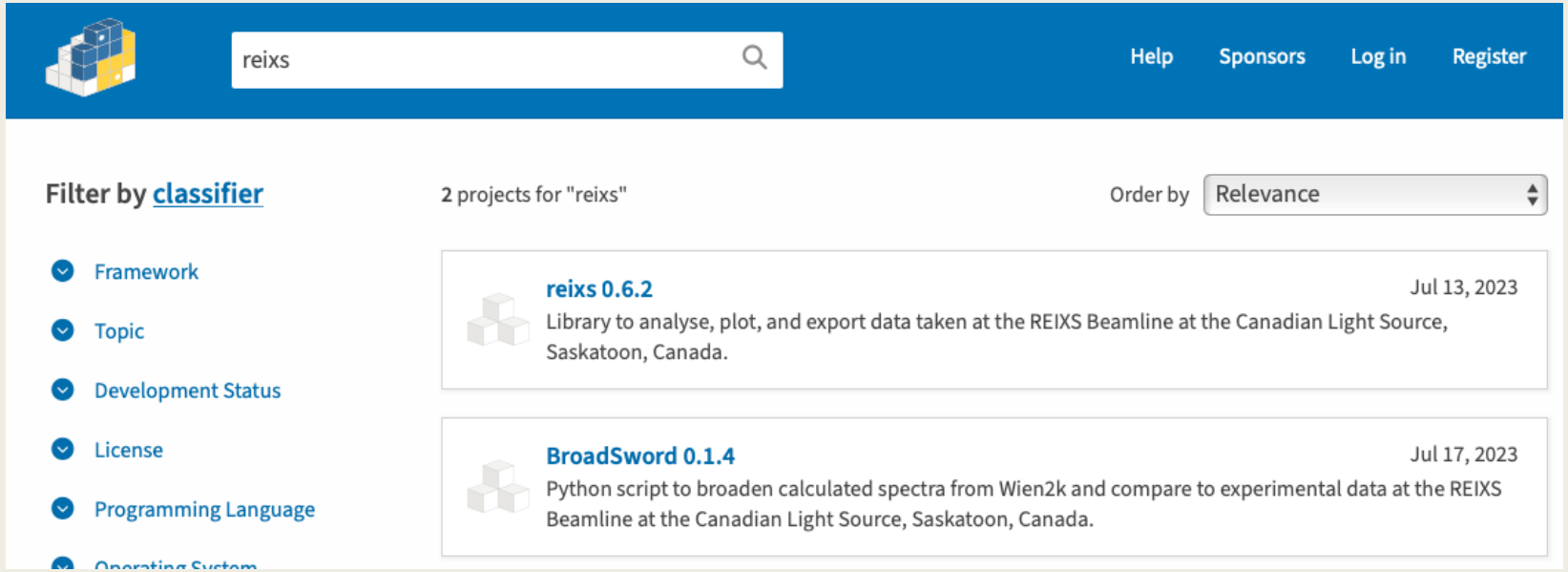
BroadSword Motivations

- Having the ability to save and reload a broadened calculation
- Something more compatible with the .csv output of the reixs software
- The ability for our group to modify the code as needed
- Something written purely in python while still being reasonably fast

