SPECATMOS : "Spectroscopy and Atmosphere: Measurements and Modelling" International Summer School

Spectroscopic Databases Tutorial

Thibault Delahaye

Laboratoire de Météorologie Dynamique/IPSL, CNRS, Ecole Polytechnique, Université Paris-Saclay, 91128, Palaiseau, France

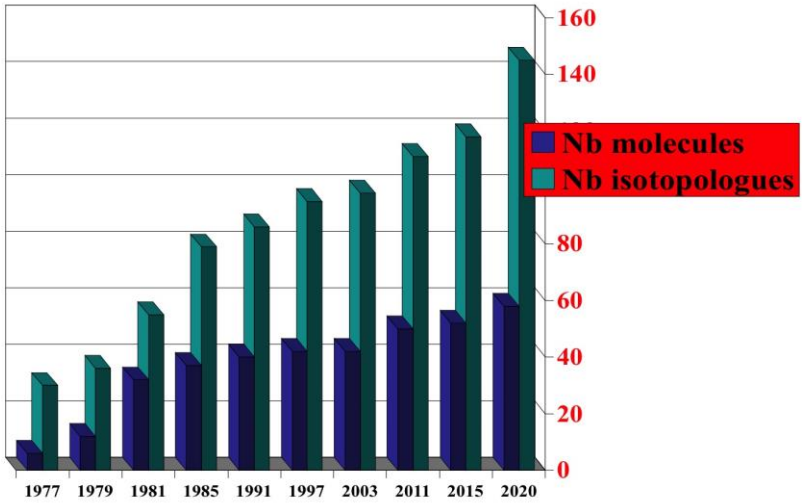
Introduction

- Adequate tools are required to perform reliable radiative transfer modelling calculations to meet the needs of communities involved in understanding the atmospheres of the Earth and other planets, especially with the emergence of highly sophisticated spectroscopic instruments (OCO-2, IASI-NG, Merlin…).
- Among these tools compilations of spectroscopic parameters are used for a vast array of applications and especially for planetary atmospheric remote sensing.
- There is an acute need for comprehensive, trustworthy and operational interactive spectroscopic databases to benefit the research in direct and inverse radiative transfer.
- The goal of spectroscopic databases is to have a self-consistent set of parameters.

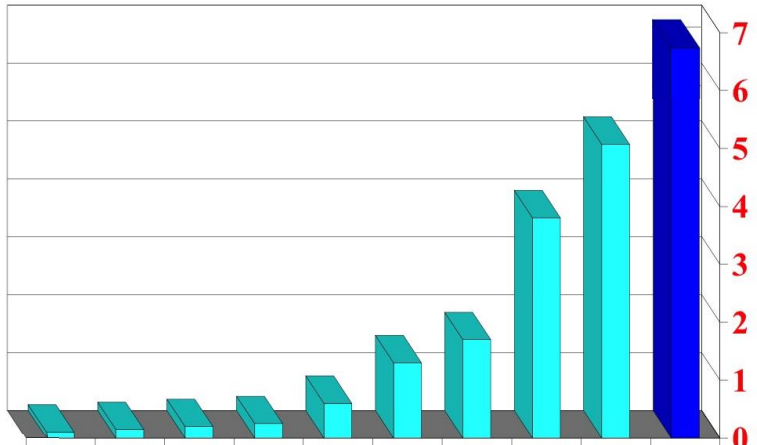
	Specific databases		Global/general databases		
Pure *ab initio* databases	ExoMol	TheoReTS	GEISA	HITRAN	Mix of experimental and theoretical data
Molecular linelists (O_3, CO_2…)	S&MPO	CDSD-4000	VAMDC Virtual Atomic and Molecular Data Centre		

GEISA2020 update

- GEISA (Gestion et Etude des Informations Spectroscopiques Atmosphériques), is developped and maintained at LMD since 1974.
- Use as reference database for several space missions: IASI, IASI-NG, MicroCarb, Merlin…
- Compilation of three databases: line-parameters, cross-sections and aerosols properties.
- **GEISA-2020 line-parameter database**: 6,746,987 lines (+33% vs GEISA-2015) on the spectral range 10^{-6} - 35,877 cm^{-1}.
- 23 updated and 6 new molecules (HONO, COFCl, CH_3F, CH_3I, RuO_4, $H_2C_3H_2$ (isomer of C_3H_4) – total of 145 isotopologues.



