = math.sqrt(mean_squared_error(hist_ref, hist_test))

        # objective = ref_grad_magn.sum() - test_grad_magn.sum()
        # objective *= objective
        # objective *= -1

        # mi = normalized_mutual_info_score(hist_ref, hist_test)
        # dmi = (1.0 - mi) / 2.0
        # objective = dmi
        objectives.append(objective)

    return objectives

```

11.2 Minimise the objective function

```

[95]: sigma1 = 2
      sigma2 = 2
      alpha = 10.5
      shift = 0
      scale = 1

      x1 = [0, 0, 0, -5, 0]
      xu = [10, 10, 15, 5, 2]
      x_init = [sigma1, sigma2, alpha, shift, scale]

      #0.003937458431052107 4012.600582499311 3.916470602237863 0.28374201341640476 6.
↪851503972136956 6.8658686847669045e-09

      x1 = [0, 1e-9, 1, 1, 0, 0.5]
      xu = [10000, 10000, 10, 10, 10000, 10000]
      x_init = [0, 1, 3, 3, 0, 1]

```

```

[96]: class SingleObjectiveProblem(Problem):

      def __init__(self):
          super().__init__(n_var=len(x_init), n_obj=1, n_constr=0,
↪n_ieq_constr=0, x1=x1, xu=xu, vtype=float)
          # super().__init__(n_var=len(x_init), n_obj=1, n_constr=0,
↪n_ieq_constr=0, vtype=float)

```

```

def _evaluate(self, x, out, *args, **kwargs):

    out["F"] = np.array(objectiveFunctionSharpen(x))
    out["F"].shape = [len(x), 1]

```

```

[97]: # The registration has already been performed. Load the results.
if os.path.isfile(output_path + "/lungman_postprocess.dat"):

    shift1, scale1, sigma1, sigma2, shift2, scale2 = np.loadtxt(output_path + "/"
↳lungman_postprocess.dat")

else:
    # Optimise
    # timeout_in_sec = 20 * 60 # 20 minutes
    # opts = cma.CMAOptions()
    # opts.set('tolfun', 1e-10)
    # opts['tolx'] = 1e-10
    # 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) * 0.05)

    problem = SingleObjectiveProblem()
    x0 = denormalize(np.random.random(problem.n_var), problem.xl, problem.xu)

    algorithm = CMAES(x0=x0,
                      sigma=0.5,
                      restarts=2,
                      maxfevals=np.inf,
                      tolfun=1e-6,
                      tolx=1e-6,
                      restart_from_best=True,
                      bipop=True)

    res = minimize(problem,
                  algorithm,
                  ('n_iter', 100),
                  seed=1,
                  save_history=True,
                  verbose=True)

    # # Optimise
    # res = minimize(problem,
    #                 algorithm,

```

```

#         ('n_iter', 100),
#         # seed=1,
#         save_history=False,
#         verbose=True)

print(f"Best solution found: \nX = {res.X}\nF = {res.F}\nCV= {res.CV}")

# Save the parameters
shift1, scale1, sigma1, sigma2, shift2, scale2 = res.X
np.savetxt(output_path + "/lungman_postprocess.dat", [shift1, scale1,
↪sigma1, sigma2, shift2, scale2], header='shift1, scale1, sigma1, sigma2,
↪shift2, scale2')

```

11.3 Apply the result of the optimisation

```

[98]: print(shift1, scale1, sigma1, sigma2, shift2, scale2) #     return scale *
↪(shift + image) + alpha * details

# Process the image
contrast = (xray_image_flat + shift1) * scale1
details = sharpen(xray_image_flat, (sigma1, sigma2), shift2, scale2)
sharpened = contrast + details
sharpened[sharpened < 1e-9] = 1e-9
log_image = np.log(contrast + details)
negative = log_image * -1
normalised = standardisation(negative)

```

```

0.0038399819169387573 9232.063565472905 7.339600967177158 7.924408749898391
11.289006641605752 0.6185266797462592

```

