Learning SciPy for Numerical and Scientific Computing

Francisco Blanco-Silva

University of South Carolina

Some Basic Principles in Scientific Computing

A personal perspective

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- Trust the Computer Scientist: Writing low-level code from scratch seldom guarantees best results.
- Find a reliable way to communicate through software.
- Big guns: Solving these problems usually require massive amounts of calculations and are often executed on supercomputers or distributed computing platforms.

Computational Resources

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- Optimized Algebra Libraries
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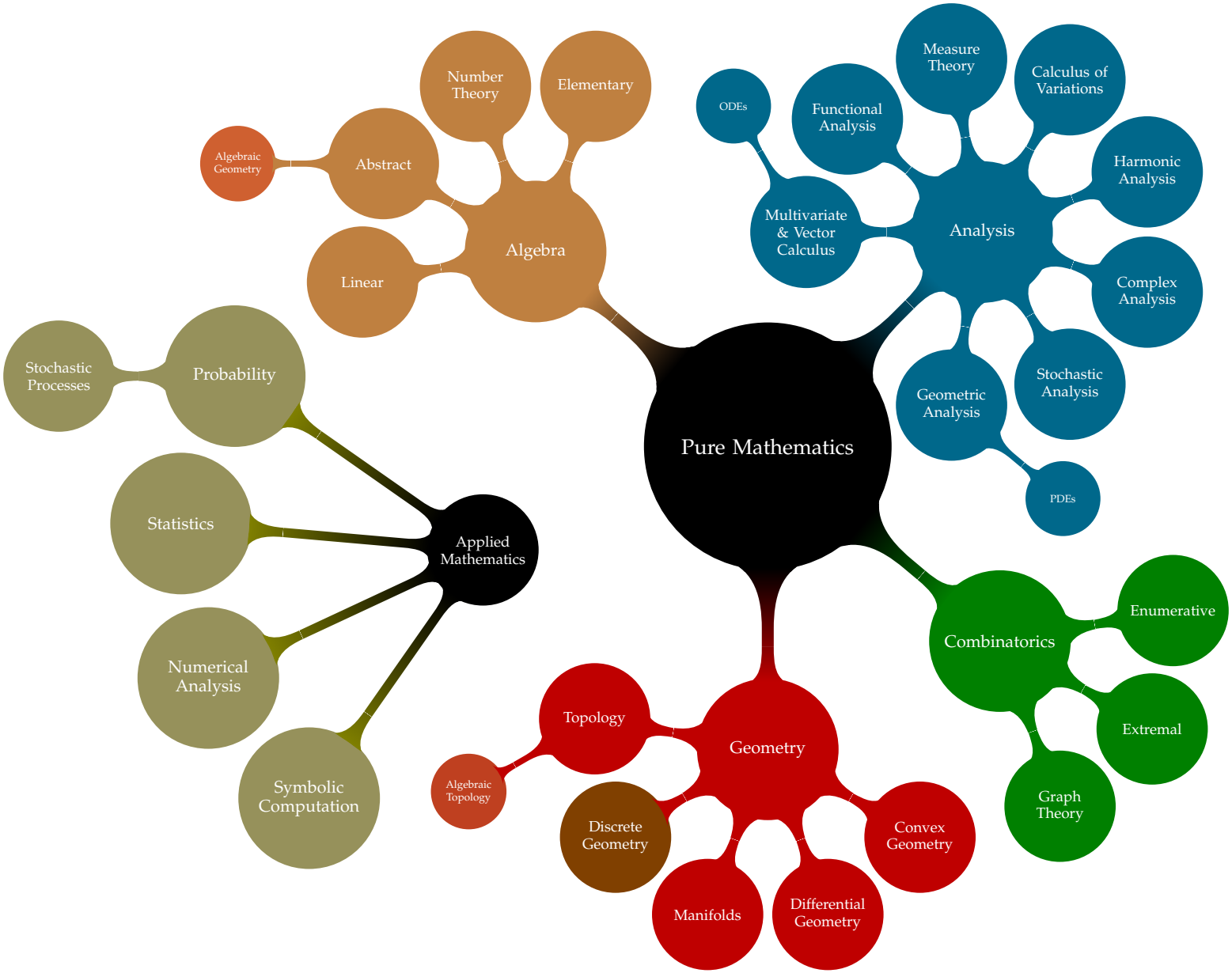
  - Python
    - with PyLab: ipython + NumPy + **SciPy** + matplotlib
    - with scikits and Pandas on top of that

