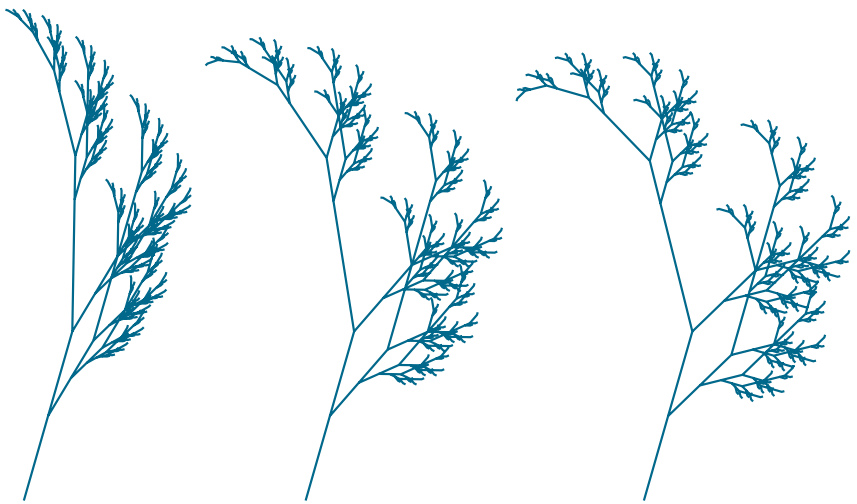
Learning SciPy for Numerical and Scientific Computing

Francisco Blanco-Silva

University of South Carolina



Some Basic Principles in Scientific Computing

A personal perspective

Scientific Computing is concerned with constructing mathematical models and quantitative analysis techniques, and using computers to analyze and solve scientific problems.

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- Trust the Engineer, Biologist, Chemist, Physicist, . . . : There are different ways to solve any problem. Rather than dismiss a different point of view, embrace it, work it out, explore the source of the problem, and look for connections with other techniques.

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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.

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Software

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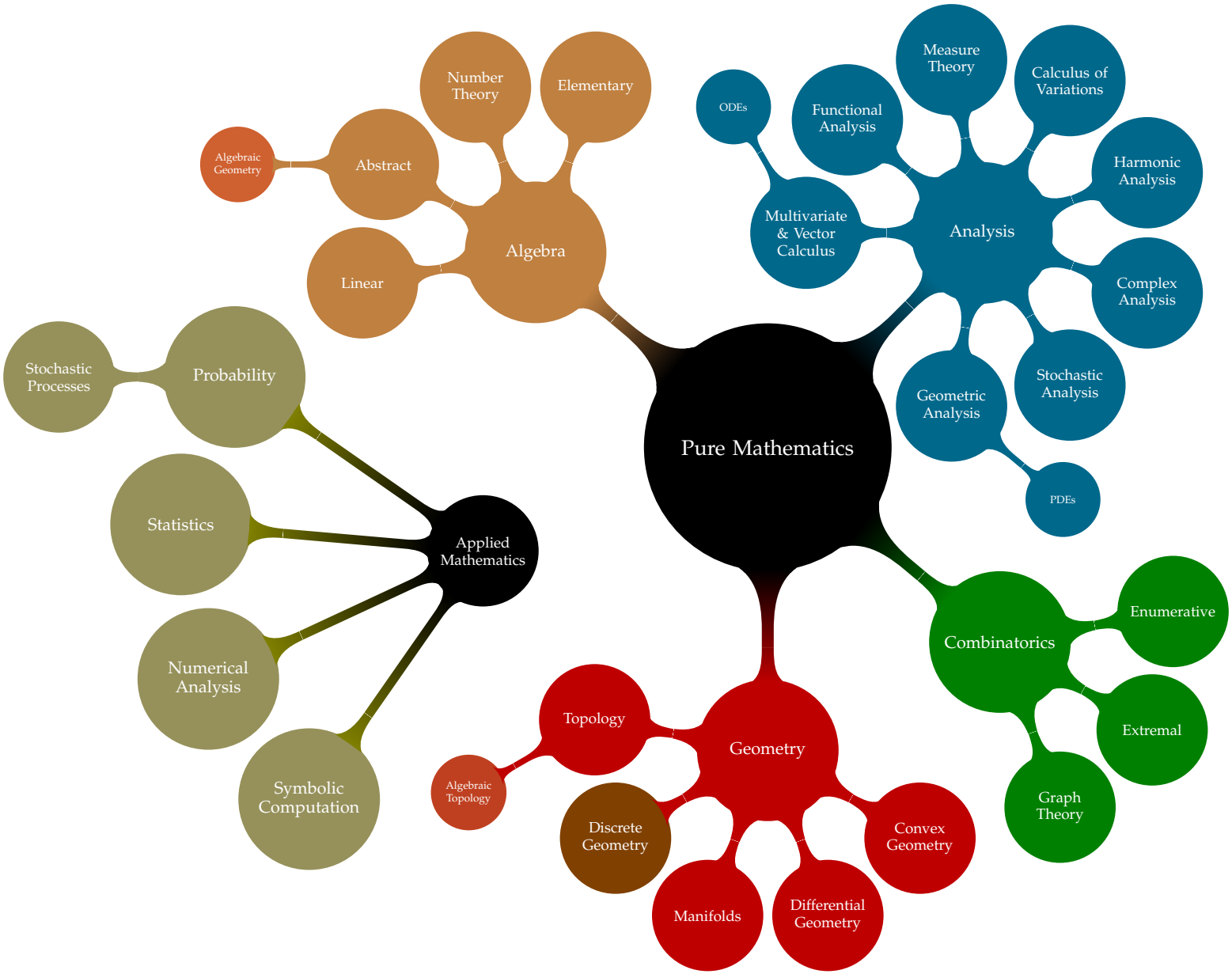
    - with `PyLab`: `ipython` + `NumPy` + **`SciPy`** + `matplotlib`
    - with `scikits` and `Pandas` on top of that