```

[99]: font = {'size' : 12.5
            }
matplotlib.rc('font', **font)

```

```

[100]: new_image_without_post_process = standardised_corrected_xray_image *
↪raw_reference.std()
new_image_without_post_process -= standardised_corrected_xray_image.mean()
new_image_without_post_process += raw_reference.mean()

new_image_with_post_process = normalised * raw_reference.std()
new_image_with_post_process -= normalised.mean()
new_image_with_post_process += raw_reference.mean()

```

```

[101]: old_zncc = np.mean(standardised_roi_ground_truth *
↪standardised_corrected_xray_image)
new_zncc = np.mean(standardised_roi_ground_truth * normalised)

```

```
[102]: old_mape = mape(raw_reference, new_image_without_post_process)
new_mape = mape(raw_reference, new_image_with_post_process)
```

```
[103]: old_ssim = ssim(raw_reference, new_image_without_post_process,
↳data_range=raw_reference.max() - raw_reference.min())
new_ssim = ssim(raw_reference, new_image_with_post_process,
↳data_range=raw_reference.max() - raw_reference.min())
```

```
[104]: print("ZNCC before sharpening:", str(100 * old_zncc) + "%")
print("ZNCC after sharpening:", str(100 * new_zncc) + "%")

print("MAPE before sharpening:", str(100 * old_mape) + "%")
print("MAPE after sharpening:", str(100 * new_mape) + "%")

print("SSIM before sharpening:", str(old_ssim))
print("SSIM after sharpening:", str(new_ssim))
```

```
ZNCC before sharpening: 98.33838407441668%
ZNCC after sharpening: 98.92364439169694%
MAPE before sharpening: 1.7763866439597007%
MAPE after sharpening: 1.54638819692157%
SSIM before sharpening: 0.9385582576217021
SSIM after sharpening: 0.9391286805711191
```

```
[105]: ground_truth_diag = np.diag(raw_reference)
gvxr_diag = np.diag(new_image_with_post_process)

print(ground_truth_diag.shape)
x = np.linspace(0, ground_truth_diag.shape[0], ground_truth_diag.shape[0]) *
↳spacing[0]
plt.figure(figsize=(15, 5))

ax = plt.subplot(111)

ax.set_title("Diagonal profiles")

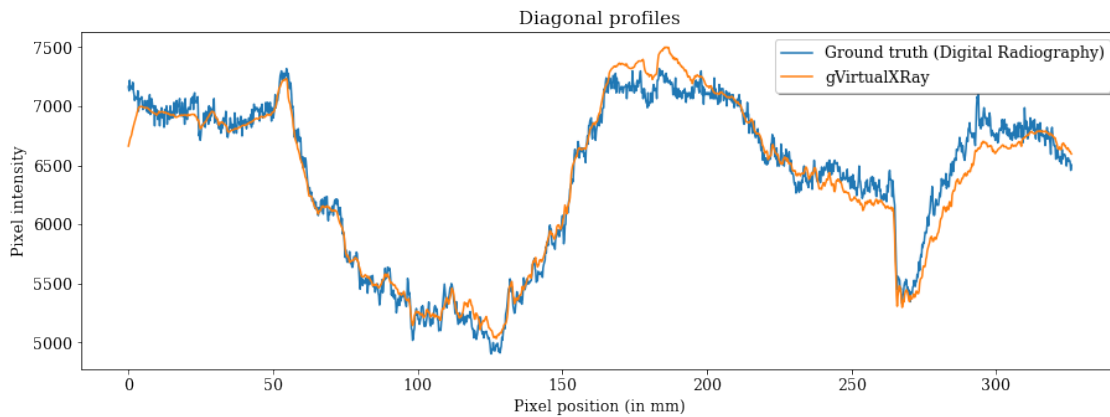
ax.plot(x, ground_truth_diag, label="Ground truth (Digital Radiography)")
ax.plot(x, gvxr_diag, label="gVirtualXRay")

ax.legend(loc='best',
        ncol=1, fancybox=True, shadow=True)

plt.xlabel("Pixel position (in mm)")
plt.ylabel("Pixel intensity")

plt.savefig(output_path + '/lungman-profiles-projection-postprocessing.pdf')
plt.savefig(output_path + '/lungman-profiles-projection-postprocessing.png')
```

(1511,)



