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Los Alamos NATIONAL LABORATORY

Using ParaView to Visualize MCNP6 Fission Matrix Eigenmodes

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Introduction

- This presentation will demonstrate how to generate MCNP6 [1] fission matrix eigenmodes for a nuclear reactor, which includes:
  - Using the KOPTS and HSRC card in MCNP6
  - Using h5py to parse the MCNP6 runtape.h5
  - Using Python to compute the eigenvalues and eigenvectors of the fission matrix, and to generate a VTI file
- This presentation will also demonstrate how to use ParaView to visualize the eigenvectors, stored in the VTI file
- The Texas A&M University Nuclear Science Center Reactor (NSCR) was used as an example

Theory: the MCNP6 fission matrix equation

The k-eigenvalue transport equation can be expressed as

$$\widehat{M}\psi\left(\vec{r},\widehat{\Omega},E\right)=\frac{1}{k}\frac{\chi(E)}{4\pi}S(\vec{r})$$

where $\widehat{M}$ is the migration operator (which includes streaming collision, and scattering) and $\boldsymbol{S(\vec{r})}$ **is the fission source** [2][3][4]

A fission-matrix eigenvalue equation can be derived via spatial discretization

$$kS_i=\sum_j^J F_{ij}S_j$$

where F_{ij} is a component of the fission matrix, which indicates the probability that a **fission neutron born in region *j*** leads to the production of a **fission neutron in region *i***

The KOPTS and HSRC cards

- Adding the following KOPTS card to an MCNP6 input deck will instruct MCNP6 to compute the fission matrix

```
KOPTS FMAT=yes
```

- The fission matrix will be evaluated for the spatial grid that is provided by the HSRC card

```
HSRC nx xmin xmax ny ymin ymax nz zmin zmax
```

- Note, the KOPTS and HSRC cards are meant to be used in conjunction with the KCODE card

Python scripts for creating VTI file (1/2) fission_matrix_eigs.py

Imports the other Python script

The **h5py** Python package is used to extract fission matrix data from the MCNP6 runtape.h5 file

The **SciPy** Python package is used to compute eigenvalues and eigenvectors

Eigenmodes are saved to a **VTI** file

```python
import h5py
import numpy as np
import scipy.sparse as sparse
import scipy.sparse.linalg as sla
import convert_numpy_to_vtk
SUPPORTED_RUNTAPES = ([1, 0, 0], [1, 0, 1])
#-----------------------------------------------------------------------
def extract_fmat(runtape: str):
    """Returns the last saved fission matrix as a scipy.sparse.csr_matrix"""
    with h5py.File(runtape, "r") as handle:
        version_file = handle["config_control"].attrs["version_file"]
        if any(SUPPORTED_RUNTAPES[0] != version_file) and any(SUPPORTED_RUNTAPES[1] != version_file):
            print("Warning: possibly incompatible runtape detected.")
        fmat = handle["results/fission_matrix"]
        n_dim = fmat["n"][()]
        indices = fmat["indices"][:]
        indptr = fmat["indptr"][:]
        data = fmat["data"][:]
        n_xyz = fmat["n_xyz"][:]
        delta_xyz = fmat["delta_xyz"][:]
        origin = fmat["origin"][:]
    return (sparse.csr_matrix((data, indices, indptr), shape=(n_dim, n_dim)),
        n_xyz, delta_xyz, origin)
#-----------------------------------------------------------------------
def get_eigs(matrix, n_xyz, n_tot=30):
    """Retrieve eigenvalues/eigenvectors, sort, reshape to 3D"""
    eigenvalues, eigenvectors = sla.eigs(matrix, k=n_tot)
    indices = np.argsort(-np.abs(eigenvalues))
    sorted_eigvals = np.sort(eigenvalues[indices].real)[::-1]
    sorted_eigvecs = [eigenvectors[:, i].reshape(n_xyz[::-1]).transpose().real for i in indices]
    sorted_eigvecs[0] = np.abs(sorted_eigvecs[0])
    return sorted_eigvals, sorted_eigvecs
#-----------------------------------------------------------------------
def eigs_to_vti_file(origin, delta_xyz, eigvals, eigvecs, output_file: str):
    """Generate VTI file containing eigenvalues/eigenvectors"""
    data_dict = dict()
    for i, eigval in enumerate(eigvals):
        data_dict[f'{i} eigenmode, eigenvalue = {eigval}'] = eigvecs[i]
    convert_numpy_to_vtk.image_data_to_vti_file(origin, delta_xyz, data_dict, output_file)
#-----------------------------------------------------------------------
fission_matrix, n_xyz, delta_xyz, origin = extract_fmat("nscr.r.h5")
eigvals, eigvecs = get_eigs(fission_matrix, n_xyz, n_tot=30)
eigs_to_vti_file(origin, delta_xyz, eigvals, eigvecs, "nscr_eigs.vti")
```