The Structure of SciPy

Similarity to the different areas of Mathematics



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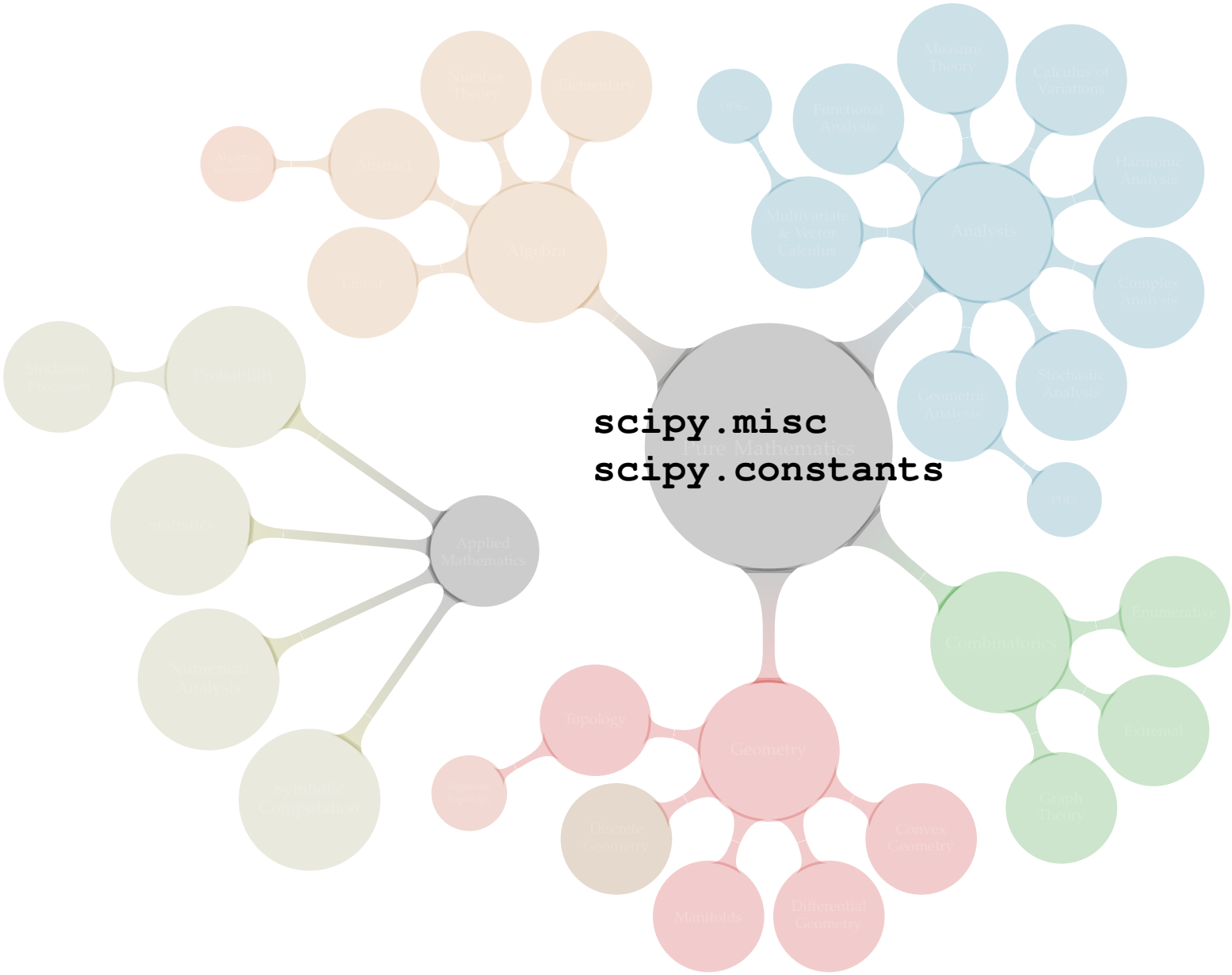