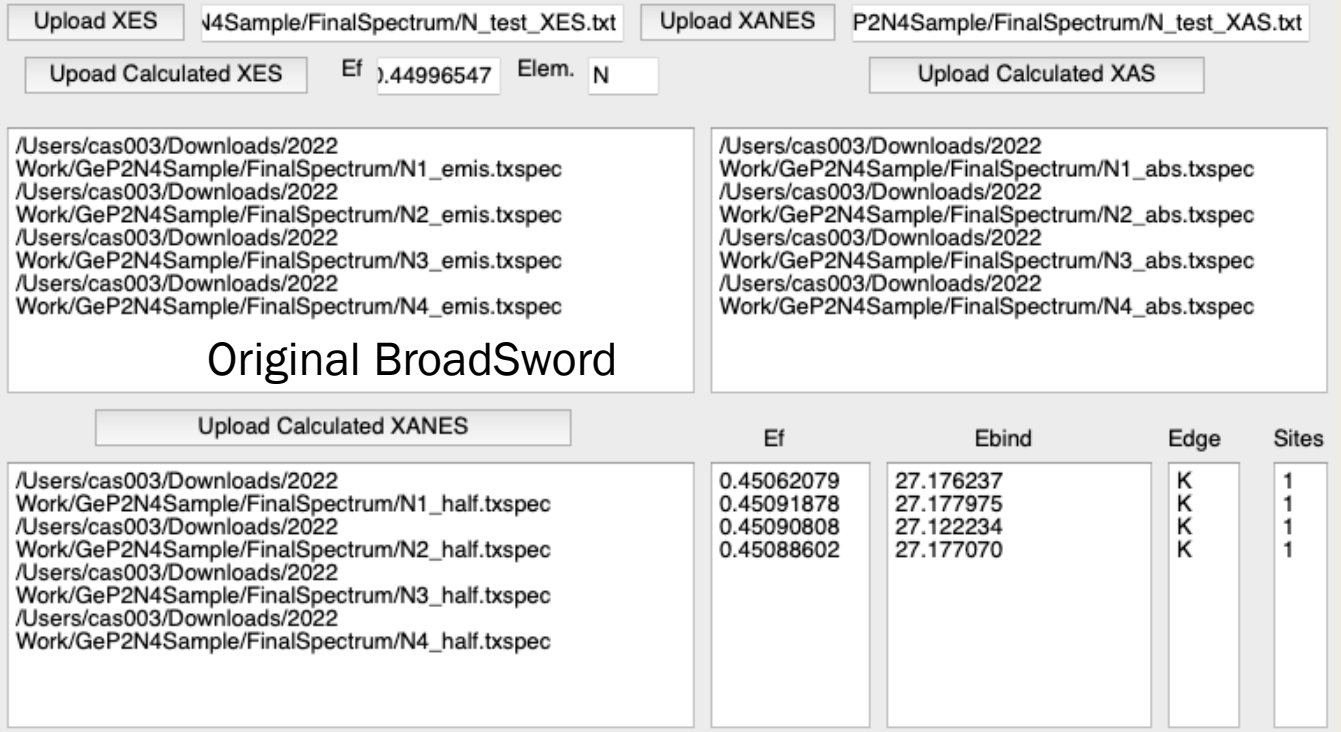
Downloading BroadSword

- Similar to downloading Patrick's reixs package through the terminal
  - *pip install BroadSword (First time)*
  - *pip install --upgrade BroadSword (To update to newest version)*
- Found on PyPi by searching for BroadSword or reixs
  - *https://pypi.org/project/BroadSword/*



Input Parameters

- Specify the base directory
- Enter name of input file
  - LoadExp takes in .txt or .csv, and you can specify the number of header lines to ignore, allowing direct input from the reixs software into broadsword
- Some parameters can be left empty (Ex: sites) and it will assume a value for them. (sites=1)
  - If XANES calculation file is not specified, it will simply duplicate the XAS into that parameter. (See bottom line for minimum required inputs)
- GS = Ground state, ES = Excited state