** adapted from [4]*

Python scripts for creating VTI file (2/2)

convert_numpy_to_vtk.py

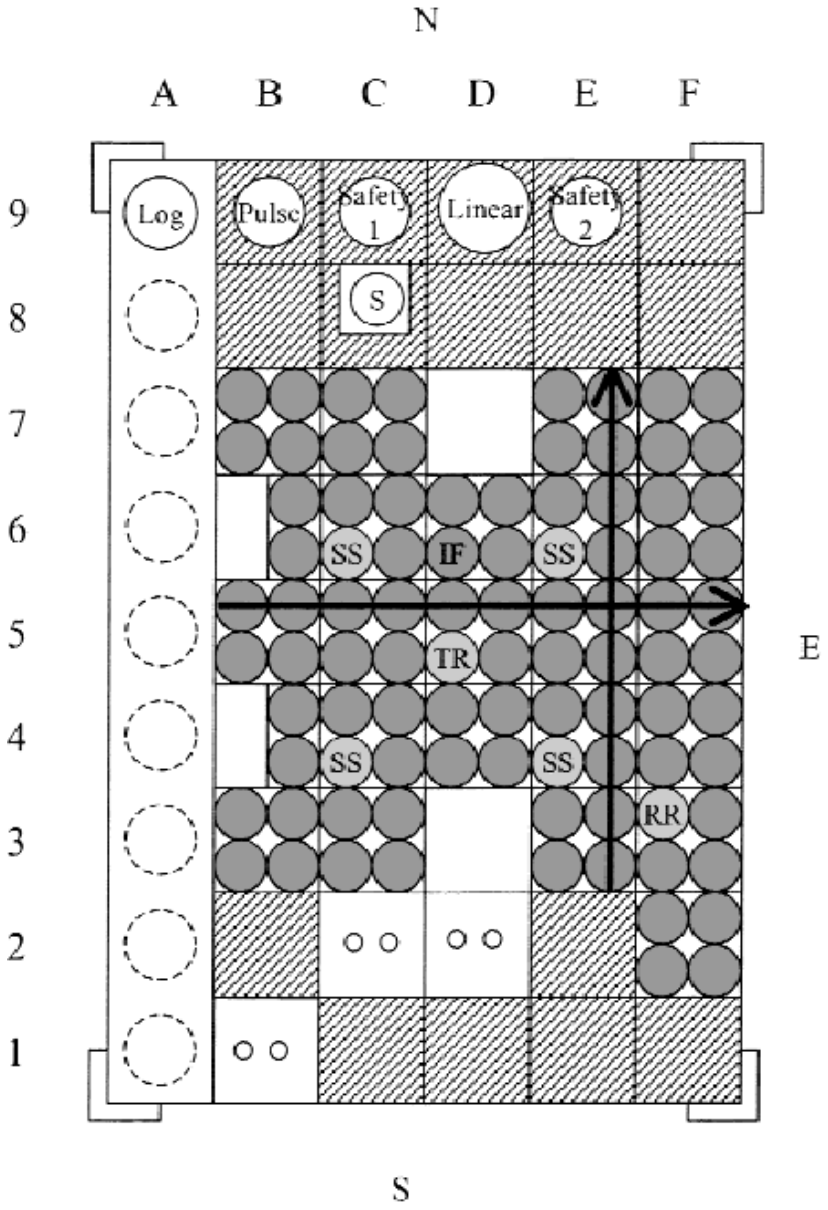
Writes a VTI **file**

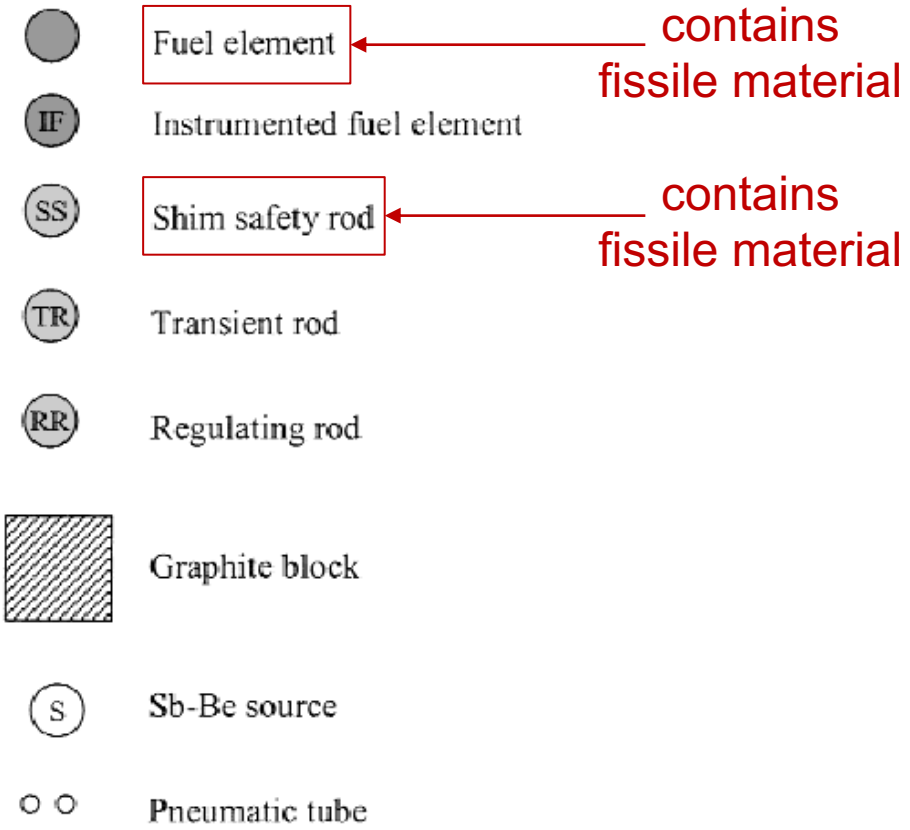
Uses image data, stored as NumPy arrays and dictionaries, and converts them in a VTI **object**

Combines the two functions above to produce a VTI **file**

```
import vtk
import vtk.util.numpy_support as numpy_support
#-----------------------------------------------------------------------------
def write_vti_file(vti, output_file: str):
    """Write VTI file"""
    writer = vtk.vtkXMLImageDataWriter()
    writer.SetFileName(output_file)
    writer.SetInputData(vti)
    writer.Write()
#-----------------------------------------------------------------------------
def image_data_to_vti_object(origin, spacing, data_dict: dict):
    """Convert image data stored as numpy arrays to a VTI object"""
    assert len(origin) == 3
    assert len(spacing) == 3
    vti = vtk.vtkImageData()
    vti.SetOrigin(origin[0], origin[1], origin[2])
    vti.SetSpacing(spacing[0], spacing[1], spacing[2])
    for field_name, data in data_dict.items():
        vti.SetDimensions(data.shape[0]+1, data.shape[1]+1, data.shape[2]+1)
        vtk_data = numpy_support.numpy_to_vtk(num_array=data.transpose().flatten(),
            deep=True, array_type=vtk.VTK_FLOAT)
        vtk_data.SetName(field_name)
        vti.GetCellData().AddArray(vtk_data)
    return vti
#-----------------------------------------------------------------------------
def image_data_to_vti_file(origin, spacing, data_dict: dict, output_file: str):
    """Convert image data stored as numpy arrays to a VTI file"""
    vti = image_data_to_vti_object(origin, spacing, data_dict)
    write_vti_file(vti, output_file)
#-----------------------------------------------------------------------------
```

