



Development of Graphical User Interface and Spectral Fitting Tool for NEQAIR

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Overview



- Background
- Motivation
- Conceptual Design of GUI
- Spectral Fitting
- Demo
- Installation
- Future Work
- Acknowledgments

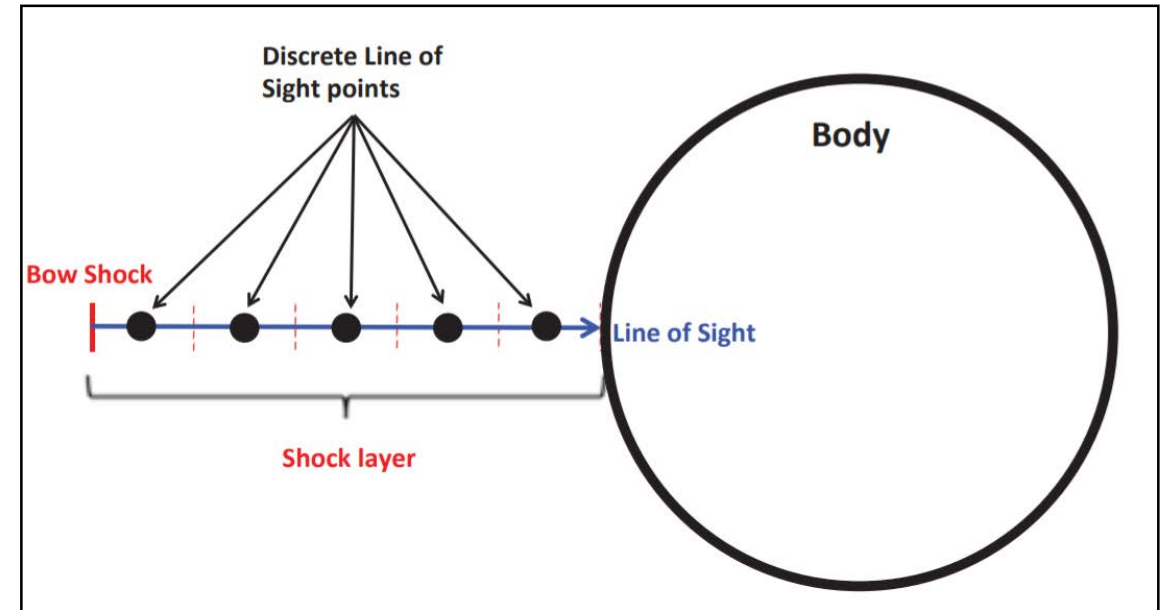




Background

NEQAIR: Nonequilibrium and Equilibrium Radiative Transport Spectra Program.

- Performs line-by-line calculation of radiation along a Line of Sight, LOS.
 - Calculates emission and absorption spectra for atoms and molecules as well as radiation from electron interaction.
 - Calculates radiative heating on a body.