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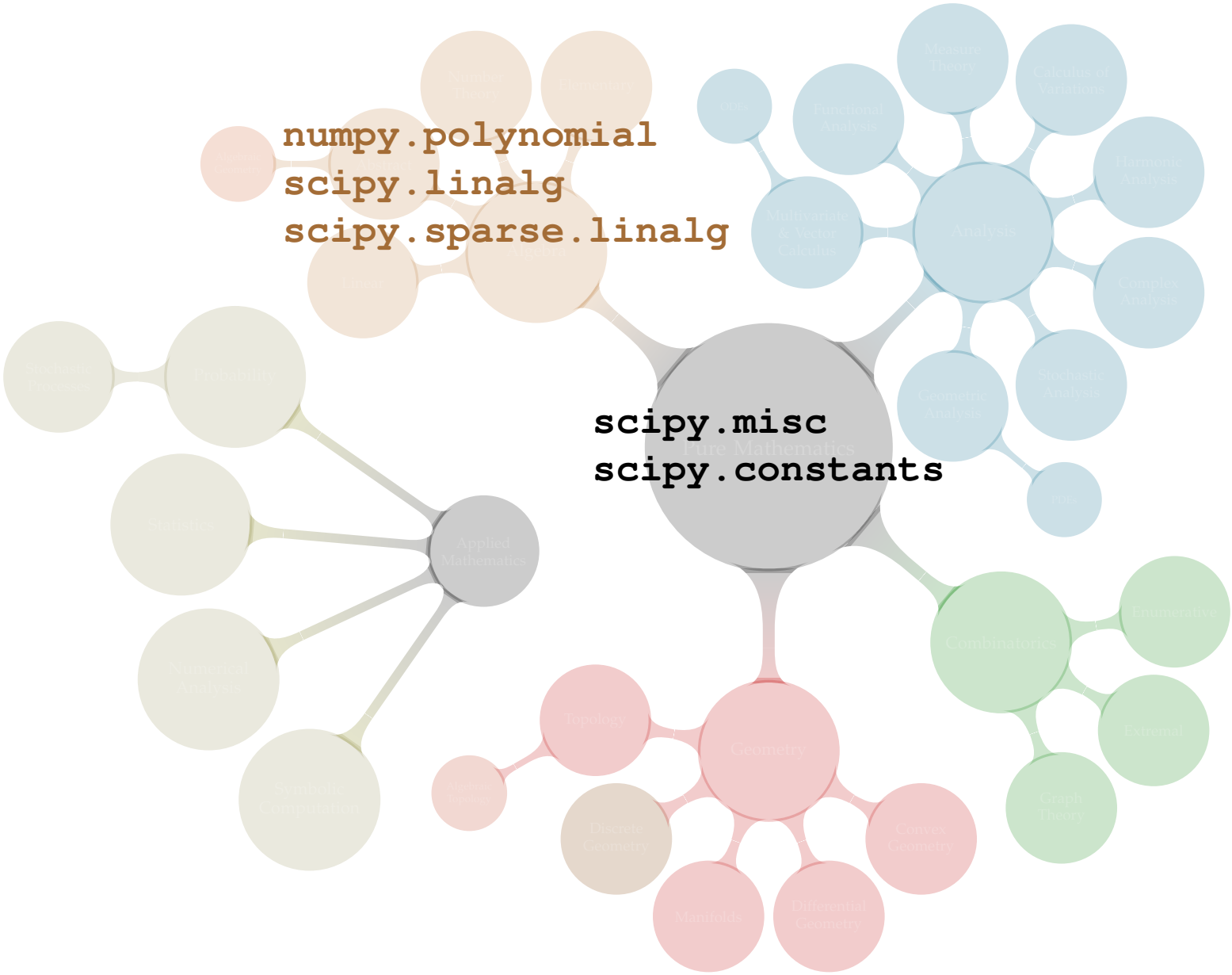

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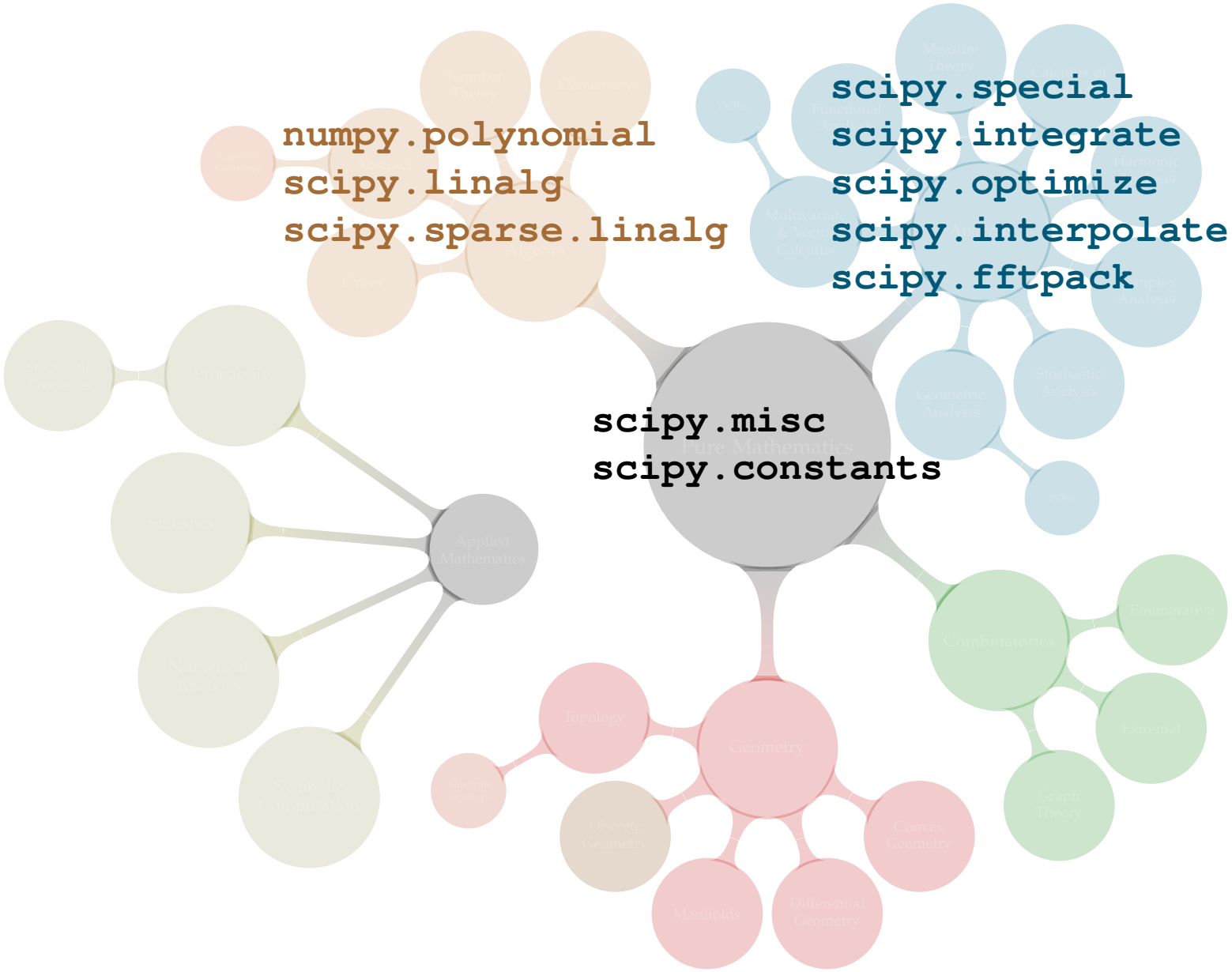