The Structure of SciPy

Similarity to the different areas of Mathematics



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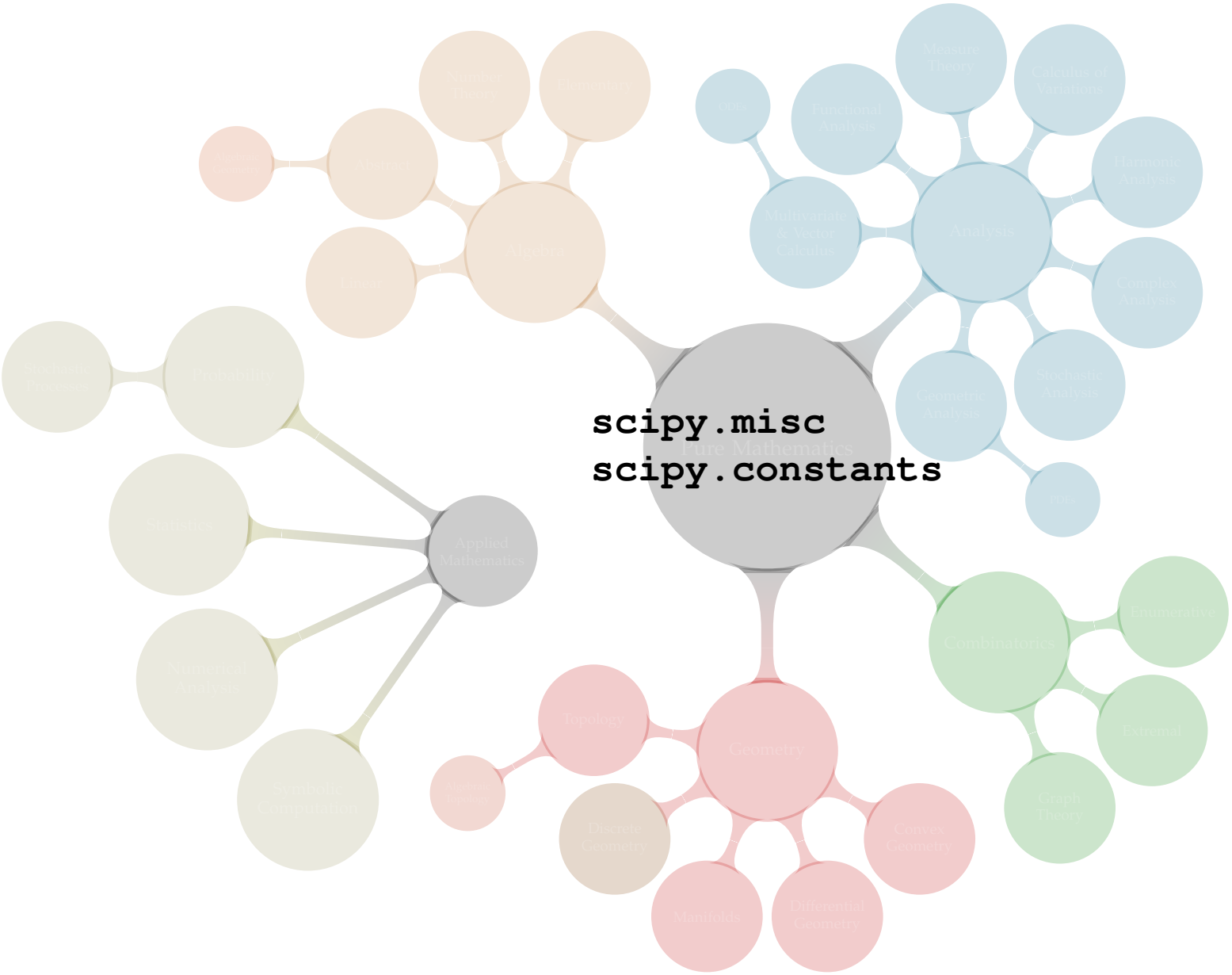

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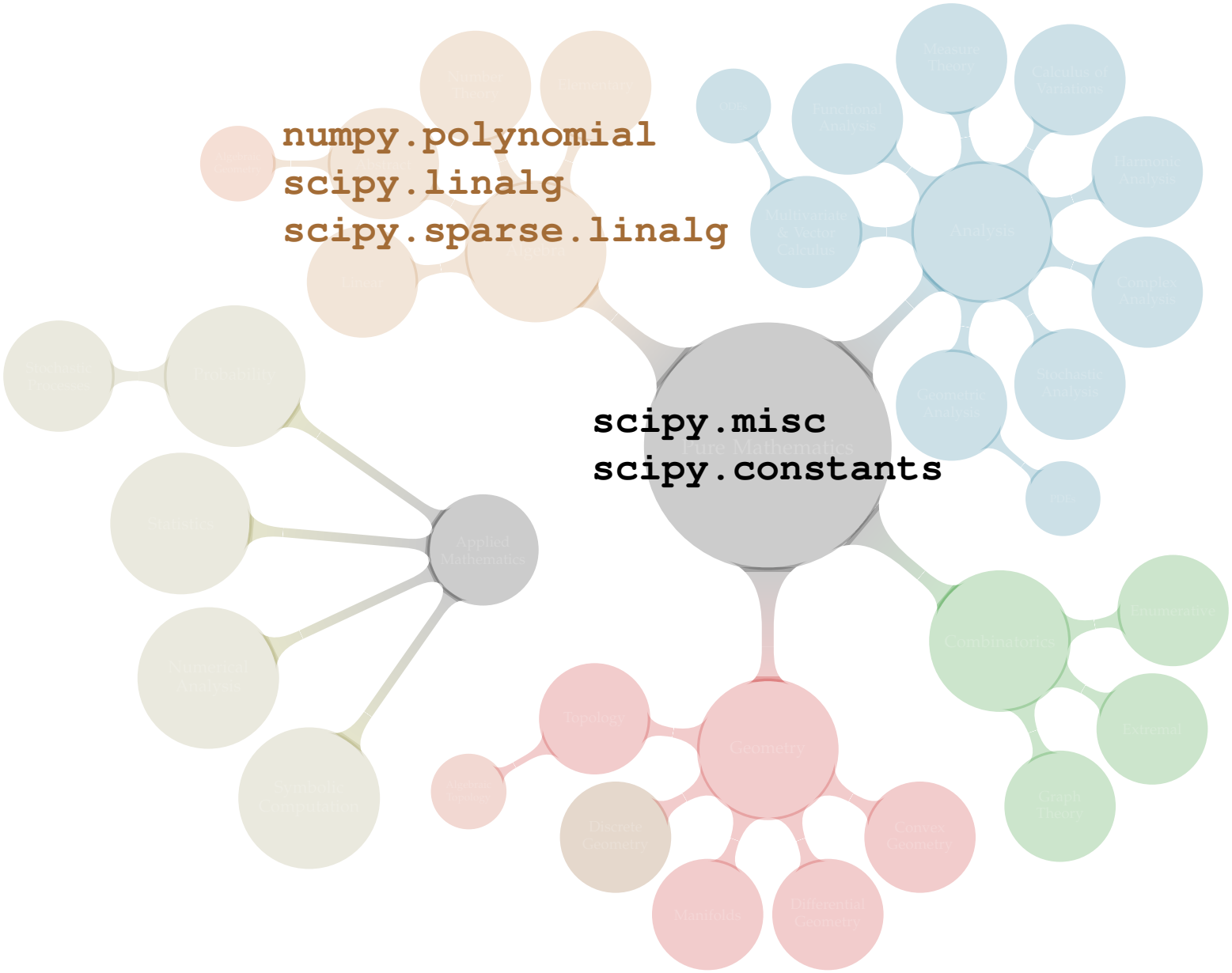