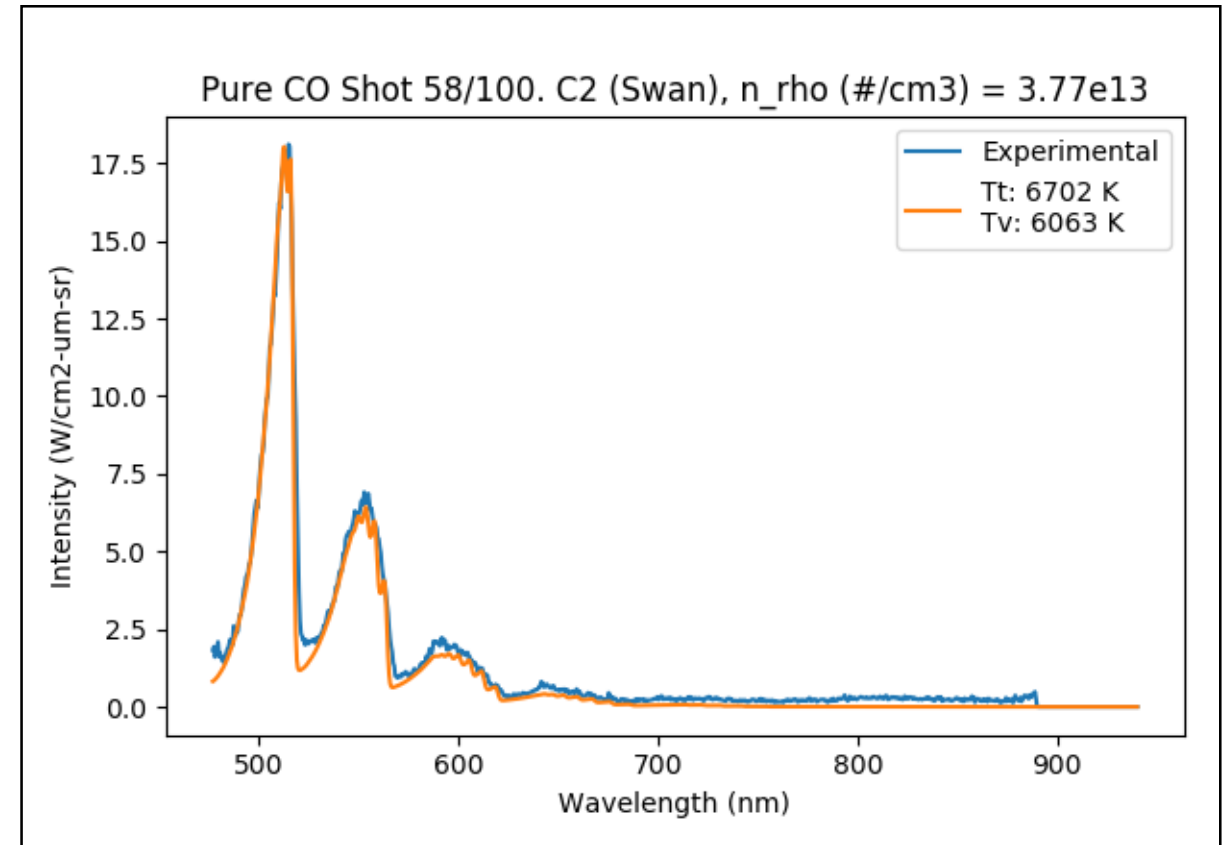


¹Line of sight calculation from shock to body.