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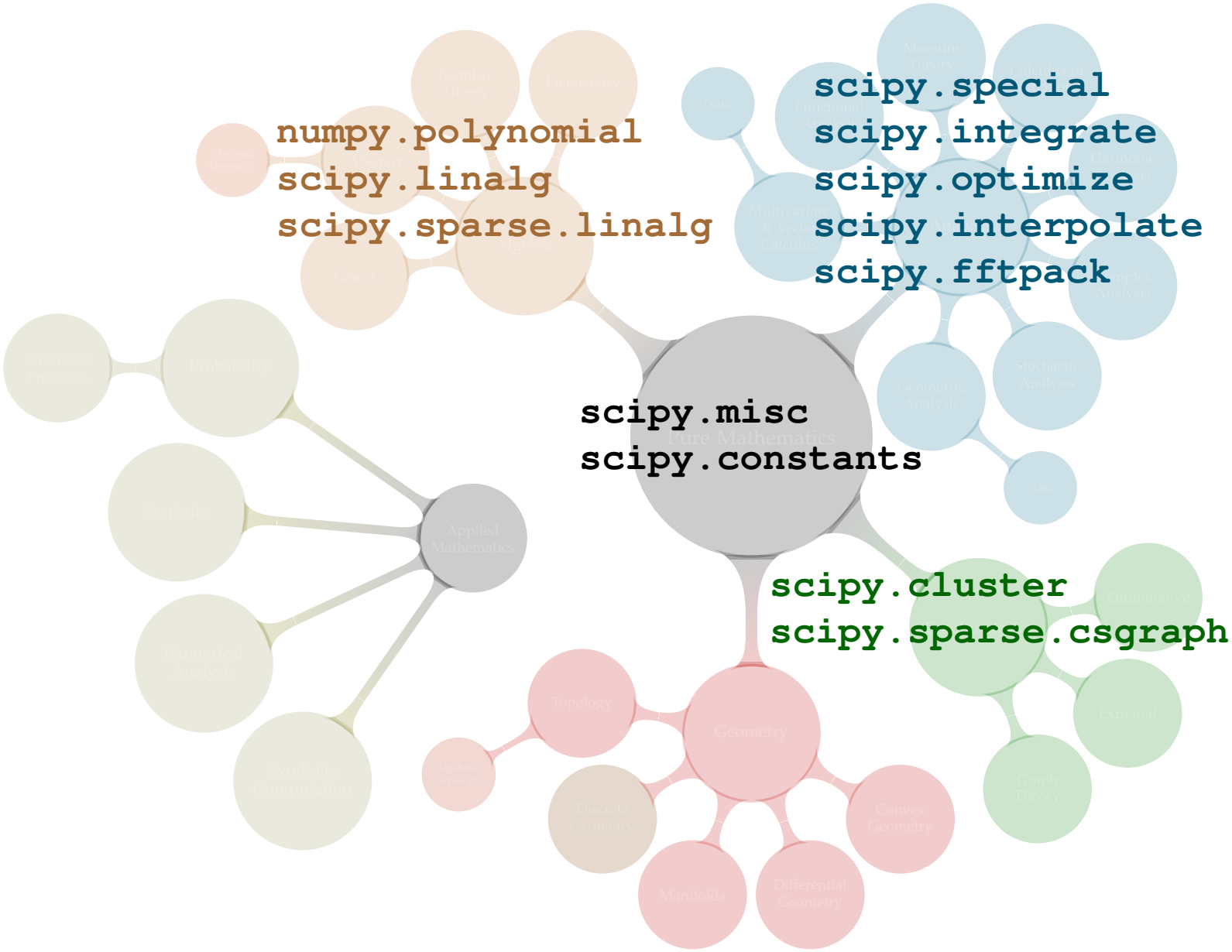