Nuclear Science Center Reactor (NSCR) Layout



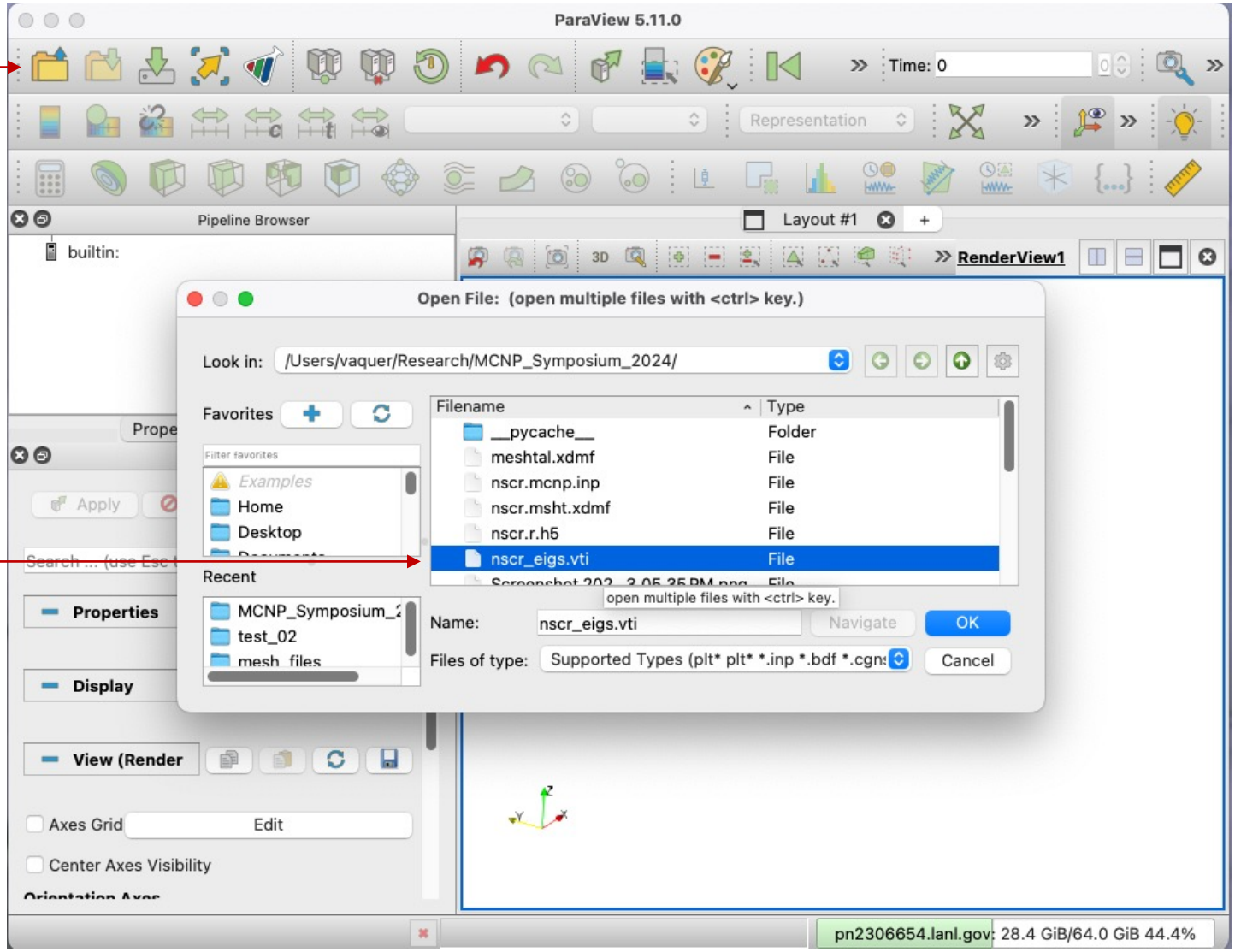


* *image from [5]*

Opening the VTI file with ParaView

Click to open file

Select VTI file



