Scientific Software Development with Python

Visualizing scientific data

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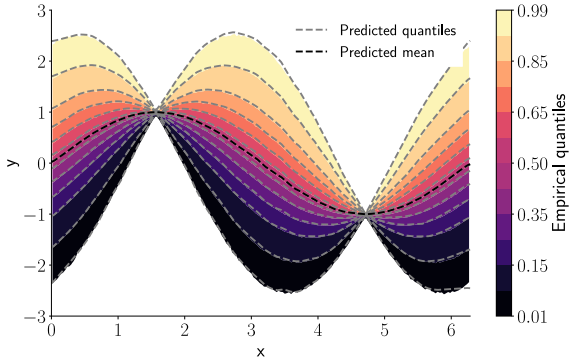
Agenda

1. Introduction

2. Visualizing 3D data with PyVista

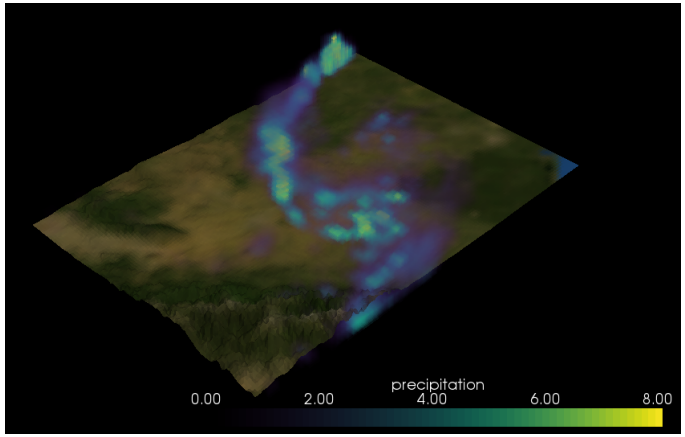
2D

- Matplotlib
  - Arguably one of the most popular scientific Python packages
  - Limited 3D capability
- plotly, bokeh
  - Web-based, interactive plotting



3D

- VTK
  - Powerful but complex
- MayaVi, PyVista
  - High-level interfaces to VTK



Agenda

1. Introduction

2. Visualizing 3D data with PyVista

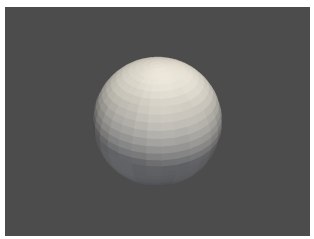
Installation

```
pip install pyvista
```

Basic workflow

- Create a mesh[1] and plot directly:

```
import pyvista as pv

# Create a mesh
mesh = pv.Sphere()
mesh.plot()
```



- Or explicitly create a plotter:

```
plotter = pv.Plotter()
plotter.add_mesh(mesh)
plotter.show()
```

[1] We use the term mesh to designate any object we create and visualize in PyVista

Primitives

- Complex visualizations are typically built from basic, visual primitives.
- In 3D we have the following primitives:
  - points
  - lines
  - surfaces
  - volumes

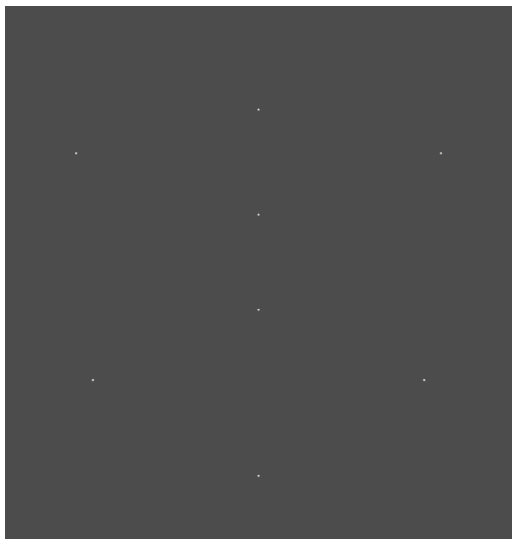
- `PolyData`: Represent surfaces points, lines and surfaces
- `UnstructuredGrid`:
  - Can represent surfaces and volumes
  - Connections between grid points must be added explicitly
  - Therefore seldomly used directly
- `StructuredGrid`:
  - Cells between neighboring points are implicitly assumed
  - Easiest way to represent gridded surfaces and volumes

Points

- The `PolyData` class allows us to build 3D shapes from these primitives
- To begin, we add a dataset with eight points.