Motivation

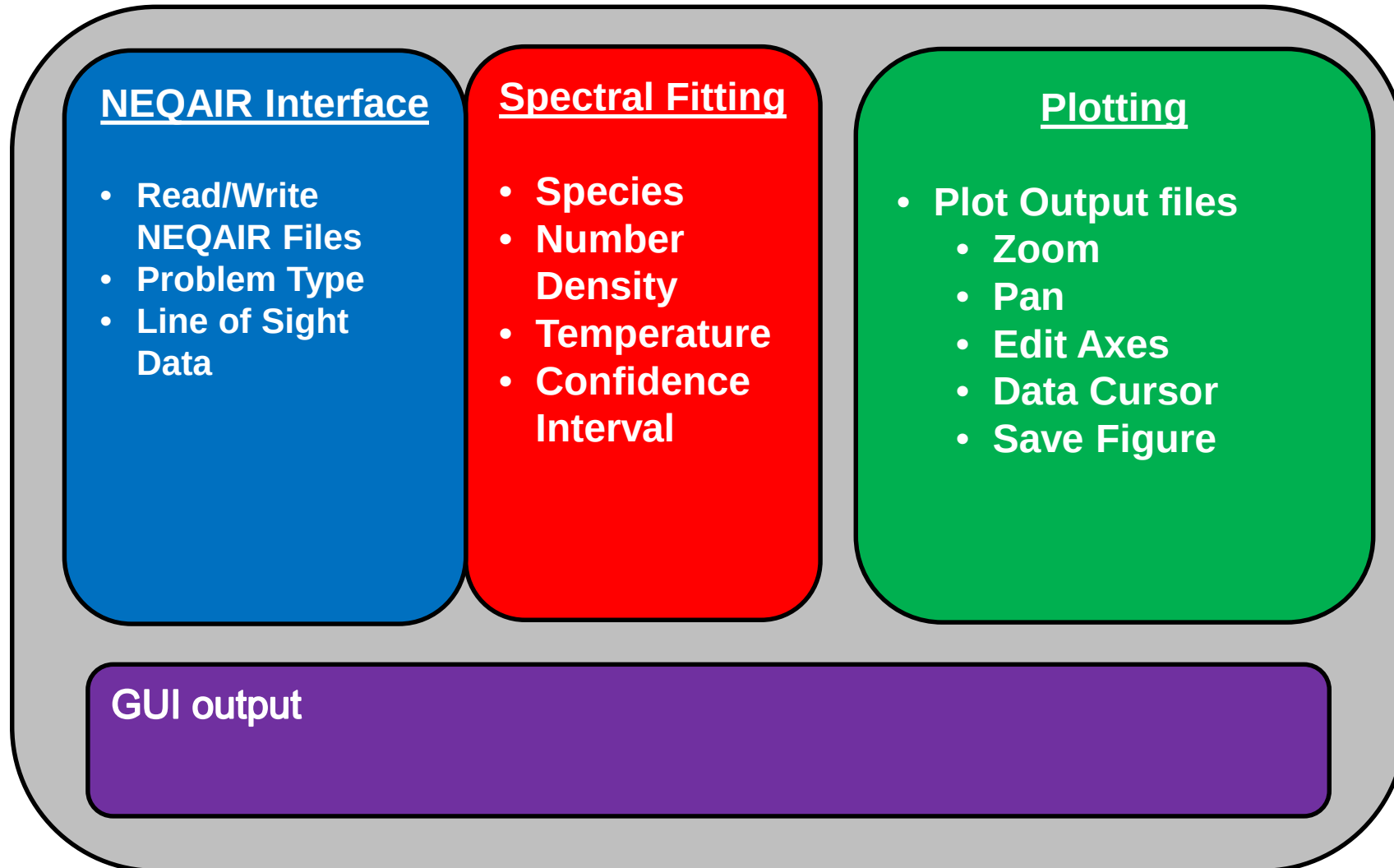
- Create a graphical user interface for creating NEQAIR input files, running simulations and viewing results.
- Add a new feature to allow NEQAIR to infer temperature and species number density from experimental data.
 - This tool can be used to make a fit of EAST shock tube results in a “hands-off” approach.
 - A fit is made by guessing the species composition and temperature rather than evaluating the data itself.



