**Research Experience Placement (REP) Scheme 2024**

**Supervisor Project Proforma**

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| **Project title:** | Atmospheric spectroscopy: Using spectral simulations to investigate uncertainties in multispectrum non-linear least-squares fitting |
| **Host Institution:** | National Centre for Earth Observation, University of Leicester |
| **Project supervisor (name, department):** | Dr Jeremy Harrison, National Centre for Earth Observation |
| **Project enquiries (supervisor email):** | [jh592@leicester.ac.uk](mailto:jh592@leicester.ac.uk) |
| **Co-Supervisor, if any (name, department):** |  |
| **Proposed start date:** | Any time from the end of June 2024 (flexible) |
| **Project description:** | |
| Remote sensing of the Earth’s atmosphere provides us with a wealth of information on the distribution of trace gases. This information is obtained from direct measurements made by instruments on a variety of platforms, including satellites, that measure infrared radiation passing through the Earth’s atmosphere. From these measurements, we can extract the abundances of atmospheric trace gases via their unique absorption patterns in the infrared, in a process known as a retrieval. However, this first requires the availability of accurate quantitative spectroscopic data, normally derived from laboratory measurements and contained in databases such as HITRAN.  The HITRAN database represents our best knowledge for calculating atmospheric molecular transmission. It consists of spectroscopic line parameters for the individual absorption lines of atmospheric molecules. The uncertainties in these line parameters are variable and can be up to 20% or higher. There is a great push to improve the accuracy of HITRAN line parameters. In order to reduce uncertainties in the retrievals of trace gases from satellite measurements, we need to be able to calculate atmospheric spectra to sub-percent accuracy. This can only be achieved by i) using metrological principles to ensure the traceability of experimental sample conditions directly back to SI units, and ii) deriving spectroscopic line parameters using non-Voigt lineshapes (e.g. speed-dependent Voigt or Rautian) and a multi-spectrum fitting approach.  It is well known, however, that some line parameters determined from multi-spectrum fitting are correlated with each other, for example Dicke narrowing and speed dependence of the Lorentz halfwidth. The purpose of this project is to investigate whether there is an optimum set of laboratory conditions from which to determine a robust set of spectroscopic line parameters that reduce correlations between parameters as far as possible, and then determine how these correlations might propagate into uncertainties in atmospheric spectra calculations. This will be done by simulating spectra of carbon dioxide in air over a range of pressures, and using these to derive line parameters via multi-spectrum non-linear least squares fitting. The candidate will then perform simulations over typical atmospheric conditions to determine the uncertainty propagation.  The successful applicant will also have the opportunity to measure infrared spectra of CO2 at the Spectroscopy for Environmental Sensing Research (SPENSER) facility at Space Park Leicester. This facility, co-funded by NERC and the University of Leicester, houses a Bruker IFS 125HR Fourier transform spectrometer. The purpose of this state-of-the-art facility is to provide accurate, SI-traceable quantitative spectroscopic data for satellite remote sensing. | |
| **Project timeline:** | |
| The project duration is flexible, but expected to be at least 6 weeks. A possible timeline could be:  Week 1: Learn about gas phase molecular spectroscopy and the technique of infrared Fourier transform spectroscopy  Week 2: Simulate laboratory spectra for a band of CO2 over a range of pressures using existing line parameters  Week 3-4: Use the multispectrum non-linear least-squares fitting program LabFit to derive new spectroscopic line parameters from different combinations of simulated spectra; compare different fits  Week 5-6+: Investigate correlations between derived parameters, and how these might propagate into the uncertainties of spectra calculated at atmospheric conditions; optimise the selection of laboratory conditions for line parameter determination | |
| **Candidate requirements:** | |
| This project is largely computer-based, but will include some laboratory work. You must have experience with scientific computer programming. Some experience with Python is desirable. The placement will be based at Space Park Leicester, but there could be some flexibility in terms of remote working. Overall, this project is suitable for anyone who is eager to learn new things. | |
| **Background reading and references:** | |
| HITRAN2020 molecular spectroscopic database: <https://hitran.org/media/refs/HITRAN-2020.pdf>  HAPI: The HITRAN Application Programming Interface: <https://hitran.org/hapi/> | |

**To be completed by institutional CENTA PoC**

I confirm that:

* The host institution takes responsibility for selecting a suitable undergraduate student and ensuring eligibility (see NERC REP student eligibility requirements above) and confirming their eligibility using the UKRI criteria listed under the NERC REP student eligibility criteria
* This REP project falls within the NERC remit and is of suitable quality
* Appropriate supervisory arrangements are in place
* The student recruited to undertake this placement will have a PhD student mentor from the DTP/CDT
* The application processes used will be inclusive and accessible
* Reasonable adjustments will be made for students that need them whilst undertaking placements
* The placement will be carried out in accordance with all applicable ethical, legal and regulatory requirements including but not limited to relevant provisions of the General Data Protection Regulation, the Data Protection Act 2018, the Bribery Act 2010, the Fraud Act 2006, the Equality Act 2010 and the Modern Slavery Act 2015
* The host organisation takes responsibility for identification, protection and exploitation of any intellectual property rights arising from the work
* All facilities, agreements about access and collaborations necessary for the work will be obtained before the work commences and can be ensured through the period of the work
* All costs awarded by NERC for the REPs will be used and accounted for appropriately
* A report of the project by the student will be submitted no later than one week after the end date of the placement or Friday 27th September 2024, whichever falls first.

Signed: 

Date: 25/4/2024

Position: NCEO CENTA POC