Example

```
import numpy as np
import pyvista as pv

points = np.array([0.0, 1.0, 2.0])
x, y, z = np.meshgrid(points, points, points)
point_coords = np.hstack([x.reshape(-1, 1),
                          y.reshape(-1, 1),
                          z.reshape(-1, 1)])
# Dataset has eight points.
points = pv.PolyData(point_coords)
points.plot()
```



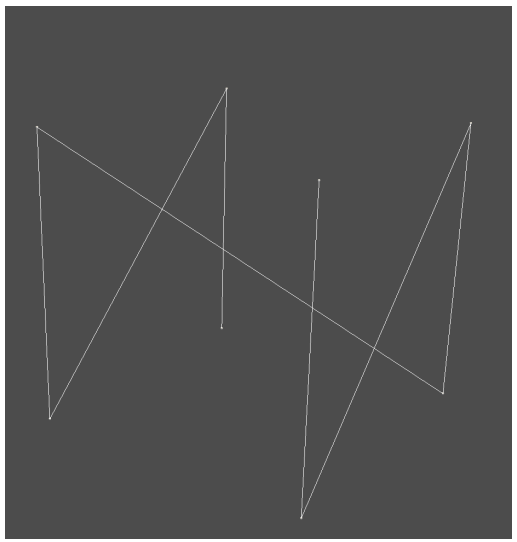
Adding lines

- Lines are described by arrays of the form:

```
[n, point_index_0, ..., point_index_n-1]
```

Example

```
# Line consists of 8 points.
lines = np.array([8] + list(range(8)))
points_and_lines = pv.PolyData(point_coords)
points_and_lines.lines = lines
```



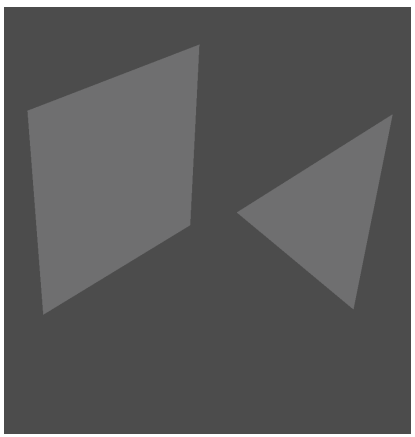
Adding faces

- Similar to lines, faces are described by arrays of the form:

```
[[n, point_index_0, ..., point_index_n-1], # First face
 [...],                                    # Second face
 ...
```

Example

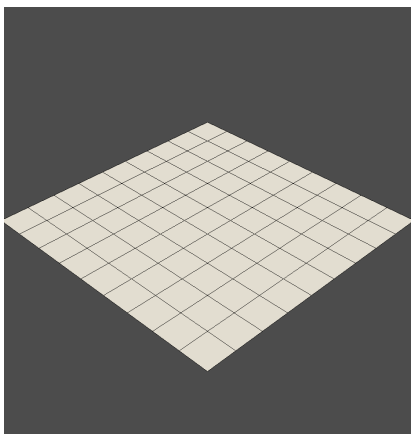
```
faces = np.hstack([[4, 0, 1, 3, 2], # A rectangle
                   [3, 4, 5, 7]],)   # A triangle
# Faces can be passed directly to the constructor.
points_with_faces = pv.PolyData(point_coords, faces)
```



- We could use `PolyData` to represent gridded surfaces, but that is typically too complicated.
- To create a gridded surface it is easier to use the `StructuredGrid` class:

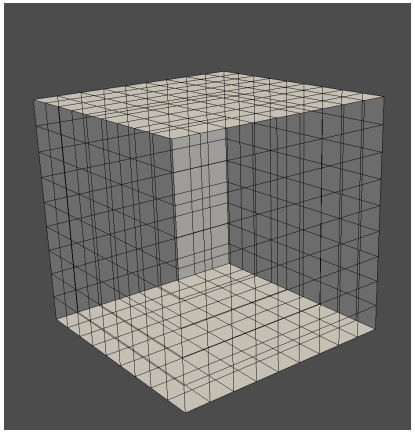
Example

```
x = np.arange(10)
y = np.arange(10)

x_coords, y_coords = np.meshgrid(x, y)
z_coords = np.zeros(x_coords.shape)
surface = pv.StructuredGrid(x_coords, # 10 x 10 array
                            y_coords, # 10 x 10 array
                            z_coords) # 10 x 10 array

plotter = pvqt.BackgroundPlotter()
plotter.add_mesh(surface, show_edges=True)
```



- Similarly, we can use the `StructuredGrid` to represent volumes:

```
x = np.arange(10)
y = np.arange(10)
z = np.arange(10)

x_coords, y_coords, z_coords = np.meshgrid(x, y, z)
volume = pv.StructuredGrid(x_coords, # 10 x 10 x 10 array
                           y_coords, # 10 x 10 x 10 array
                           z_coords) # 10 x 10 x 10 array
plotter = pvqt.BackgroundPlotter()
plotter.add_mesh(volume, show_edges=True)
```