Sample spectral fit output from the program

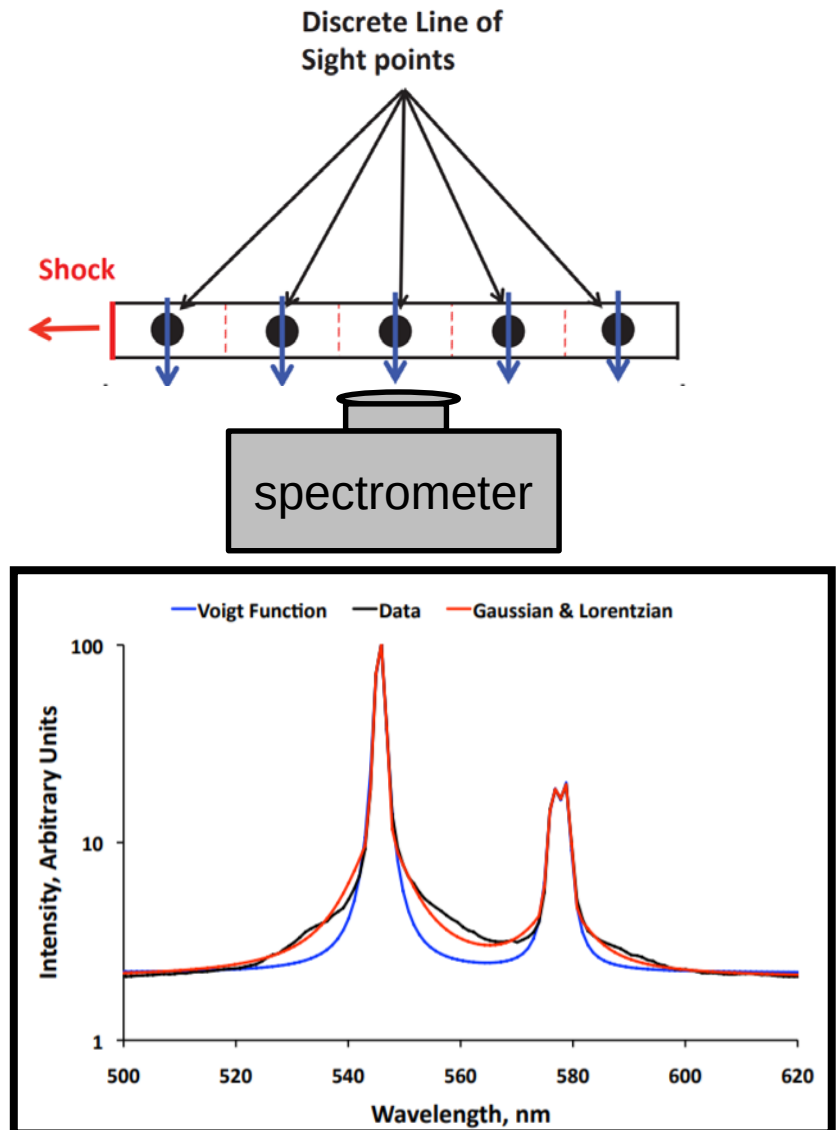
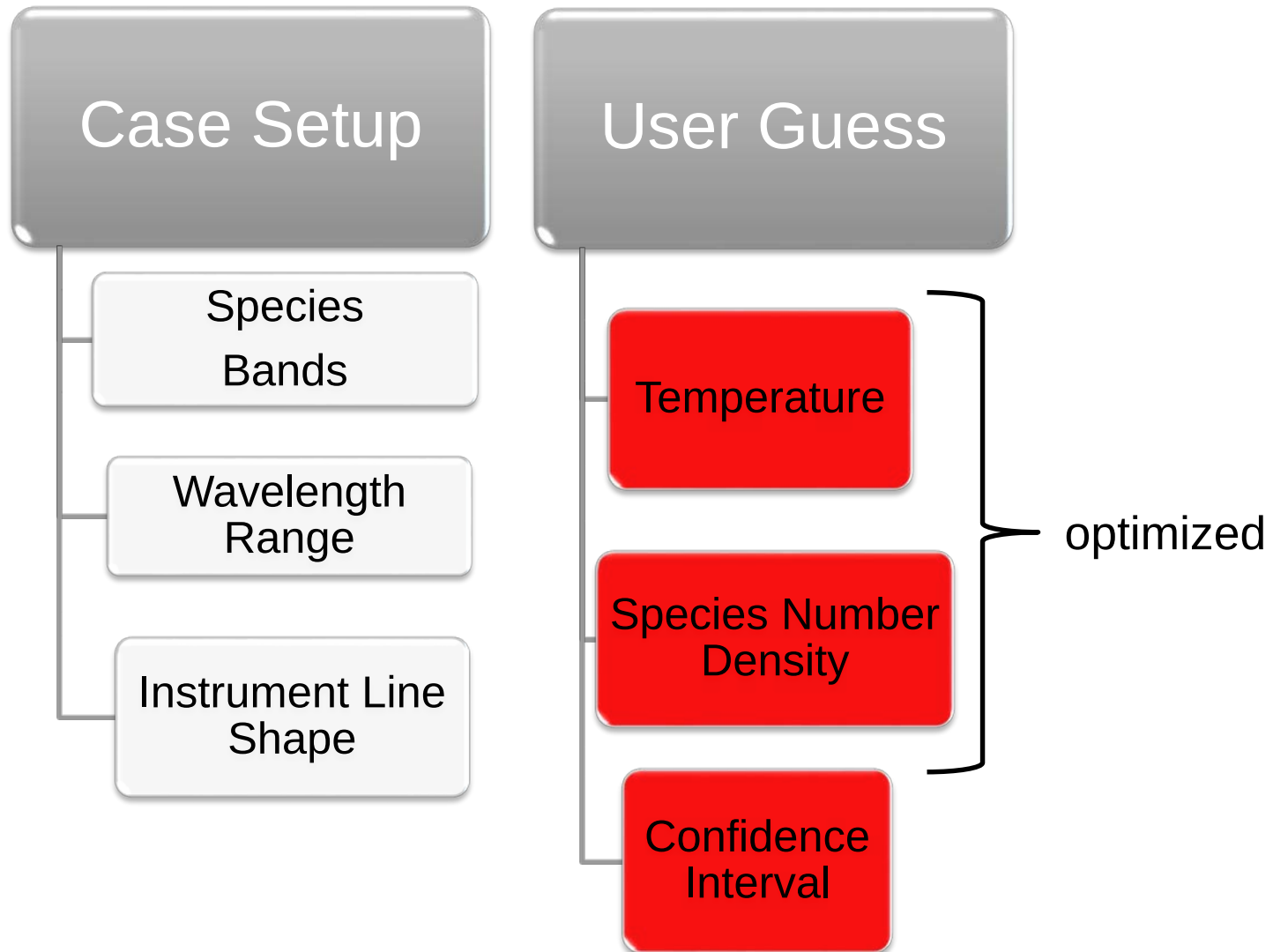