New BroadSword

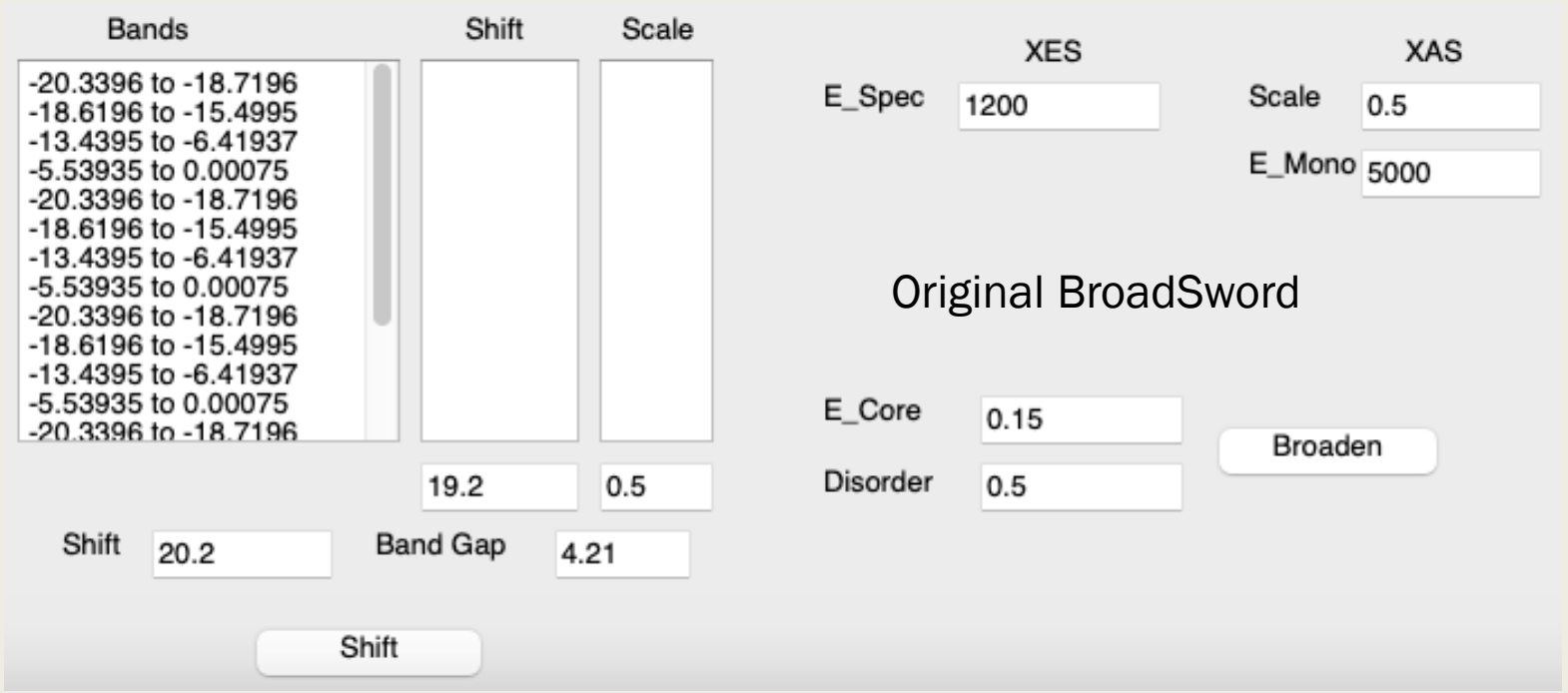
```
# Create an instance of the class
broad = Broaden()

# Load the experimental and calculations
broad.loadExp(basedir,XES="N_test_XES.txt",XANES="N_test_XAS.txt",GS_fermi=0.44996547,headerlines=[2,2])
broad.loadCalc(basedir,XES="N1_emis.txspec",XAS="N1_abs.txspec",GS_bindingEnergy=27.176237,XANES="N1_half.txspec",ES_fermi=0.45062079,sites=1,edge="L2")
broad.loadCalc(basedir,XES="N2_emis.txspec",XAS="N2_abs.txspec",GS_bindingEnergy=27.177975,XANES="N2_half.txspec",ES_fermi=0.45091878)
broad.loadCalc(basedir,XES="N3_emis.txspec",XAS="N3_abs.txspec",GS_bindingEnergy=27.122234,XANES="N3_half.txspec",ES_fermi=0.45090808)
broad.loadCalc(basedir,XES="N4_emis.txspec",XAS="N4_abs.txspec",GS_bindingEnergy=27.177070,XANES="N4_half.txspec",ES_fermi=0.45088602)

# broad.loadCalc(basedir,XES="N1_emis.txspec",XAS="N1_abs.txspec",GS_bindingEnergy=27.177070) # Minimum required inputs to broaden a spectra.
```