Adding information

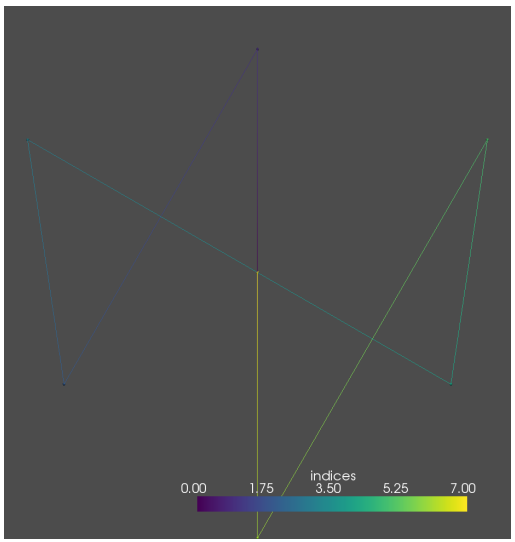
- So far we can represent geometries
- Next we will see how to associate these geometries with data

`PolyData`

- To display information we need to add data arrays to our mesh
- We can do this for each point

Example

```
points = pv.PolyData(point_coords)
points.point_arrays["indices"] = np.arange(8)
points.plot(scalars="indices")
```

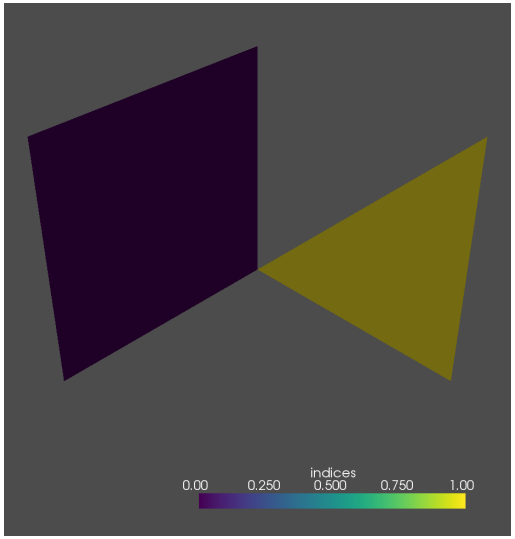


`PolyData`

- Or for each cell

Example

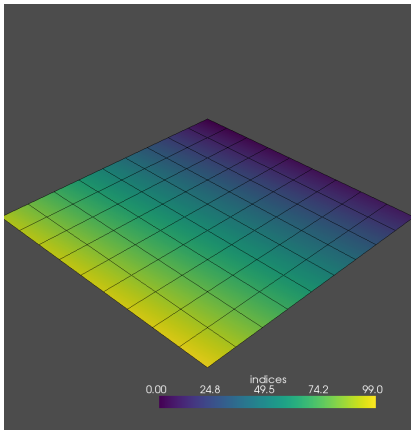
```
faces = np.hstack([[4, 0, 1, 3, 2],
                   [3, 4, 5, 7]],)
points_with_faces = pv.PolyData(point_coords, faces)
points_with_faces.cell_arrays["indices"] = [0, 1]

plotter = pvqt.BackgroundPlotter()
plotter.add_mesh(points_with_faces, scalars="indices")
```



`StructuredGrid`

- Adding data to a structured grid works in the same way

```
x = np.arange(10)
y = np.arange(10)

x_coords, y_coords = np.meshgrid(x, y)
z_coords = np.zeros(x_coords.shape)
surface = pv.StructuredGrid(x_coords, # 10 x 10 array
                            y_coords, # 10 x 10 array
                            z_coords) # 10 x 10 array

surface.cell_arrays["indices"] = np.arange(81)
plotter = pvqt.BackgroundPlotter()
plotter.add_mesh(surface, show_edges=True)
```



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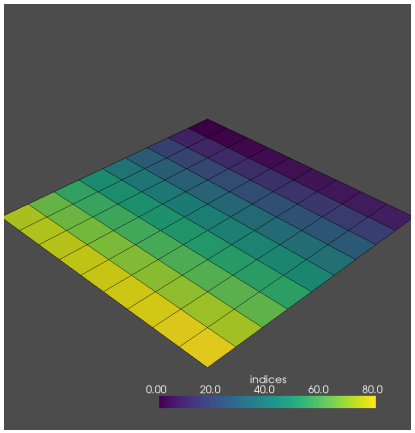
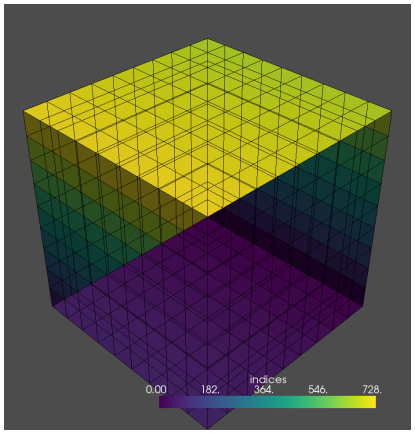


`StructuredGrid`

- Adding data to a 3D `StructuredGrid` works in the same way.