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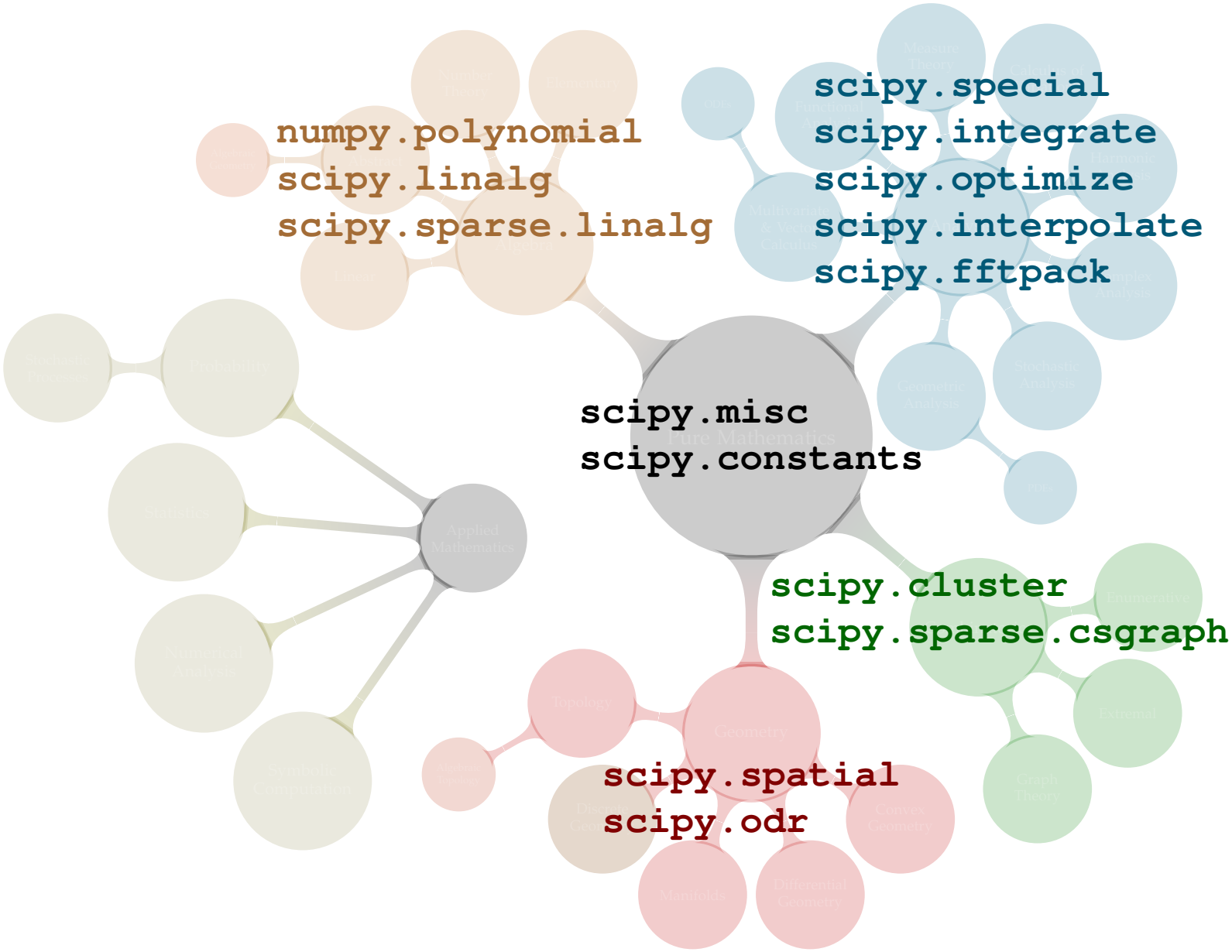