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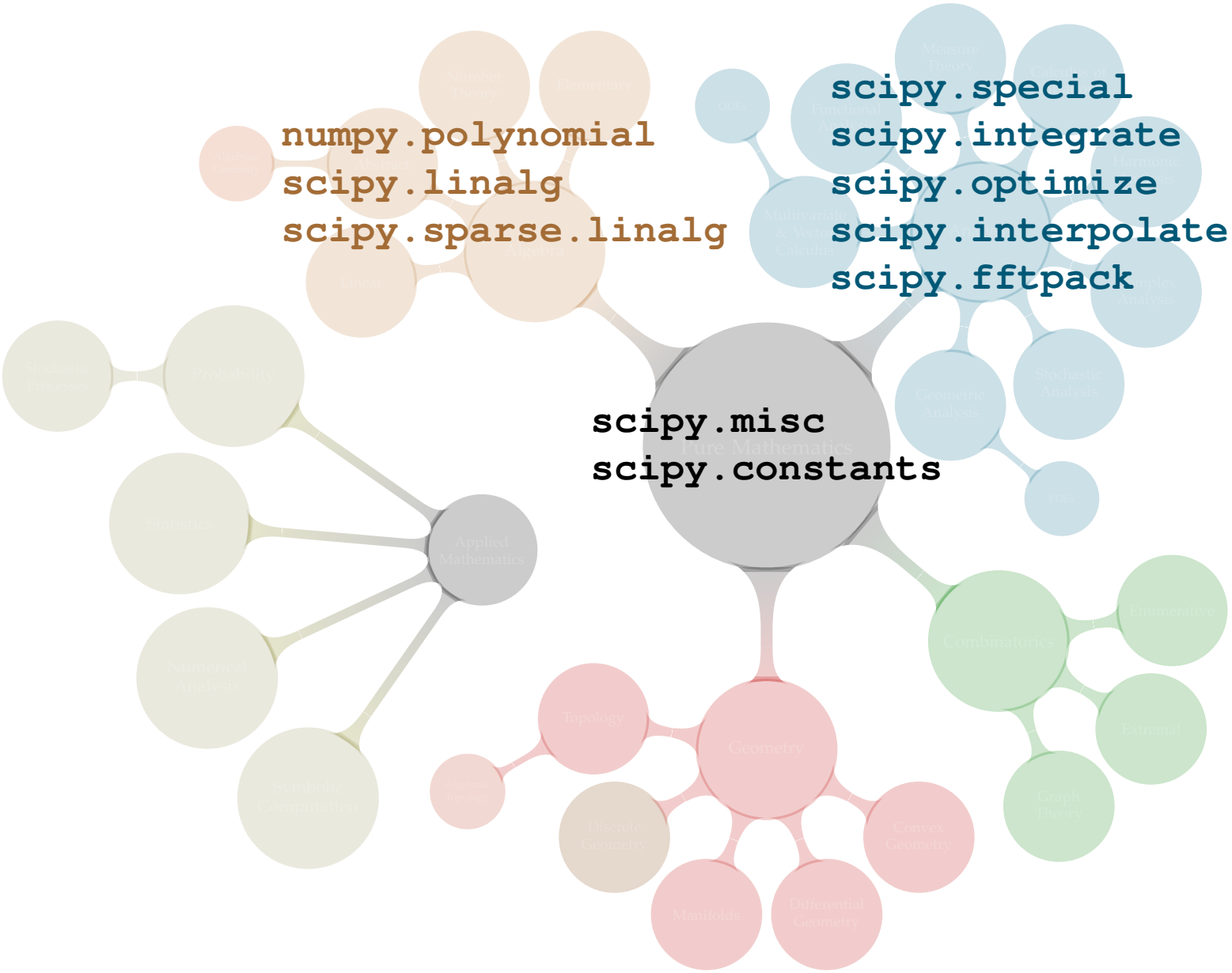