Broadening Parameters

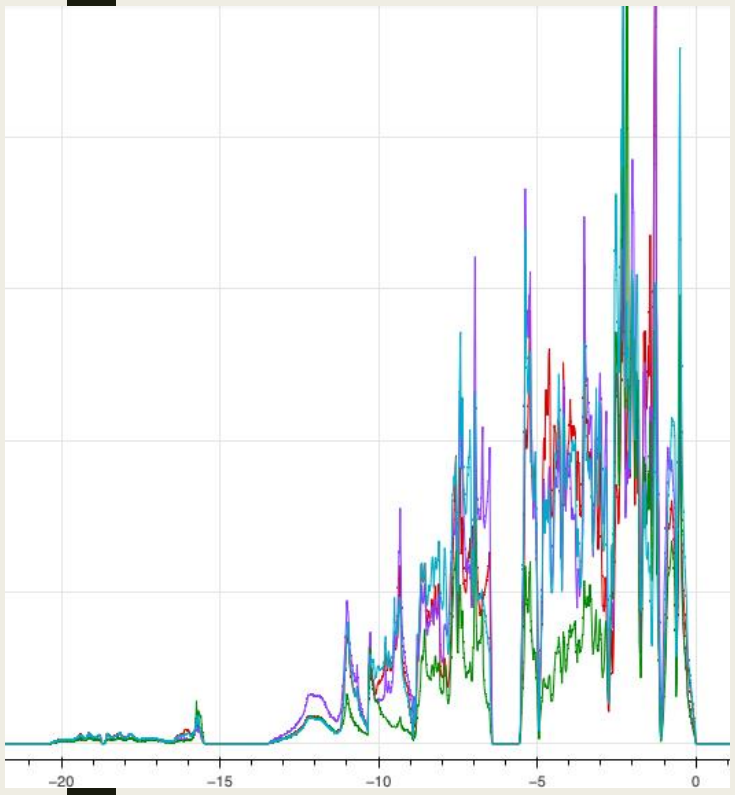
- Specify the broadening parameters the same way as in original program
- Specify the shifting parameters
  - Will produce an output graph to show the shift
- Broaden the spectra
  - ‘separate’ simply refers to plotting the XES in a different plot window than the XAS for visual purposes



New BroadSword

```
# Initialize the broadening parameters
broad.initResolution(corelifetime=0.15,specResolution=1200,monoResolution=5000,disorder=0.5,XESscaling=0.5,XASscaling=0.5)
# Shift the spectra until the calculation aligns with the experimental
broad.Shift(XESshift=19.2,XASshift=20.2,separate=False)
# Broaden the spectra
broad.broaden(separate=False)
```

Targeting Specific XES Bands



Output of .printBands()

```
In inequivalent atom #0
Band #0 is located at -20.33963 to -18.7196
Band #1 is located at -18.6196 to -15.49954
Band #2 is located at -13.4395 to -6.41937
Band #3 is located at -5.53935 to 0.00075
In inequivalent atom #1
Band #0 is located at -20.33963 to -18.7196
Band #1 is located at -18.6196 to -15.49954
Band #2 is located at -13.4395 to -6.41937
Band #3 is located at -5.53935 to 0.00075
In inequivalent atom #2
Band #0 is located at -20.33963 to -18.7196
Band #1 is located at -18.6196 to -15.49954
Band #2 is located at -13.4395 to -6.41937
Band #3 is located at -5.53935 to 0.00075
In inequivalent atom #3
Band #0 is located at -20.33963 to -18.7196
Band #1 is located at -18.6196 to -15.49954
Band #2 is located at -13.4395 to -6.41937
Band #3 is located at -5.53935 to 0.00075
```

Bands	Shift	Scale
-20.3396 to -18.7196	30	0.1
-18.6196 to -15.4995	33	0.2
-13.4395 to -6.41937	30	0.2
-5.53935 to 0.00075	20	0.4
-20.3396 to -18.7196	15	0.2
-18.6196 to -15.4995	19.2	0.2
-13.4395 to -6.41937	19.2	0.4
-5.53935 to 0.00075	19.2	0.2
-20.3396 to -18.7196	30	0.3
-18.6196 to -15.4995	33	0.2
-13.4395 to -6.41937	30	0.1
-5.53935 to 0.00075	20	0.5
-20.3396 to -18.7196	15	0.3
Original BroadSword	0	0