```
[106]: window_centre = int(volume.GetMetaData("0028|1050").split("\\")[1]) # Use 0 for normal, 1 for harder, 2 for softer
        window_width = int(volume.GetMetaData("0028|1051").split("\\")[1]) # Use 0 for normal, 1 for harder, 2 for softer

        print("Window Center used: ", window_centre)
        print("Window Width used: ", window_width)

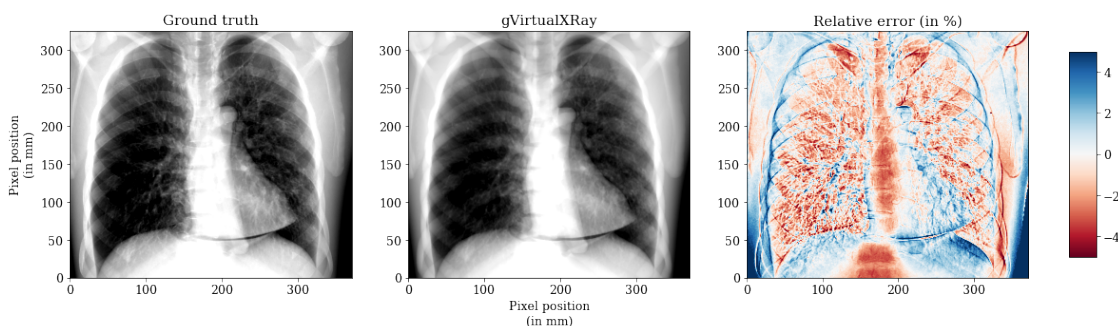
        vmin = window_centre - window_width / 2
        vmax = window_centre + window_width / 2

        view_position = volume.GetMetaData("0018|5101")
```

Window Center used: 6032

Window Width used: 2245

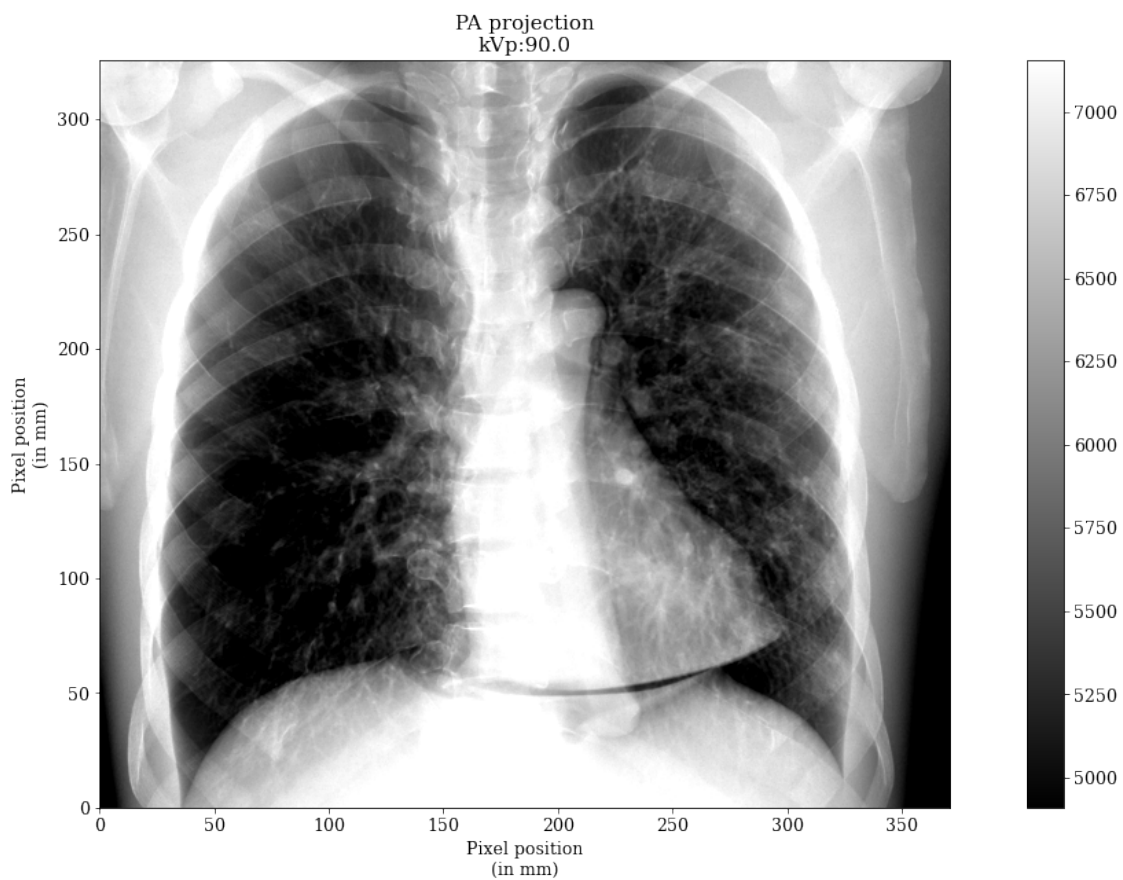
```
[107]: fullCompareImages(raw_reference,
                        new_image_with_post_process,
                        "gVirtualXRay",
                        output_path + "/lungman-projection-harder", spacing,
                        log=False, vmin=vmin, vmax=vmax)
```