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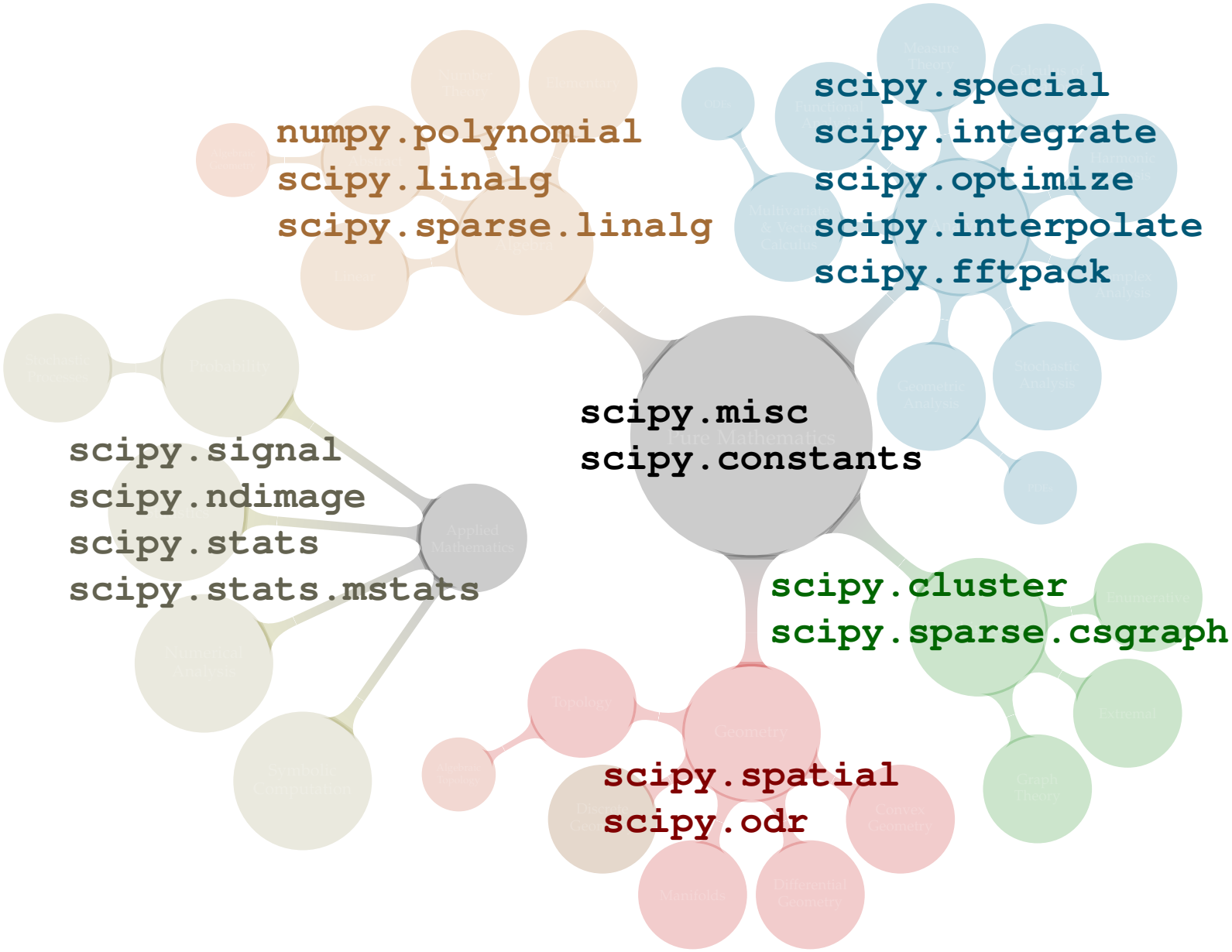
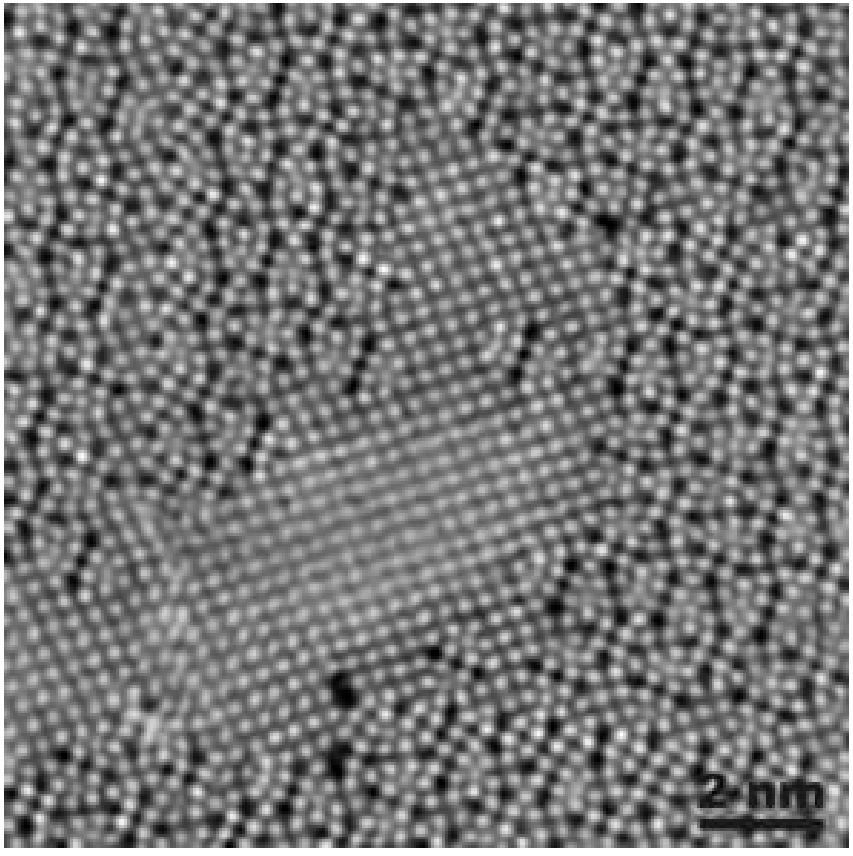