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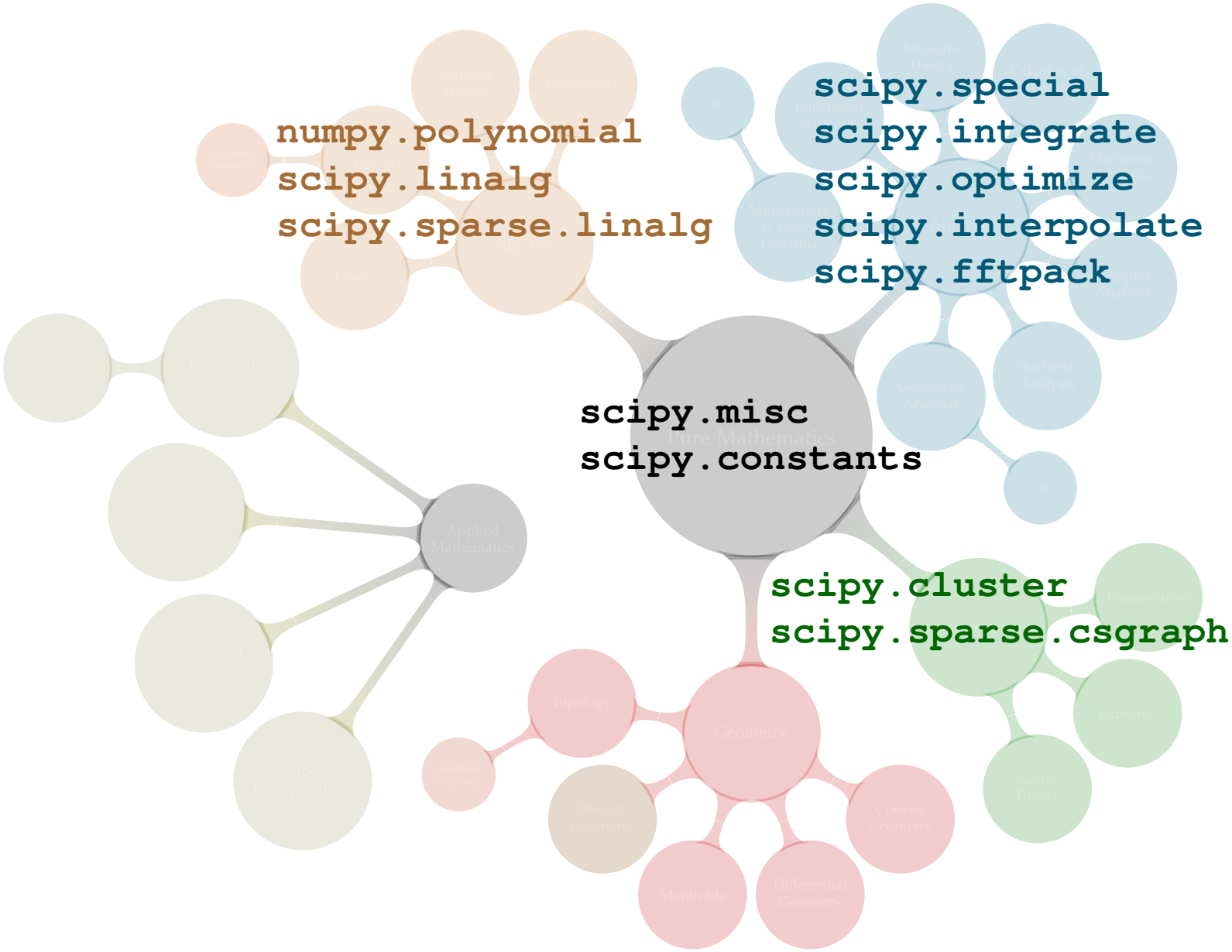

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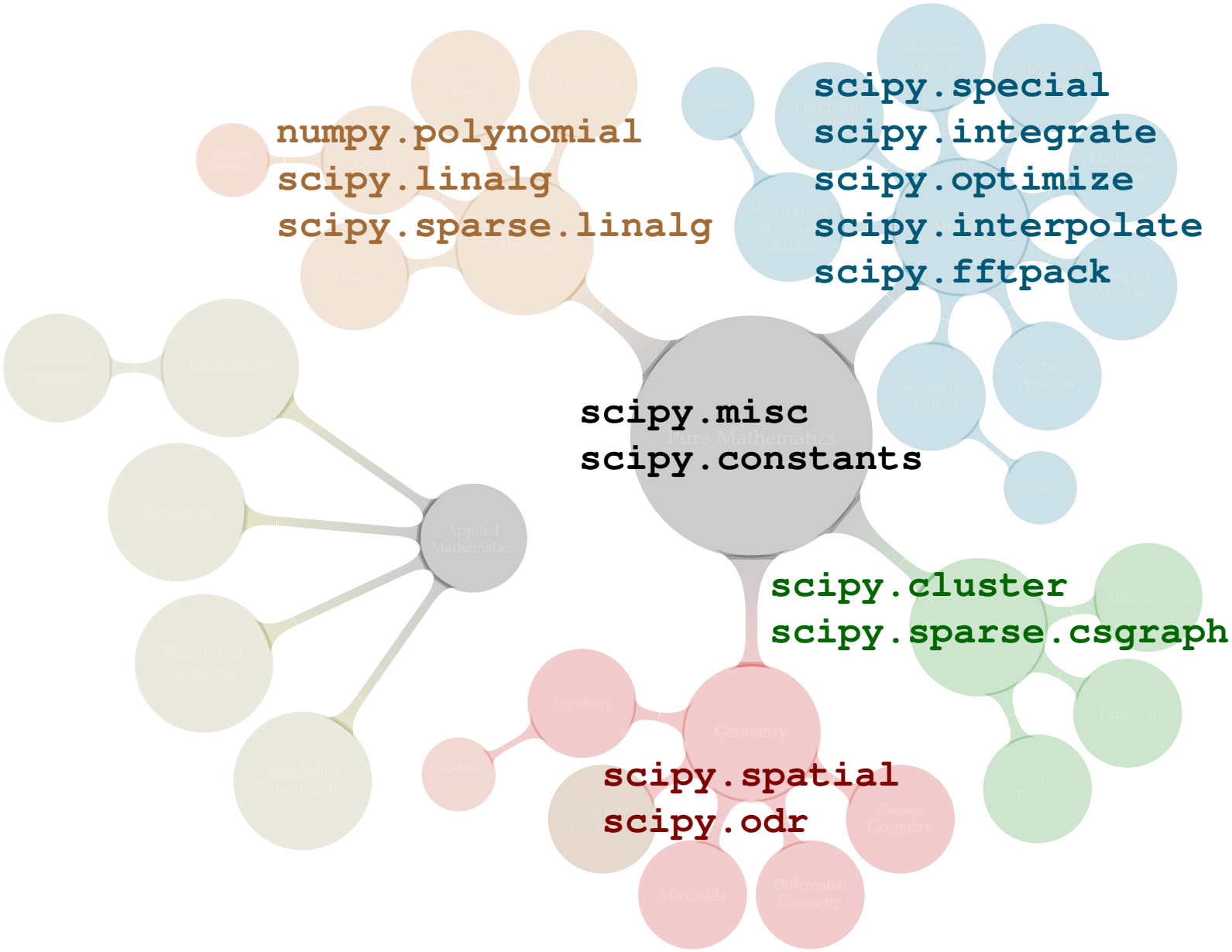