```
[108]: plt.figure(figsize= (20,10))
xrange=range(raw_reference.shape[1])
yrange=range(raw_reference.shape[0])

plt.xlabel("Pixel position\n(in mm)")
plt.ylabel("Pixel position\n(in mm)")
plt.title(view_position + " projection\nkVp:" + str(kVp))
plt.imshow(raw_reference, cmap="gray",
           vmin=vmin, vmax=vmax,
           extent=[0,(raw_reference.shape[1]-1)*spacing[0],0,(raw_reference.
↪shape[0]-1)*spacing[1]])
plt.colorbar(orientation='vertical')

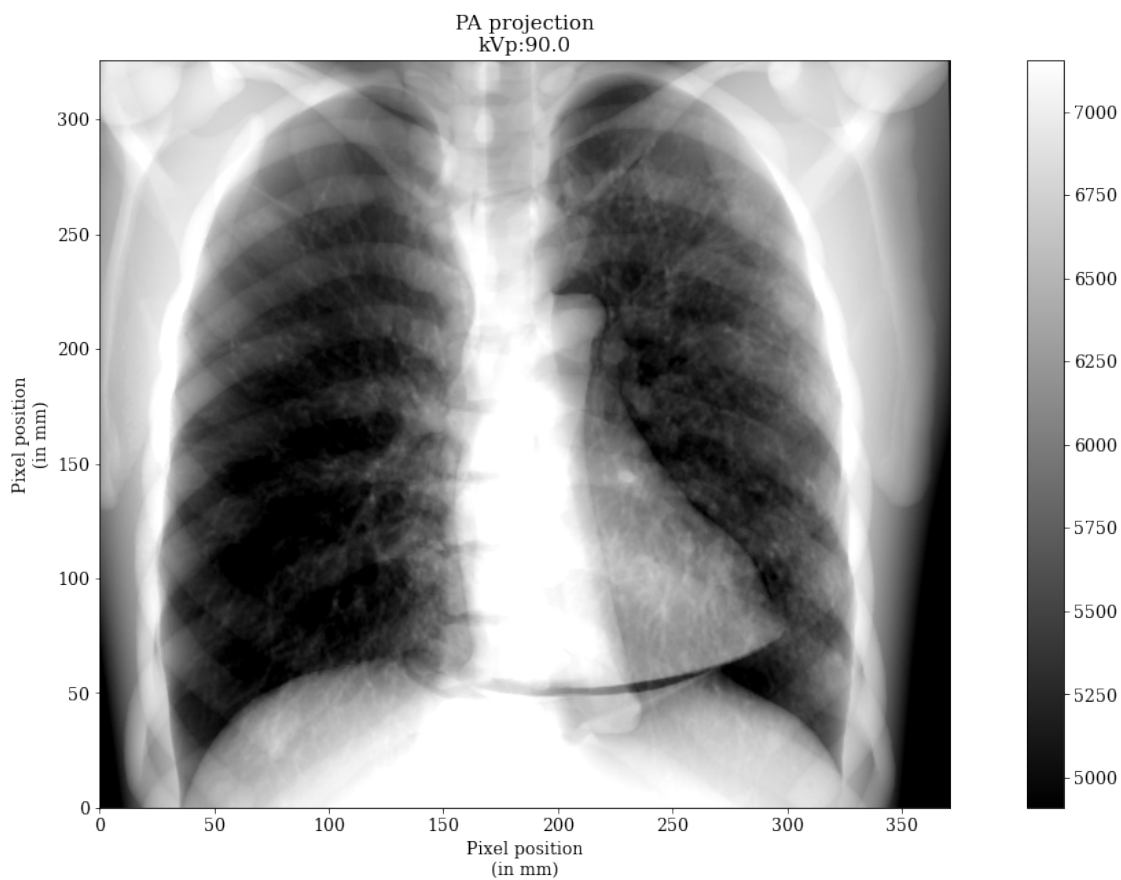
plt.savefig(output_path + '/lungman_experimental_DX_image-harder.pdf')
plt.savefig(output_path + '/lungman_experimental_DX_image-harder.png')
```