Plot of the 0th eigenmode (k_0=1.005) with ParaView

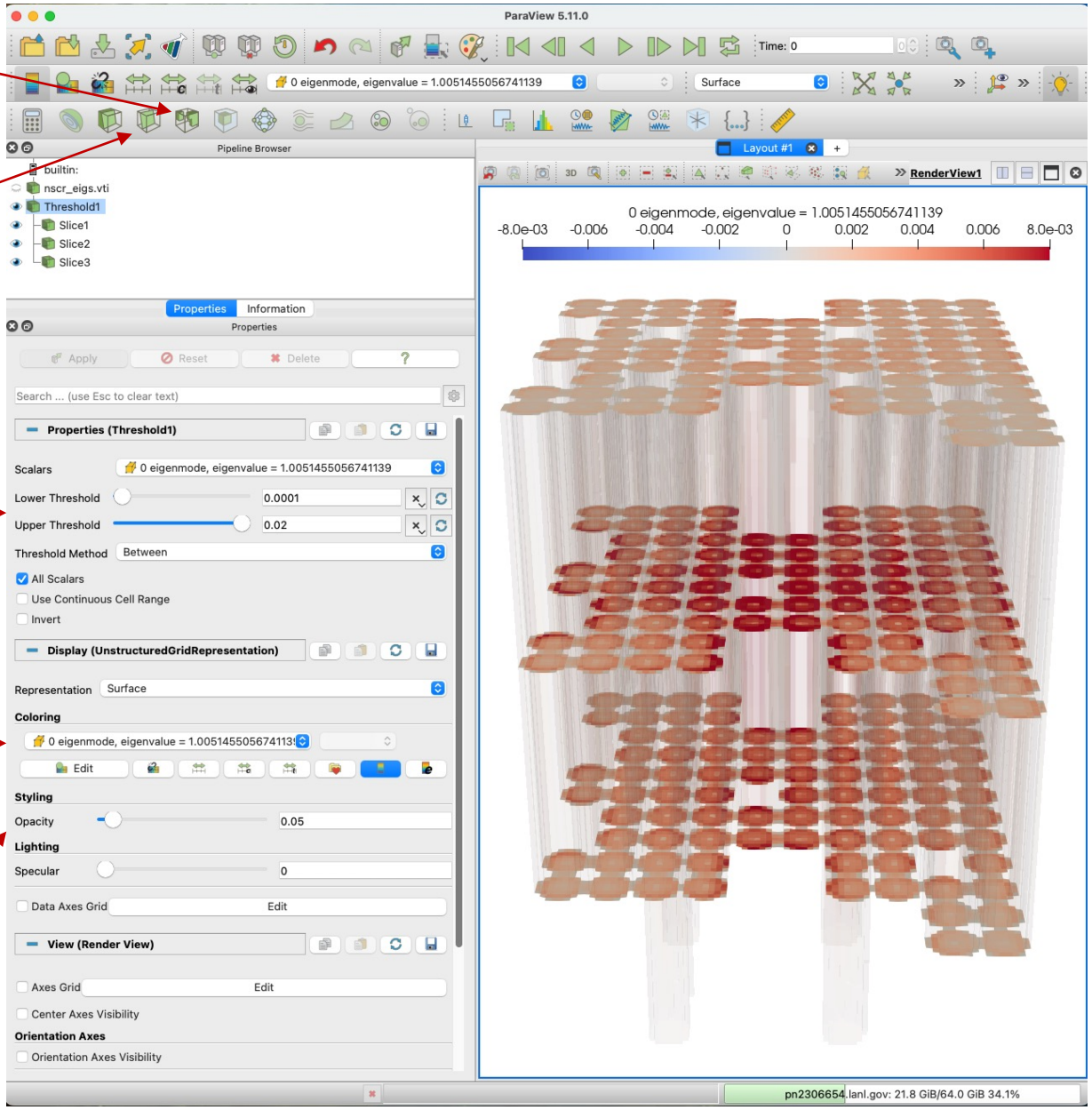
Add a threshold

Add multiple slices along Z dimension

Vary threshold values here