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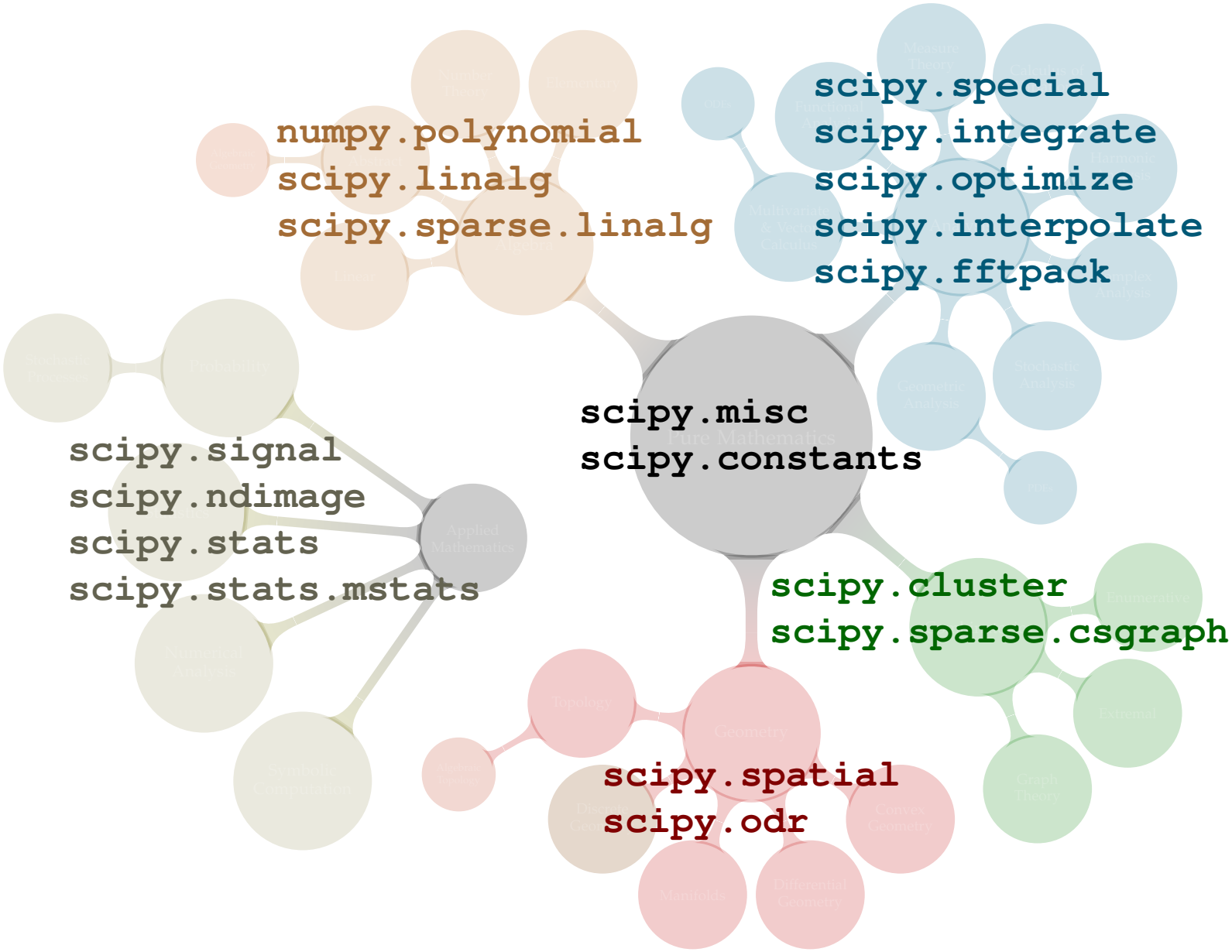
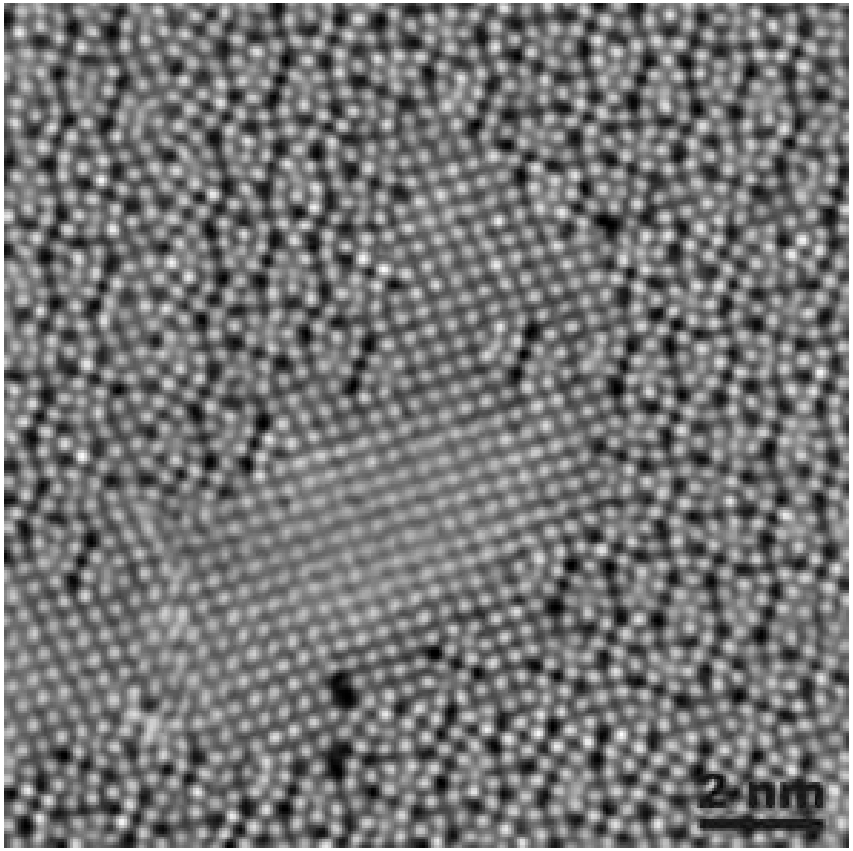


