A Collection of Scripts for Ab Initio Calculations:
Migrating from Python 2 to 3

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Usage of Scripts (Phonon)

Ab Initio: using known structures of molecules/crystals to study properties

Scripts interpret experimental data from neutron spectroscopy

Vibrational Modes of Water Molecules

v1: symmetric stretch
v3: asymmetric stretch
v2: bend

Filter-Analyzer Neutron Spectrometer (FANS)

2 Vibrational Modes of C60 Molecule
Transitioning Process

Scripts written in Python 2
• Incompatible with Python 3
• No longer supported in 2020

Total Code Transitioned (phonon + auxiliary):
123 scripts
30,818 lines

Goals:
• Transition scripts to run in Python 3
• Improve accuracy of calculations, if possible

Process:
1. Apply 2to3 Fixers
2. Adjust to stricter code behavior
3. Transition Outdated Modules / Scripts
4. Parallel Testing
5. Improve Transition Efficiency
Step 1: Apply **2to3** fixers in command line

Automated Python 2 to 3 code translator

**Python 2** \[\rightarrow\] **Python 3**

<table>
<thead>
<tr>
<th>PRINT statement</th>
<th>PRINT() function</th>
</tr>
</thead>
<tbody>
<tr>
<td>MAP()</td>
<td>LIST( MAP() )</td>
</tr>
</tbody>
</table>

Final files:

- Edited script (with Python 3 fixers)
- Backup of original script (Python 2)
Step 2: Adjust to stricter code behavior

**Python 2**

- **DIVISION** operations
  - `/` floor division
  - ex. `5/2` → 2

- **STRING** module
  - `string.split(mystr)`

- **SPACE/TAB** interchangeable

**Python 3**

- **DIVISION** operations
  - `/` true division
  - ex. `5/2` → 2.5

- **STRING** methods
  - `mystr.split()`

- **SPACE/TAB** incompatible

Require manual fixes
Step 3: Transition outdated modules

### Python 2

**NUMERIC LINEARALGEBRA** modules

- `array(a)`
- `matrixmultiply(a, b)`
- `take(a, indices, axis=0)`
- `eigenvectors(a)`

- Gives left-hand (row) evecs

### Python 3

**NUMPY** module

- `array(a)`
- `dot(a, b)`
- `take(a, indices, axis=-1)`
- `linalg.eig(a)`

- Gives right-hand (column) evecs

#### Carry over

- Exceptions

- `axis=0` ‘takes’ rows of matrix
- `axis=-1` ‘takes’ columns of matrix
**SPLINE**

Third party script (Python 2)

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**SCIPY.INTERPOLATE.CubicSpline**

Spline Comparison Using \( \cos(x) \) Data Points

Key

- **cos(x) data points**
- **Third party spline**
- **cos(x) graph**
- **Scipy CubicSpline**
Step 4: Test scripts in parallel

Same Input

Python 2 Script

Python 3 Script

Compare generated outputs
- Run diff in command line
- Plotting

Debug

Test outputs with real data
**Vibrational Spectrum of C\textsubscript{60}**

- **Neutron Energy Loss (meV)**
  - Neutrons counted by detector

- **Neutron Intensity (A.U.)**

**Vibrational Energy**

- **C\textsubscript{60} Ag(1) mode**
  - 54.38420 meV

- **C\textsubscript{60} Ag(2) mode**
  - 198.27823 meV

**Experimental Data gathered from FANS**

**Python 2 Output (Calculated Spectrum)**

**Python 3 Output (Calculated Spectrum)**

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**Filter-Analyzer Neutron Spectrometer (FANS)**

![Diagram of neutron spectrometer](Image)
5. Improving Transition Efficiency

Supplementary version of Python’s 2to3

Rewrites most Numeric & LinearAlgebra functions with NumPy

Rewrites former string functions as string methods

Replaces any tabs (\t) with 8 spaces

Prints line number & content of functions that are difficult to transition

Limitations:

- NUMERIC and MATH modules share functions (ex. pi, sin(), cos())
- int() may need to be added to index values to ensure edited scripts run
Conclusion

We successfully migrated a subset of scripts (phonon + auxiliary).
We wrote and tested a supplementary 2to3 script (addresses manual fixes).

→ Useful for other scripts (ex. thermal expansion, elastic properties)

Things I learned:

• Phonon programming
• Neutron spectroscopy
• Linear algebra applications

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References