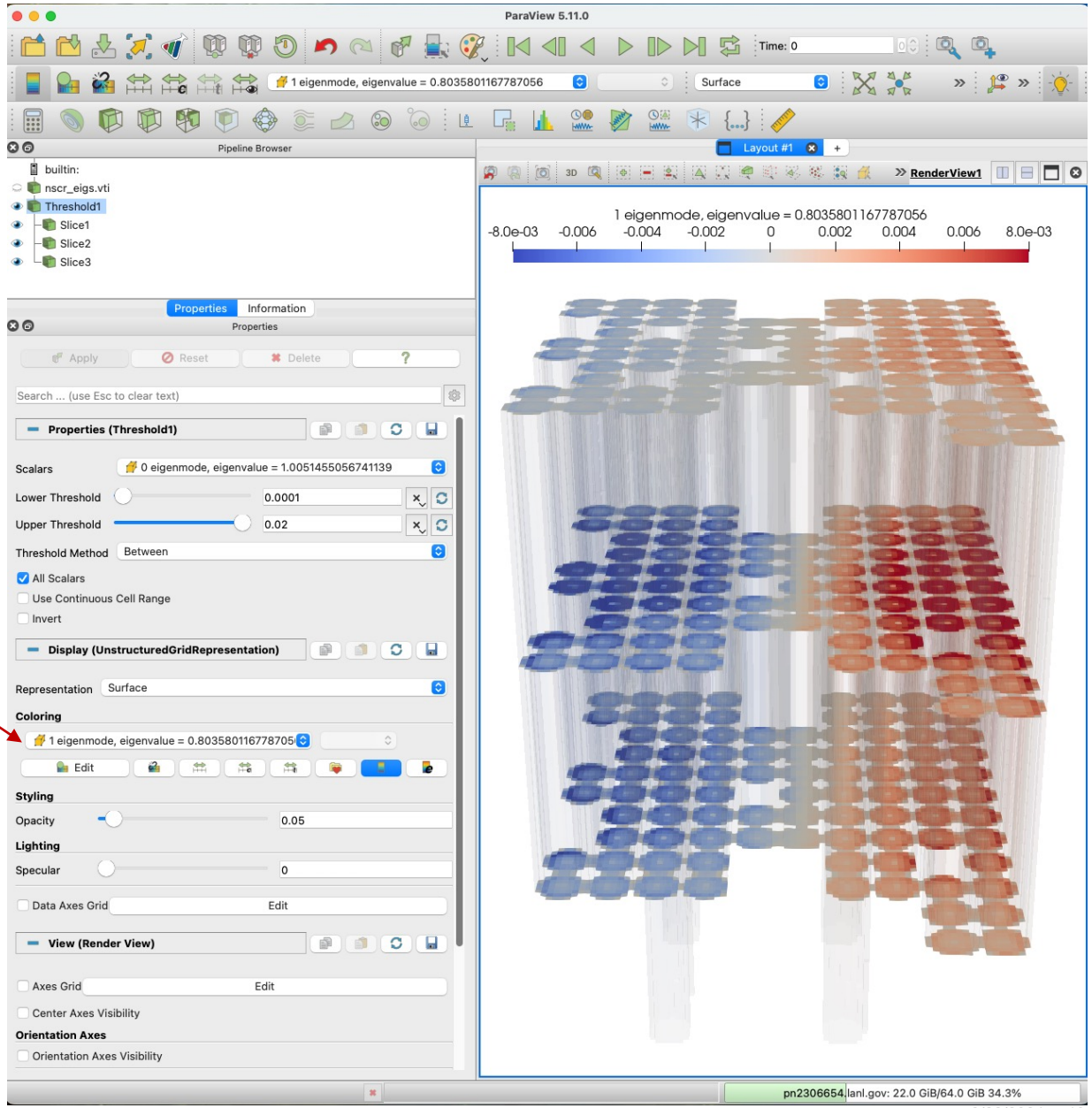
Select 0th eigenmode

Vary opacity here



Plot of the 1st eigenmode (k_1=0.804) with ParaView

Select 1st eigenmode (this must be done for all slices)