Conceptual GUI Layout





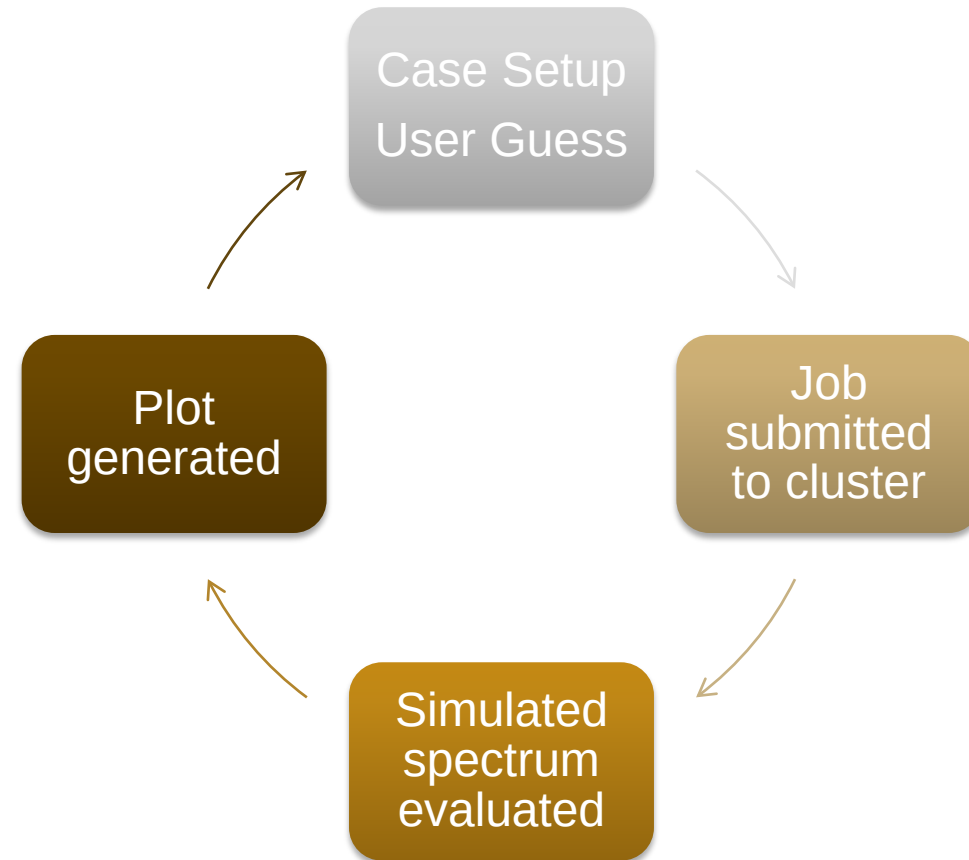
Spectral Fitting





Spectral Fitting Workflow

- User Guess data file and Case Setup file are created.
- Job submitted to cluster.
- Output files are monitored for job completion.
- Simulated spectrum is linearly interpolated to match experimental resolution.
- Optimization routine evaluation.
- Plot of experimental and simulated data are returned.