```
[109]: plt.figure(figsize= (20,10))
xrange=range(raw_reference.shape[1])
yrange=range(raw_reference.shape[0])

plt.xlabel("Pixel position\n(in mm)")
plt.ylabel("Pixel position\n(in mm)")
plt.title(view_position + " projection\nkVp:" + str(kVp))
plt.imshow(new_image_with_post_process, cmap="gray",
           vmin=vmin, vmax=vmax,
           extent=[0,(raw_reference.shape[1]-1)*spacing[0],0,(raw_reference.
↪shape[0]-1)*spacing[1]])
plt.colorbar(orientation='vertical')

plt.savefig(output_path + '/lungman_simulated_DX_image-harder.pdf')
plt.savefig(output_path + '/lungman_simulated_DX_image-harder.png')
```



```
[110]: runtimes = []

resetToDefaultParameters()
```

```

setTransformations(res_nsga3_X[best_dzncc_id])

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

    raw_x_ray_image = np.array(gvxr.computeXRayImage())

    # Process the image
    xray_image_flat = raw_x_ray_image / total_energy_in_MeV
    contrast = (xray_image_flat + shift1) * scale1
    details = sharpen(xray_image_flat, (sigma1, sigma2), shift2, scale2)
    sharpened = contrast + details
    sharpened[sharpened < 1e-9] = 1e-9
    log_image = np.log(contrast + details)
    negative = log_image * -1

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

```

```

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

raw_x_ray_image = np.array(raw_x_ray_image)

```

```

[112]: ZNCC = df_nsga3["ZNCC"].max()
SSIM = df_nsga3["SSIM"].max()
MAPE = df_nsga3["MAPE"].max()

print("Lungman PA view & Real digital radiograph & " +
      "{0:0.2f}".format(100 * new_mape) + "\\% & " +
      "{0:0.2f}".format(100 * new_zncc) + "\\% & " +
      "{0:0.2f}".format(new_ssim) + " & $" +
      str(raw_x_ray_image.shape[1]) + " \\times " + str(raw_x_ray_image.
↪shape[0]) + "$ & N/A &" +
      str(number_of_triangles) + " & " +
      "$" + str(runtime_avg) + " \\pm " + str(runtime_std) + "$ & N/A \\\\")

```

```

Lungman PA view & Real digital radiograph & 1.55\% & 98.92\% & 0.94
& $1871 \times 1881$ & N/A & 16528580 & $527 \pm 67$ & N/A \

```

11.4 All done

Destroy the window

```

[113]: gvxr.destroyAllWindows()

```