SciPy in action

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



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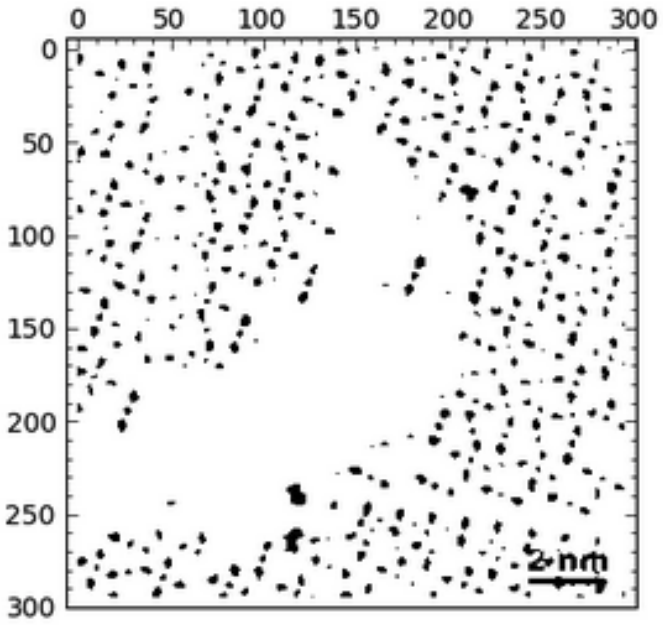
Computation of structural models

We take the following (naïve) approach:

- Segmentation of the atoms by thresholding and morphological operations.



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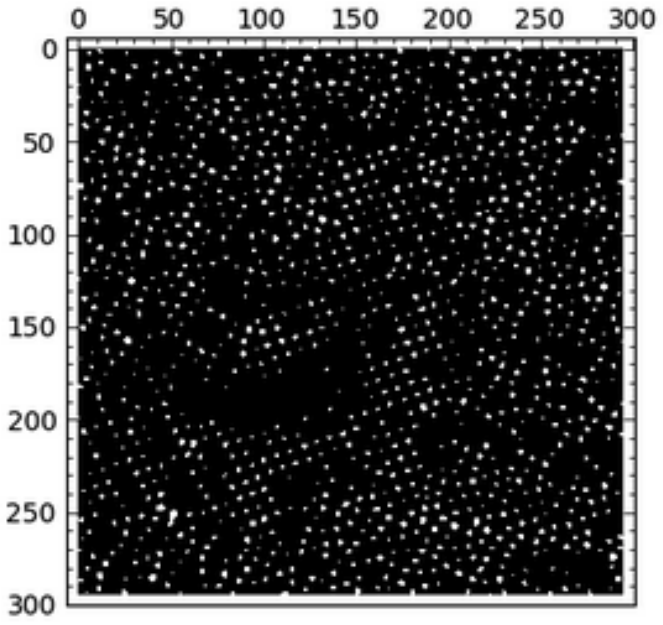

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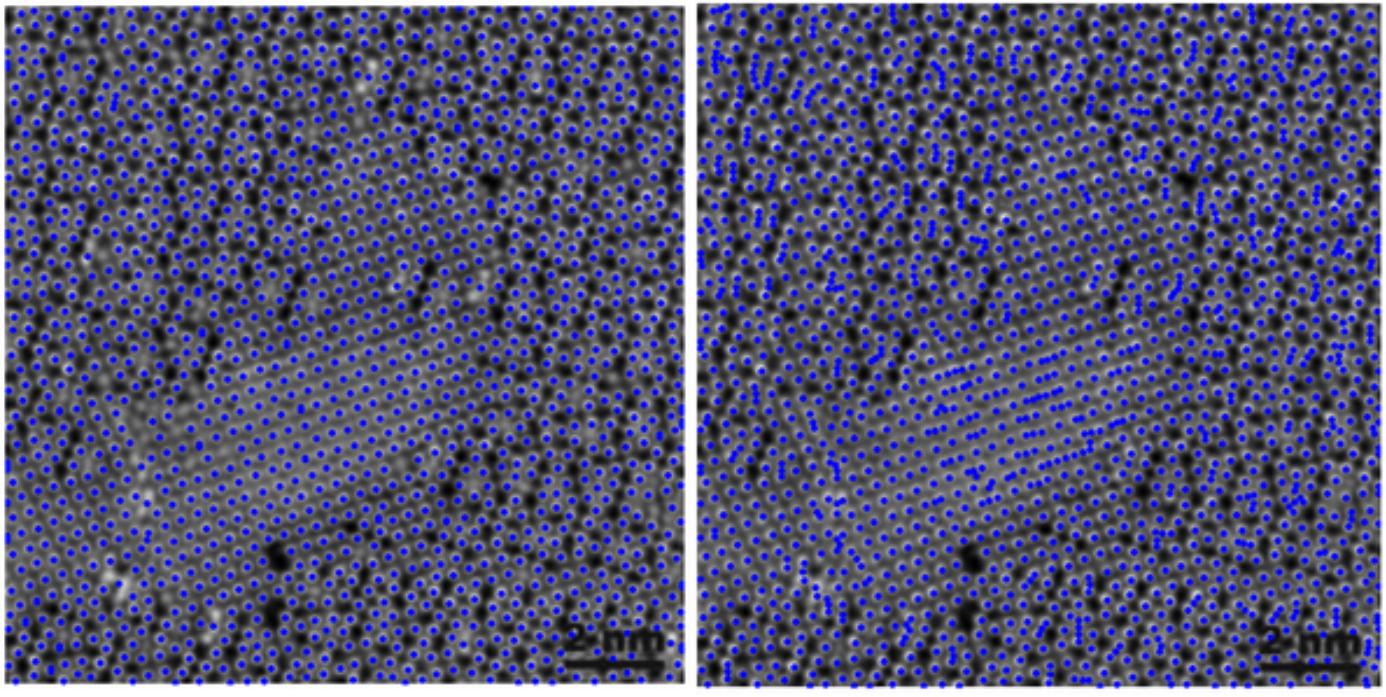