SciPy in action

Extract the structural model of a molecule of $Nb_4W_{13}O_{47}$



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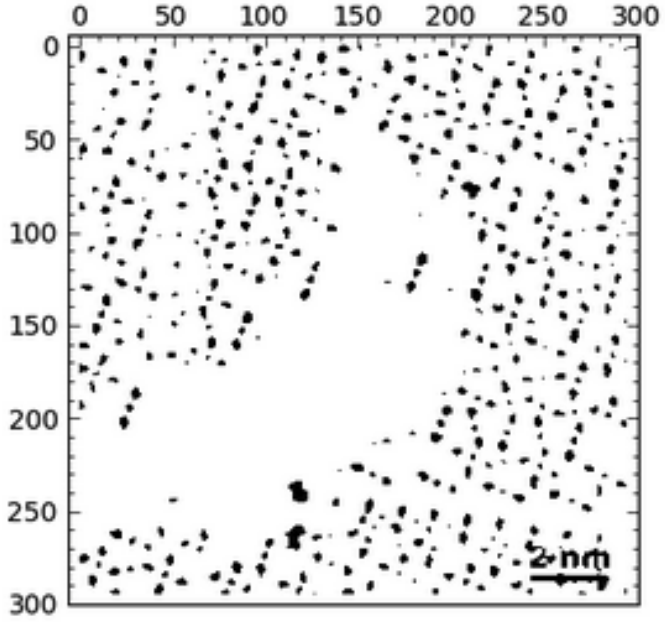
Computation of structural models

We take the following (naïve) approach:

- Segmentation of the atoms by thresholding and morphological operations.



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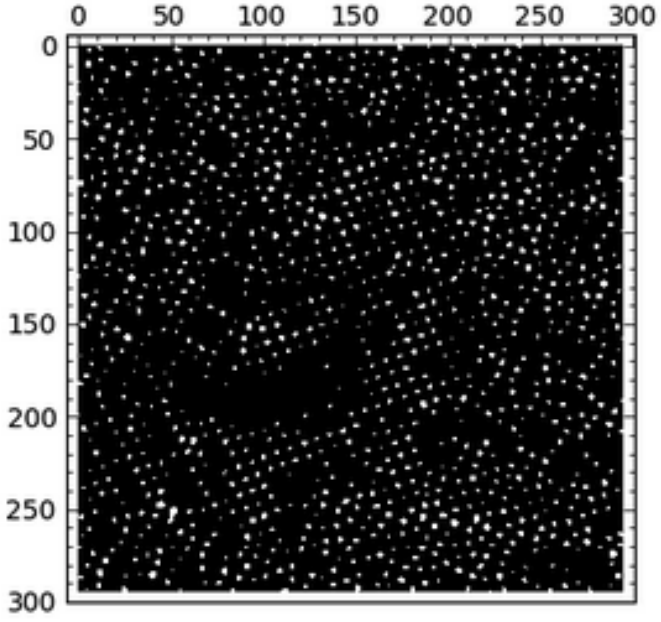