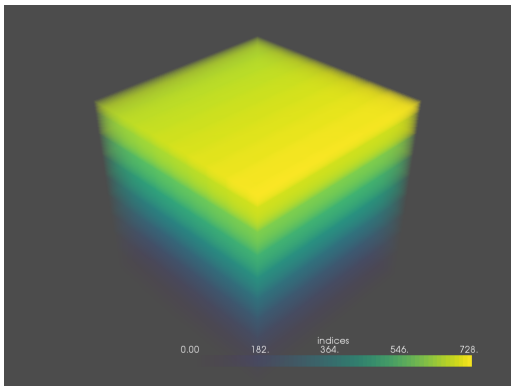
```
x = np.arange(10)
y = np.arange(10)
z = np.arange(10)

x_coords, y_coords, z_coords = np.meshgrid(x, y, z)
volume = pv.StructuredGrid(x_coords,  # 10 x 10 x 10 array
                           y_coords, # 10 x 10 x 10 array
                           z_coords) # 10 x 10 x 10 array

volume.point_arrays["indices"] = np.arange(10 * 10 * 10)
plotter = pvqt.BackgroundPlotter()
plotter.add_mesh(volume, show_edges=True)
```



Volume rendering

- Typically refers to displaying volumetric scalar data using transparency.
- In `pyvista` only works with a `UniformGrid`

```
volume = pv.UniformGrid((21, 21, 21), spacing=(1, 1, 1))
volume.cell_arrays["indices"] = np.arange(20 ** 3)
volume.plot(volume=True)
```