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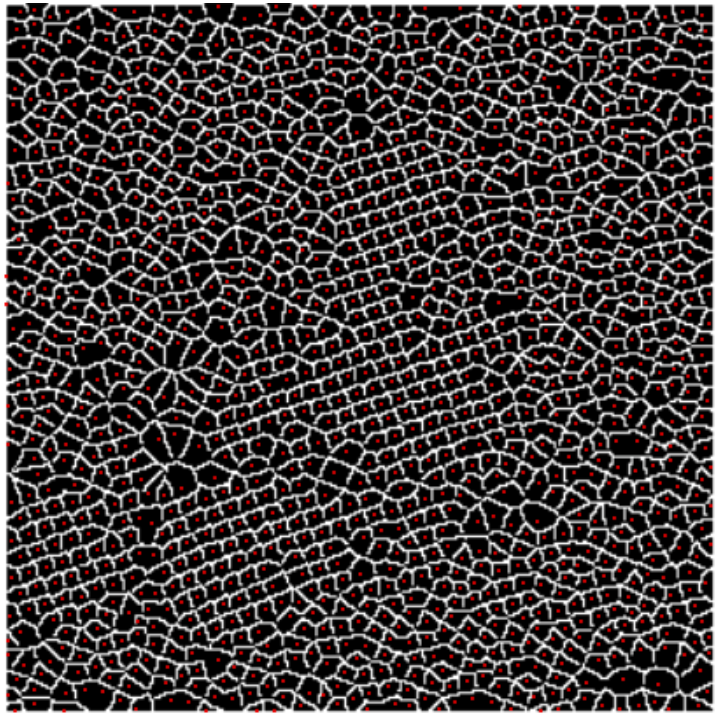
Computation of structural models

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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1  # Preamble
2  import numpy
3  import scipy
4  from scipy.ndimage import binary_opening, label, center_of_mass,
       distance_transform_edt
5  # Load the image
6  img = scipy.misc.imread('NbW-STEM.png')
7  # Apply a threshold to segment atoms
8  BWatoms = (img > 0.62)
9  # Perform a binary operation to eliminate outliers
10 BWatoms = binary_opening(BWatoms, structure=numpy.ones((2,2)))
11 # Segmentation of each atom
12 structuring_element = [[0,1,0],[1,1,1],[0,1,0]]
13 segmentation,segments = label(BWatoms, structuring_element)
14 # Computation of centers of mass of each atom
15 coords = center_of_mass(img, segmentation, range(1,segments+1))
16 xcoords = array([x[0] for x in coords])
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18 # Compute the Voronoi diagram of the lattice
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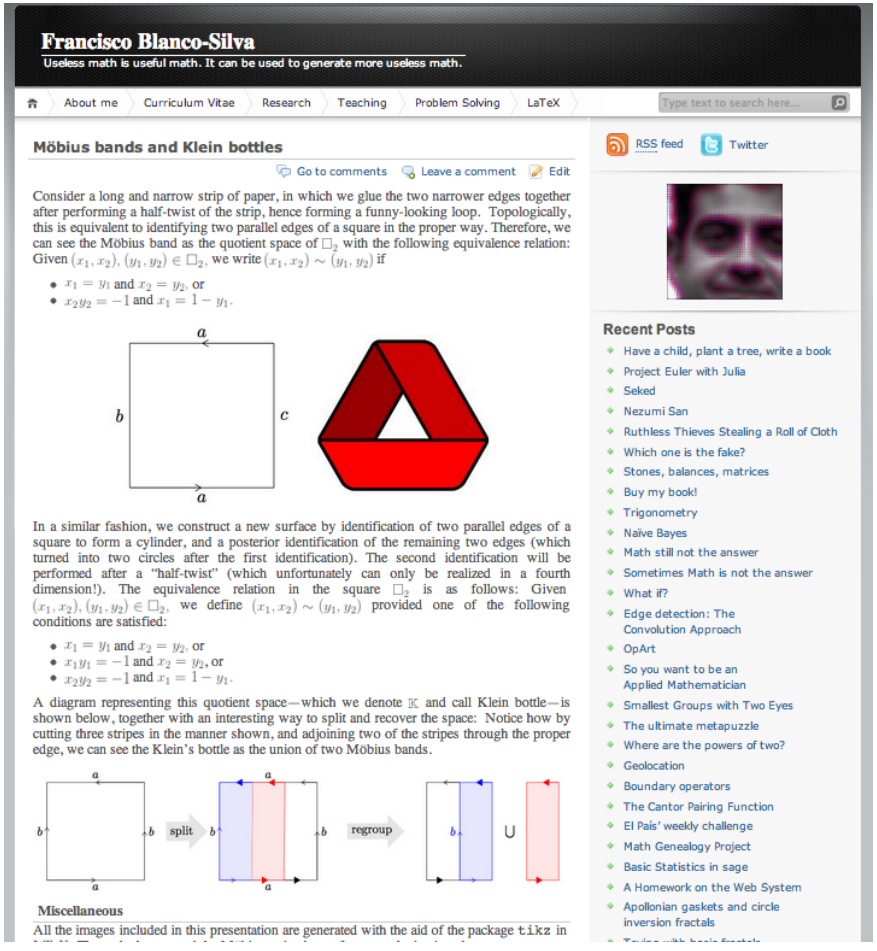

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