- Print the bands to the screen
- Add in a new parameter into the .initResolution() and .Shift() functions that were described last page
- Specify the scaling/shifting for each band
  - This is an array of arrays. Each inner array contains the band scale/shift values for a single inequivalent site

New BroadSword

```
# Optionally you can scale and shift specific bands in XES. Use printBands() to determine where the bands are located.
# Then add the new argument XESbandScaling into initResolution() and XESbandshift int Shift()
broad.printBands()
broad.initResolution(corelifetime=0.15,specResolution=1200,monoResolution=5000,disorder=0.5,XESscaling=0.5,XASscaling=0.5,XESbandScaling=[[0.1,0.2,0.2,0.4],[0.2,0.2,0.4,0.2],[0.3
broad.Shift(XESshift=19.2,XASshift=20.2,separate=False,XESbandshift=[[30,33,30,20],[15,19.2,19.2,19.2],[30,33,30,20],[15,19.2,19.2,19.2]])

# Broaden the spectra
broad.broaden(separate=False)
```

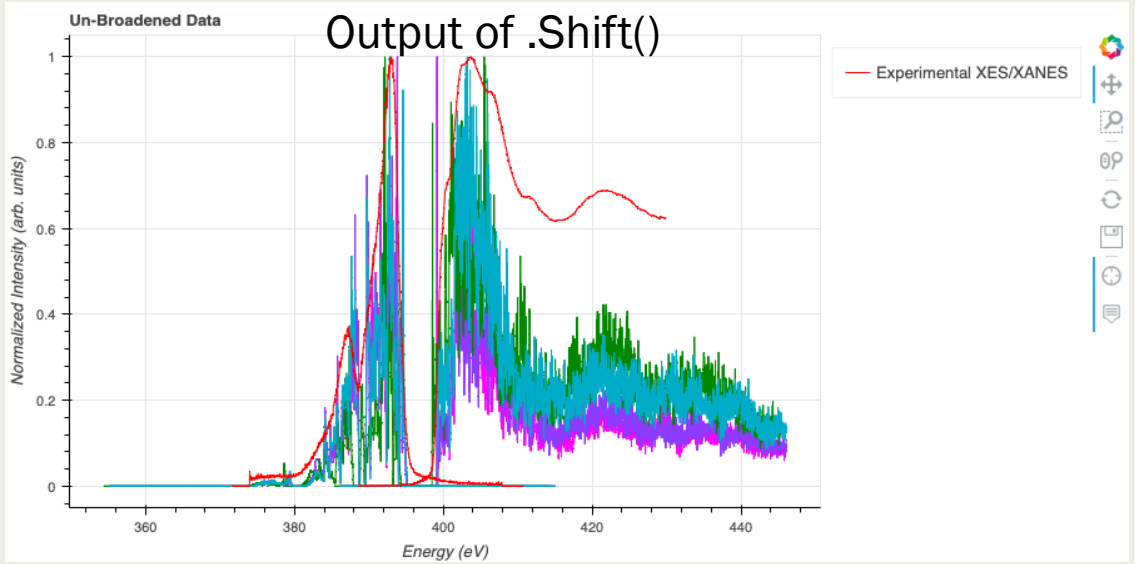
Shift value becomes obsolete

A single inequivalent atom, and the four bands associated with it

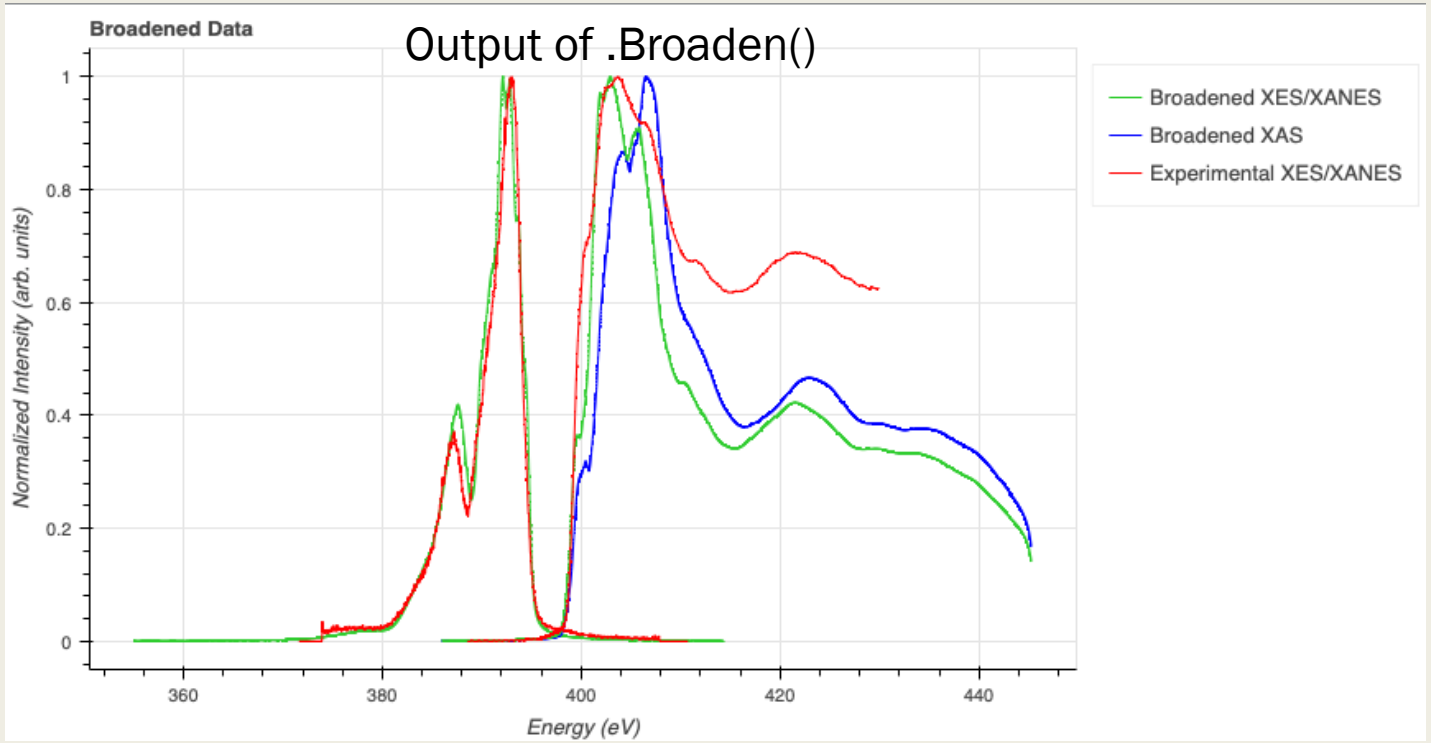
Broadened Output

```
# Export the broadened calculated spectra
broad.export(filename="GeP2N4",element="N",individual=False)
```

Output of .Shift()



Output of .Broaden()



- Returns values accurate to ~3 decimal places to original broadsword program
  - Python is using more precision in its floating-point numbers
  - (Perhaps reduce this for speed improvement???)
- Individual = False
  - Returns only the broadened sum of the inequivalent sites
  - Ex: GeP2N4_N_XES.csv
- Individual = True
  - Returns the individual broadened contributions as well
  - This is the default in original broadsword

General Comments/Future Work

- Bring back usability of the Ctypes version, as that was slightly faster, but more difficult for the user to set up, and not functional on windows yet.
- Various miscellaneous updates to the comments and example program to make it clearer to understand
- Update the plotting functions to be more code friendly
- The python code is almost a direct copy from the C program, and so it follows some very poor python practices such as having everything in a global variable.
  - *The only major difference is the use of vectorization, which is what allows it to run within a reasonable timeframe.*
- Testing has been fairly limited, so please do a couple trial runs to confirm that the output is the same from the original before assuming everything is correct