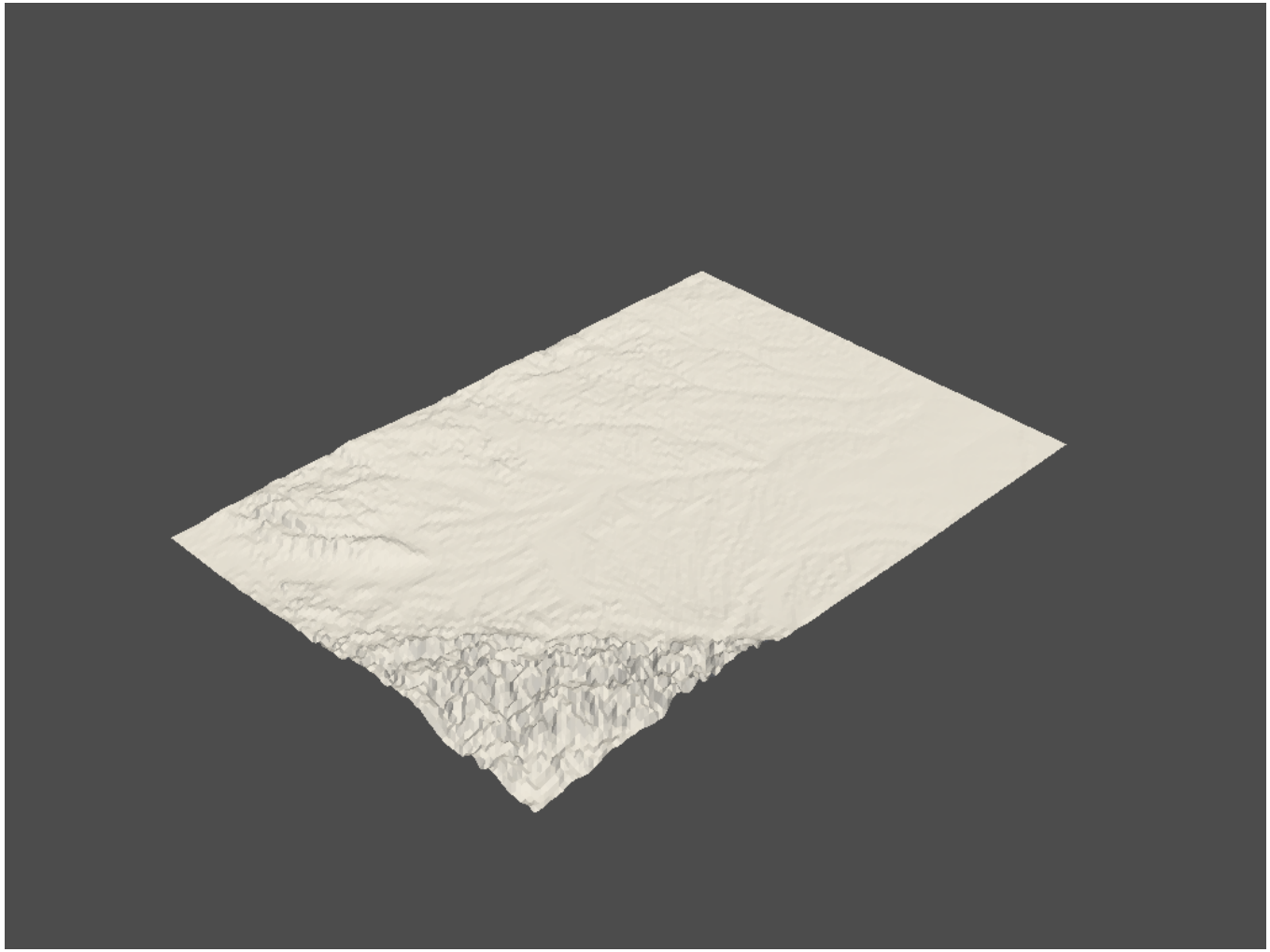
Example: Elevation data

- We can use a 2D mesh to visualize surface elevation:

```
import numpy as np
import matplotlib.pyplot as plt
import pyvista as pv

# Dimensions of the grid data.
dx = 5e3
dy = 5e3
dz = 250

x = dx * np.arange(lats.shape[0])
y = dy * np.arange(lats.shape[1])
x_coords, y_coords = np.meshgrid(x, y, indexing="ij")
elevation = np.load("elevation.npy")

# We scale the z dimensions because surface elevation
# would hardly be visible, otherwise.
z_scaling = 10.0
z_coords = z_scaling * elevation

surface = pv.StructuredGrid(x_coords, # 10 x 10 array
                            y_coords, # 10 x 10 array
                            z_coords) # 10 x 10 array
```

Example: Elevation data

- We can use a 2D mesh to visualize surface elevation:

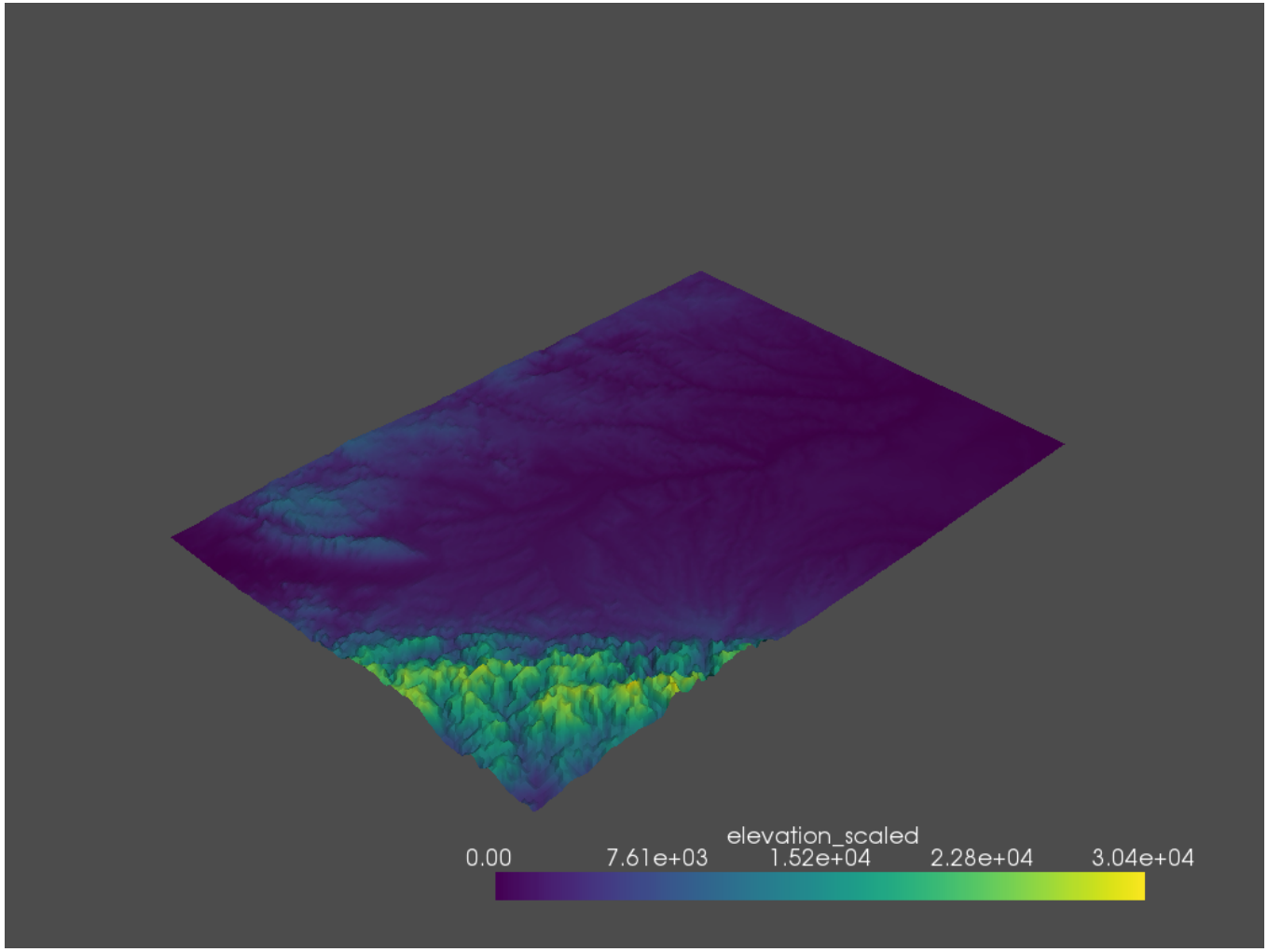


Example: Elevation data

- Anohter way to achieve this is to start with a flat grid and warp it.

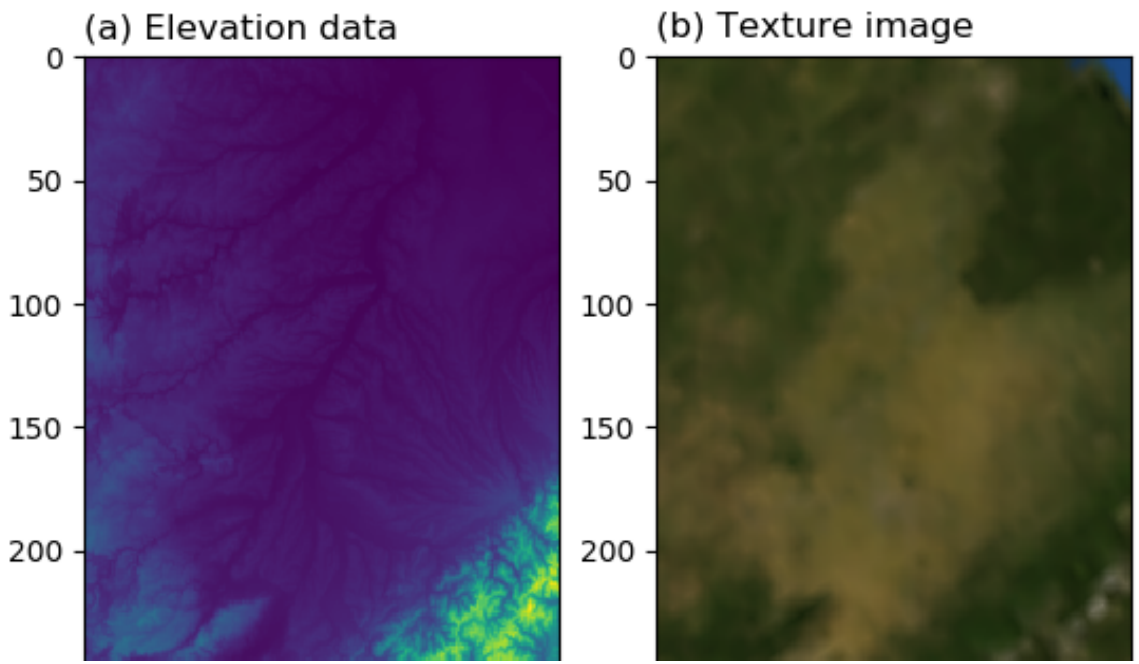
```
nx, ny = lats.shape
surface = pv.UniformGrid((nx, ny, 1),
                         (dx, dy, 1.0))

z_scaling = 10.0
surface.point_arrays["elevation"] = elevation.ravel(order="F")
surface_warped = surface.warp_by_scalar(z_factor * elevation)
```

Example: Elevation data



Textures

- Textures allow displaying image data on a 3-dimensional surface
- For example, we may want to combine the elevation data with realistic surface texture