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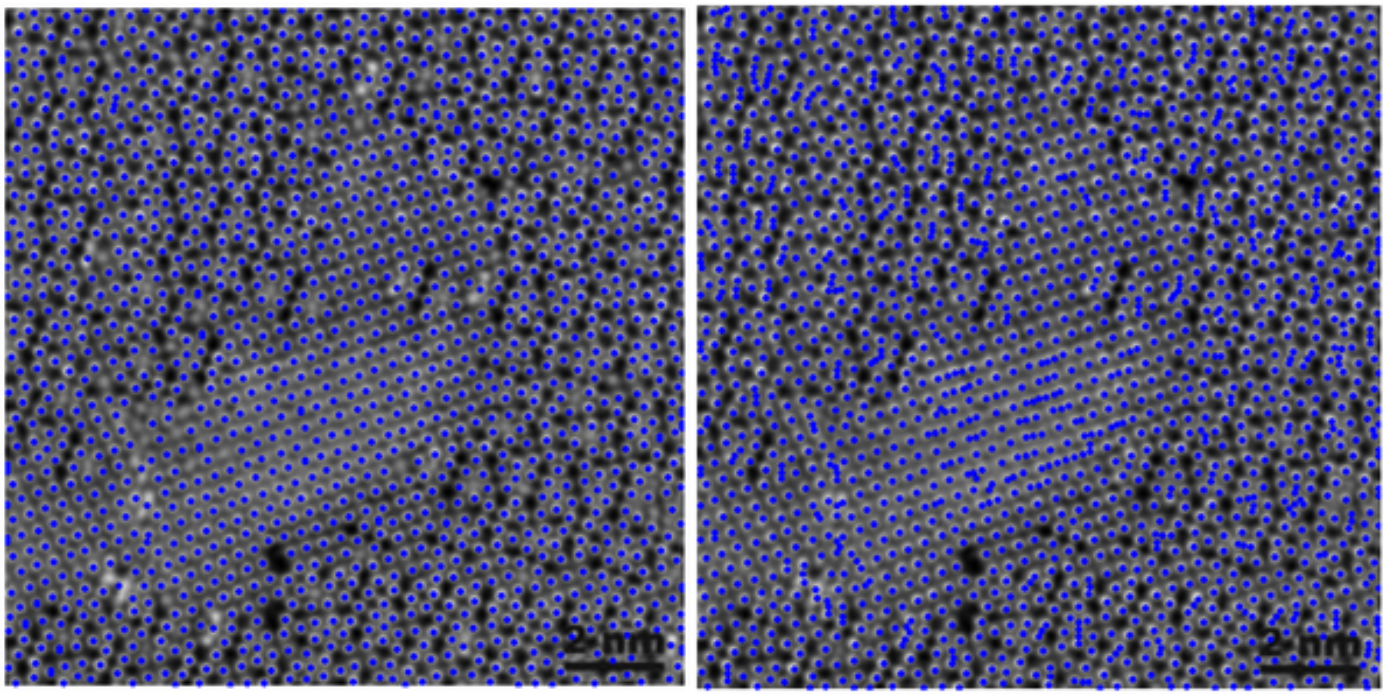

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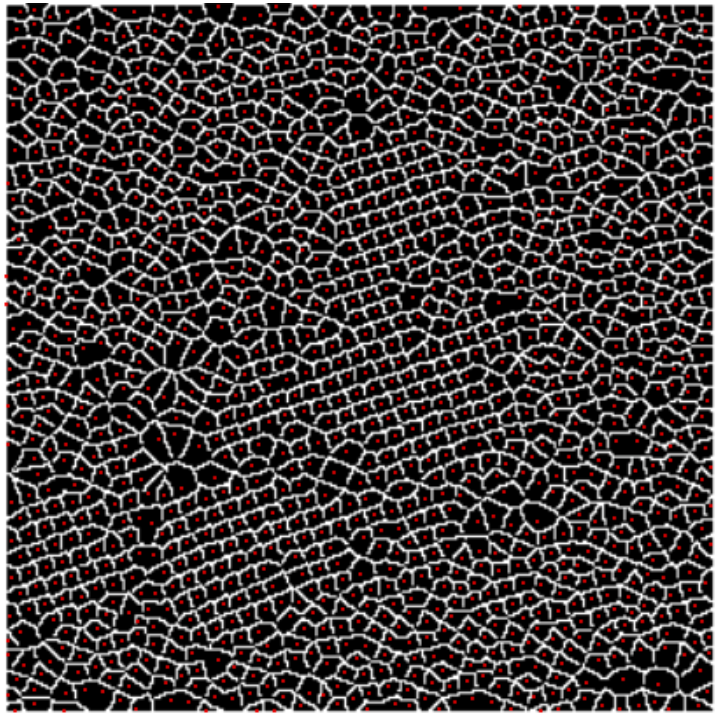
We take the following (naïve) approach:

- Segmentation of the atoms by thresholding and morphological operations.
- Connected component labeling to extract each atom for posterior examination.
- Computation of the centers of mass of each label identified as an atom.
- Computation of the Voronoi diagram of the lattice formed by the previous points.