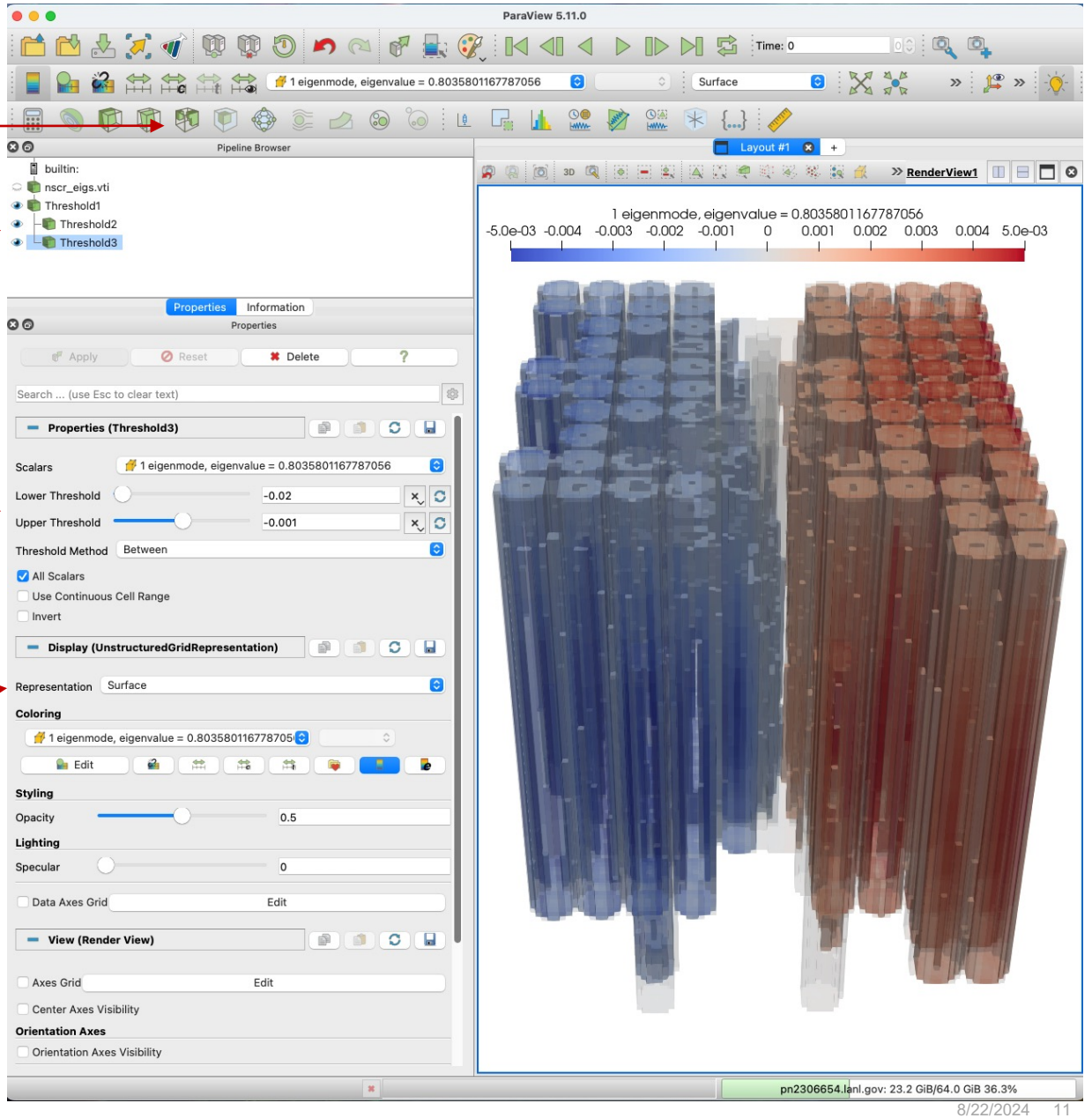
Alternative plot of the 1st eigenmode (k_1=0.804)

Add separate thresholds for negative and positive values

Vary threshold values here

Many other representations can be plotted:

- points
- wireframes
- volumes



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