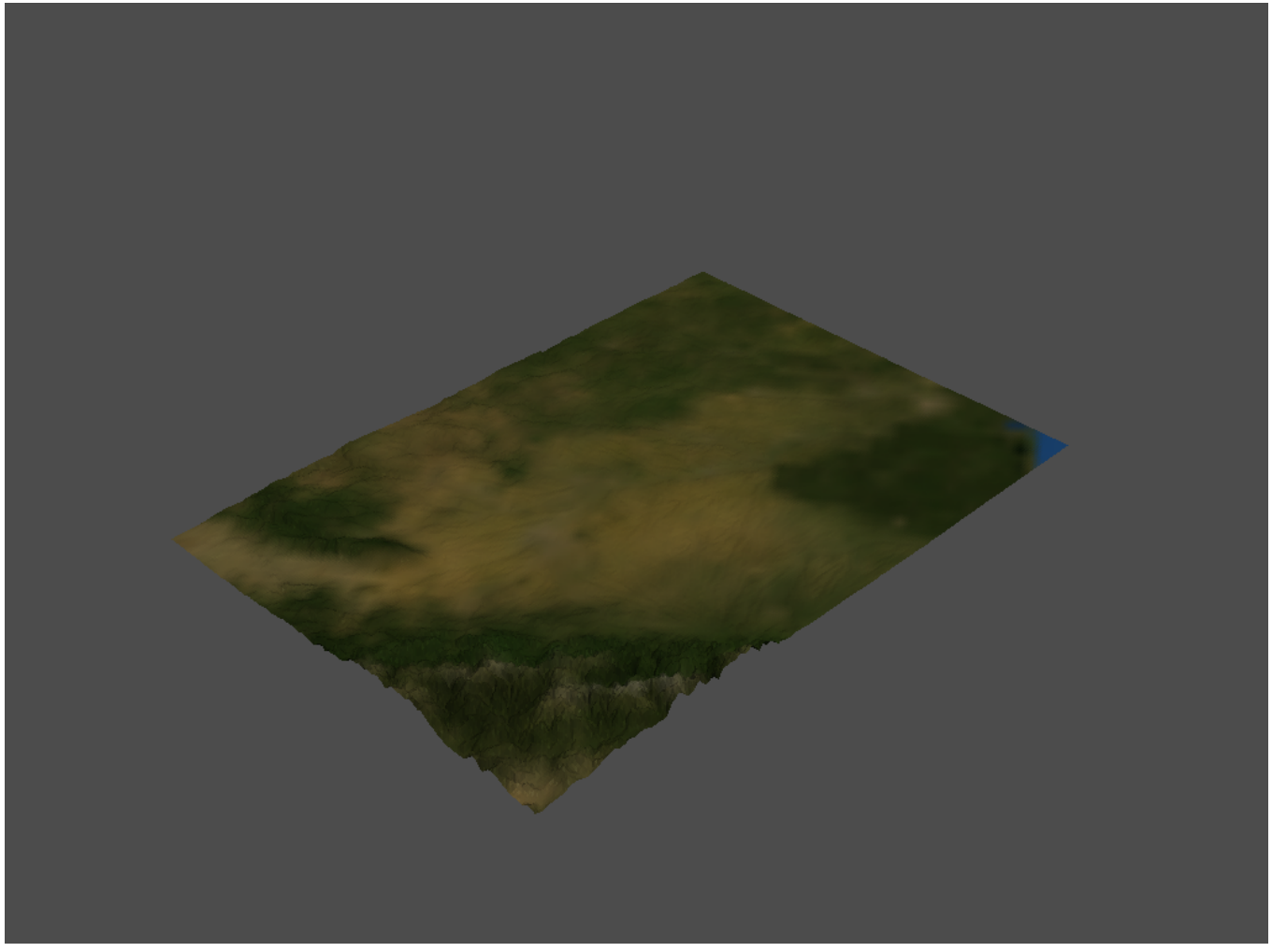


Mapping a texture to a mesh

1. Load texture (typically RGB image)
   - Note that we need to flip the data along the first axis before converting it.
2. Add texture coordinates to mesh.
   - Usually done using `texture_map_to_plane` or `texture_map_to_sphere`
   - Complex geometries may require setting `mesh.t_coords` explicitly
3. Plot mesh with texture.
   - Need to provide `texture` argument to `plot` or `add_mesh`

```
# Step 1: Load texture
texture_image = np.load("texture.npy")
texture = pv.numpy_to_texture(np.flipud(texture_image))

# Step 2: Add texture coordinates to surface.
surface_warped.texture_map_to_plane(inplace=True)

# Step 3: Add texture to mesh
surface_warped.plot(texture=texture)
```

Texture



Combining surface and volume plots

- To render 3D data above the surface, we need to add a new mesh:

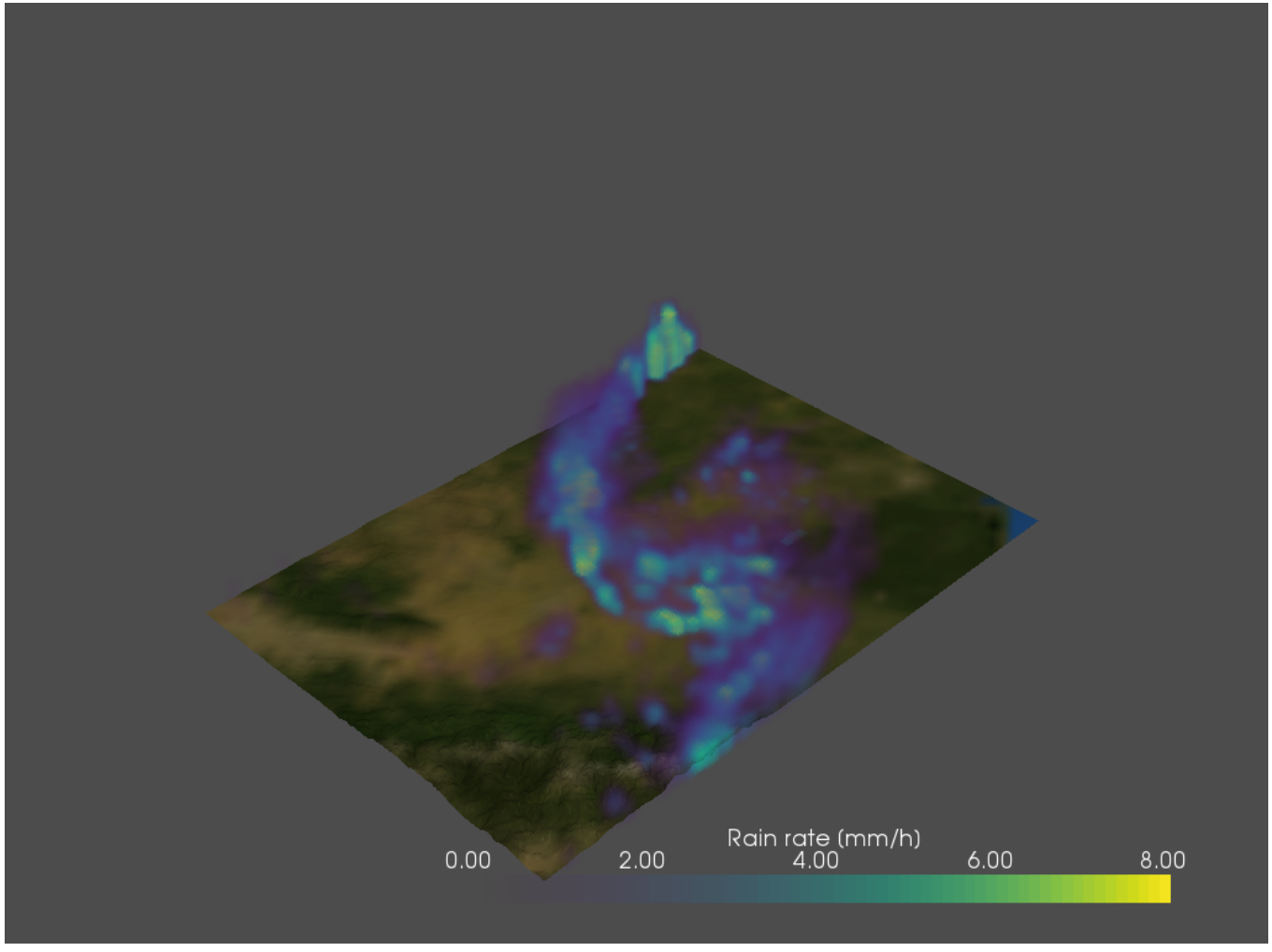
```
precipitation = np.load("precipitation.npy")[:, :, :]
nx, ny, nz = precipitation.shape
volume = pv.UniformGrid((nx + 1, ny + 1, nz + 1),
                        (dx, dy, dz * z_scaling))
volume.cell_arrays["Rain rate [mm/h]"] = np.minimum(precipitation.ravel("F"), 8.0)
```

Combining surface and volume plots

- We can then combine surface and volume in one plot:

```
plotter = pv.Plotter()
plotter.add_volume(volume)
plotter.add_mesh(surface_warped, texture=texture, specular=1)
plotter.show()
```

Result



Summary

- PyVista allows creating advanced 3D visualization in a fairly simple way
- The package is still relatively new and a few things still under development
- For the future: Further integration with web-based viewers will likely make it easier to distribute 3D graphics and animations.