Optimization

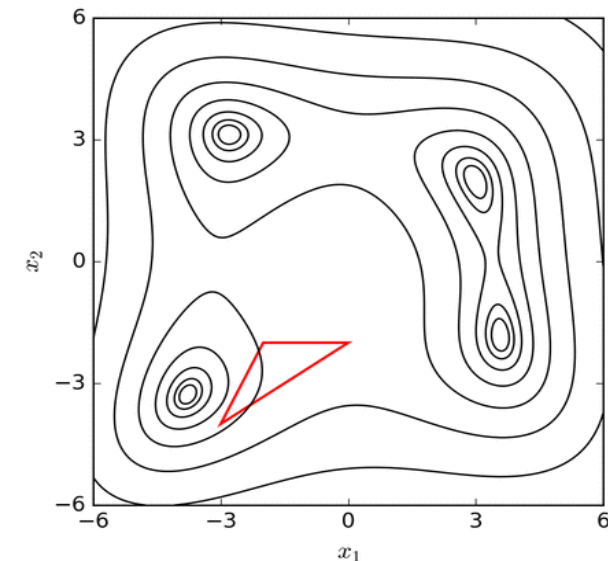
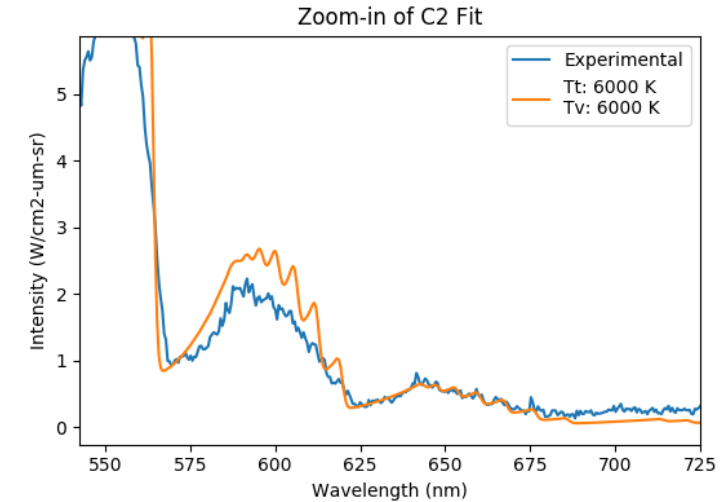


Why optimization?

- Our objective is to minimize differences between spectra:

$$objective = \sum_i |\exp_i - sim_i| I_{\exp_i}^2$$

- The Nelder-Mead “Down-hill” Simplex Method was chosen:
 - Requires very little input on the user end.
 - May quantify and define a confidence interval on the initial guess.
- Shortcomings:
 - This algorithm typically takes more iterations than other schemes to converge.



<https://commons.wikimedia.org/w/index.php?curid=51597577>



Demo







Install



How does the user get the GUI?



At NASA?

- GUI be installed on Cedar cluster.
- Packaged with NEQAIR v15.0
- Script will be made to run install commands for you.

- With Anaconda as your Python Distribution, you only need these items:
 - NeQtPy.py
 - setup.py
 - README.md
- Anaconda will setup an environmental variable which points to its path.
- Setup.py is used to install the NEQAIR GUI.



Future Work

- **Make direct use of NEQAIR modules to speed up spectral fitting process.**
 - Waiting for the job in the queue is what takes the longest in each iteration, so bypassing that will improve calculation time.
- **Add selection for optimization schemes.**
 - Nelder-Mead is simple, but other optimizers are available that are faster, and easy to use.
 - The Sequential Least Squares Programming routine allows the user to set bounds and constraints on variables.
- **Accept a user's instrument line shape function.**
 - Different instruments take in radiation in different profiles, giving the user the option add their own that may have been measured decreases the error in the fit.
- **Saved file of successfully fit spectrum.**
 - A simple file of the scanned intensity with information of the temperatures used, species, bands, and even instrument line shape parameters.



Acknowledgements

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Brett Cruden

Aaron Brandis

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David Hash

References

1. Brandis, Aaron M., and Brett A. Cruden. "NEQAIRv14. 0 Release Notes: Nonequilibrium and Equilibrium Radiative Transport Spectra Program." (2014).
2. Brandis, Aaron M., and Brett A. Cruden. "Benchmark Shock Tube Experiments of Radiative Heating Relevant to Earth Re-entry." *55th AIAA Aerospace Sciences Meeting*. 2017.



QUESTIONS?