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Computation of structural models

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# Preamble
import numpy
import scipy
from scipy.ndimage import binary_opening, label, center_of_mass,
     distance_transform_edt
# Load the image
img = scipy.misc.imread('NbW-STEM.png')
# Apply a threshold to segment atoms
BWatoms = (img > 0.62)
# Perform a binary operation to eliminate outliers
BWatoms = binary_opening(BWatoms, structure=numpy.ones((2,2)))
# Segmentation of each atom
structuring_element = [[0,1,0],[1,1,1],[0,1,0]]
segmentation,segments = label(BWatoms, structuring_element)
# Computation of centers of mass of each atom
coords = center_of_mass(img, segmentation, range(1,segments+1))
xcoords = array([x[0] for x in coords])
ycoords = array([x[1] for x in coords])
# Compute the Voronoi diagram of the lattice
L1, L2 = distance_transform_edt(segmentation==0, return_distances=False,
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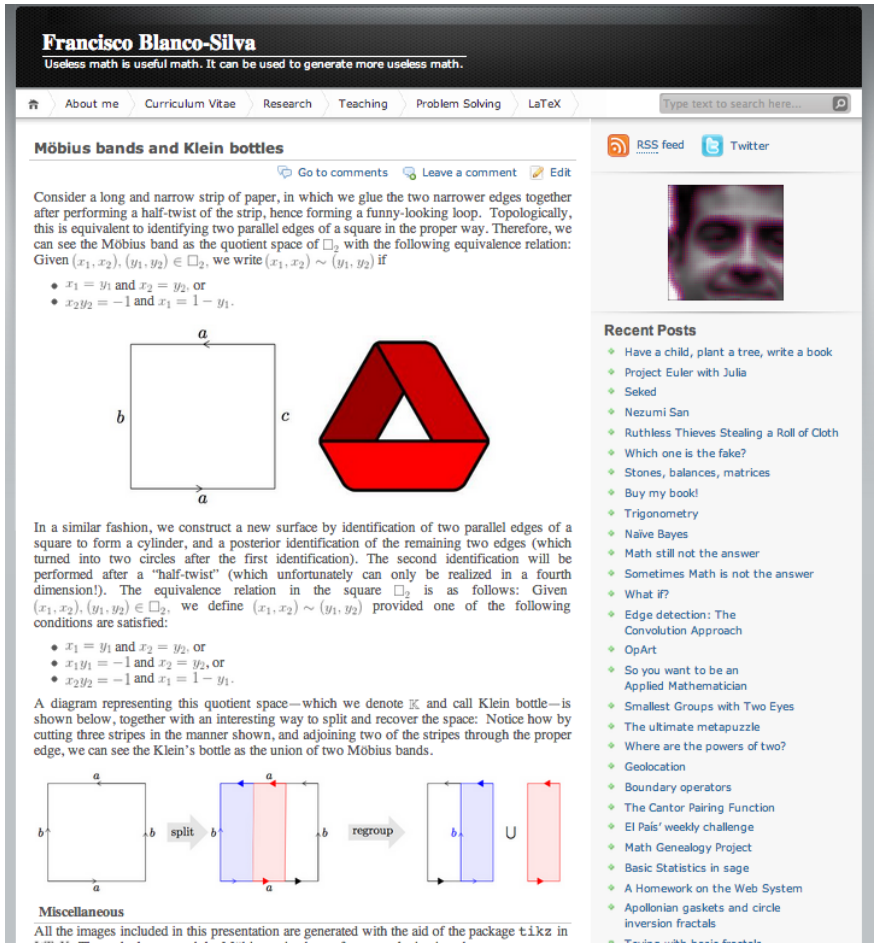

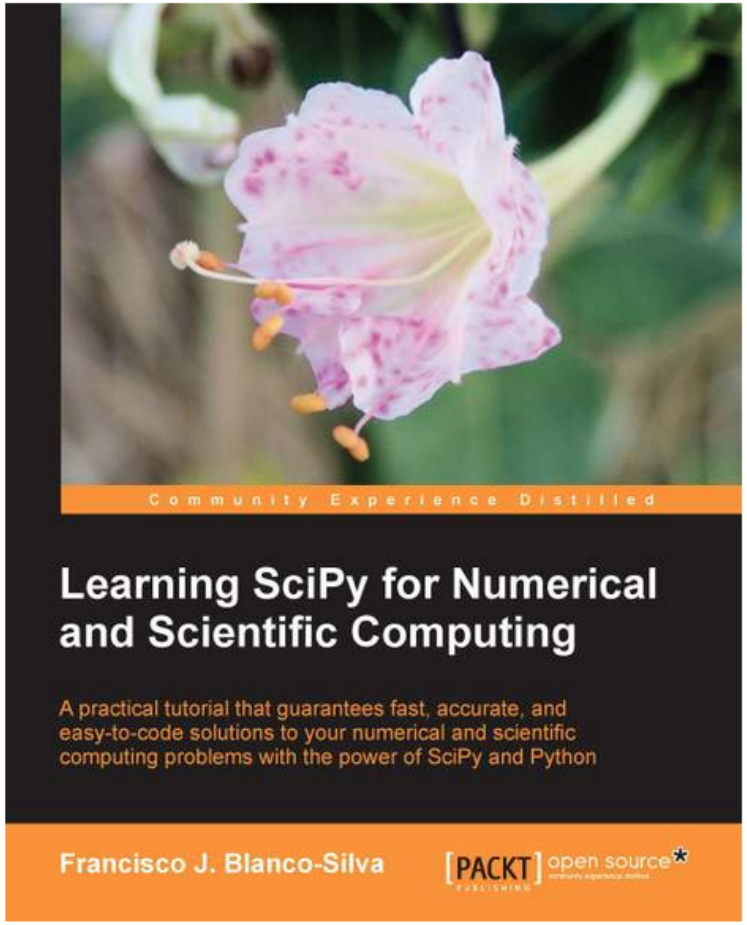

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