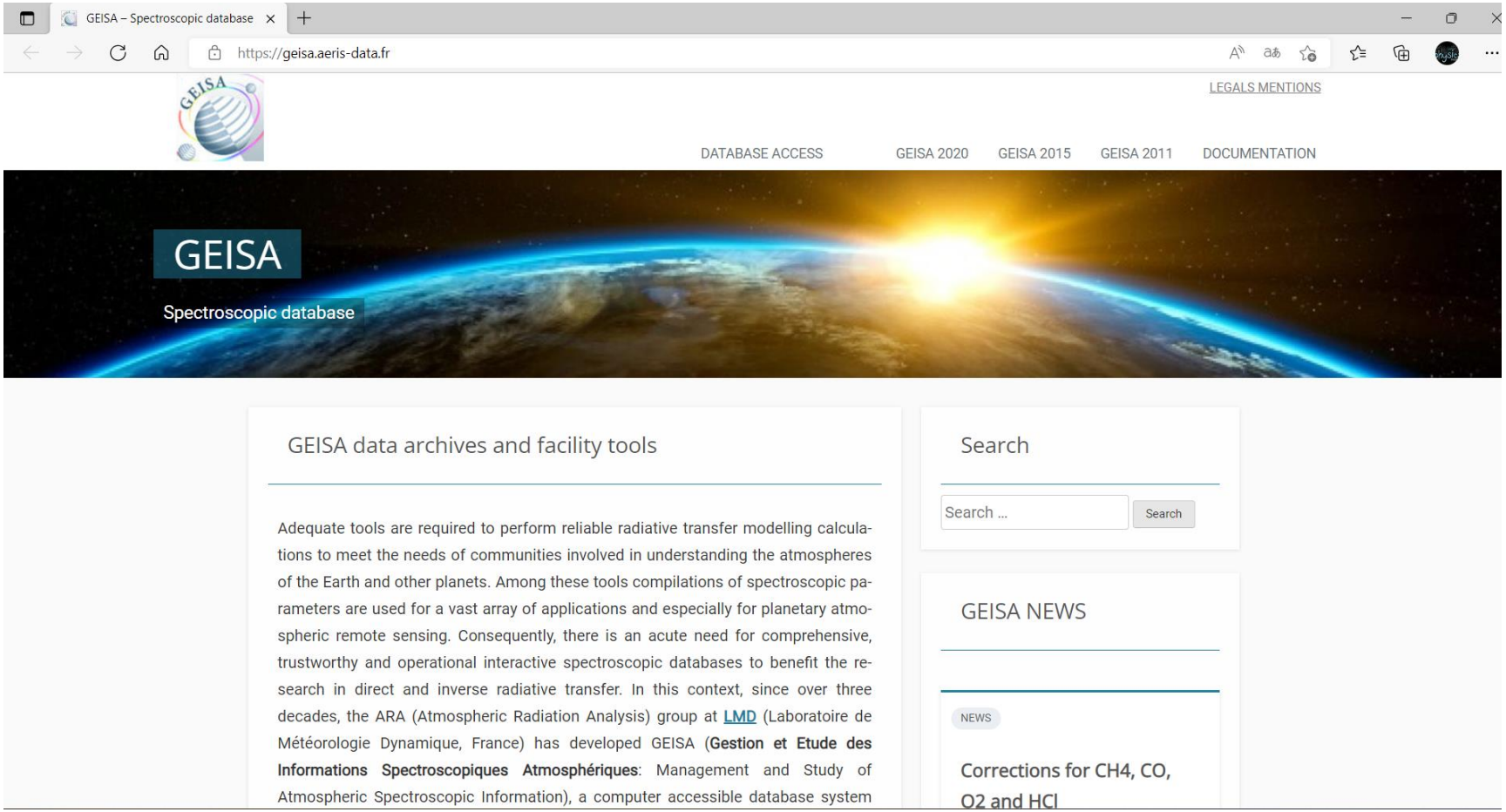
	1977	1979	1981	1985	1991	1997	2003	2011	2015	2020
Nb molecules	6	12	32	37	40	42	42	50	52	58
Nb isotopologues	30	36	55	79	86	95	98	111	118	145



	1977	1979	1981	1985	1991	1997	2003	2011	2015	2020
Nb lines (million)	0,1	0,15	0,2	0,25	0,6	1,30	1,70	3,80	5,07	6,75

GEISA access

https://geisa.aeris-data.fr/

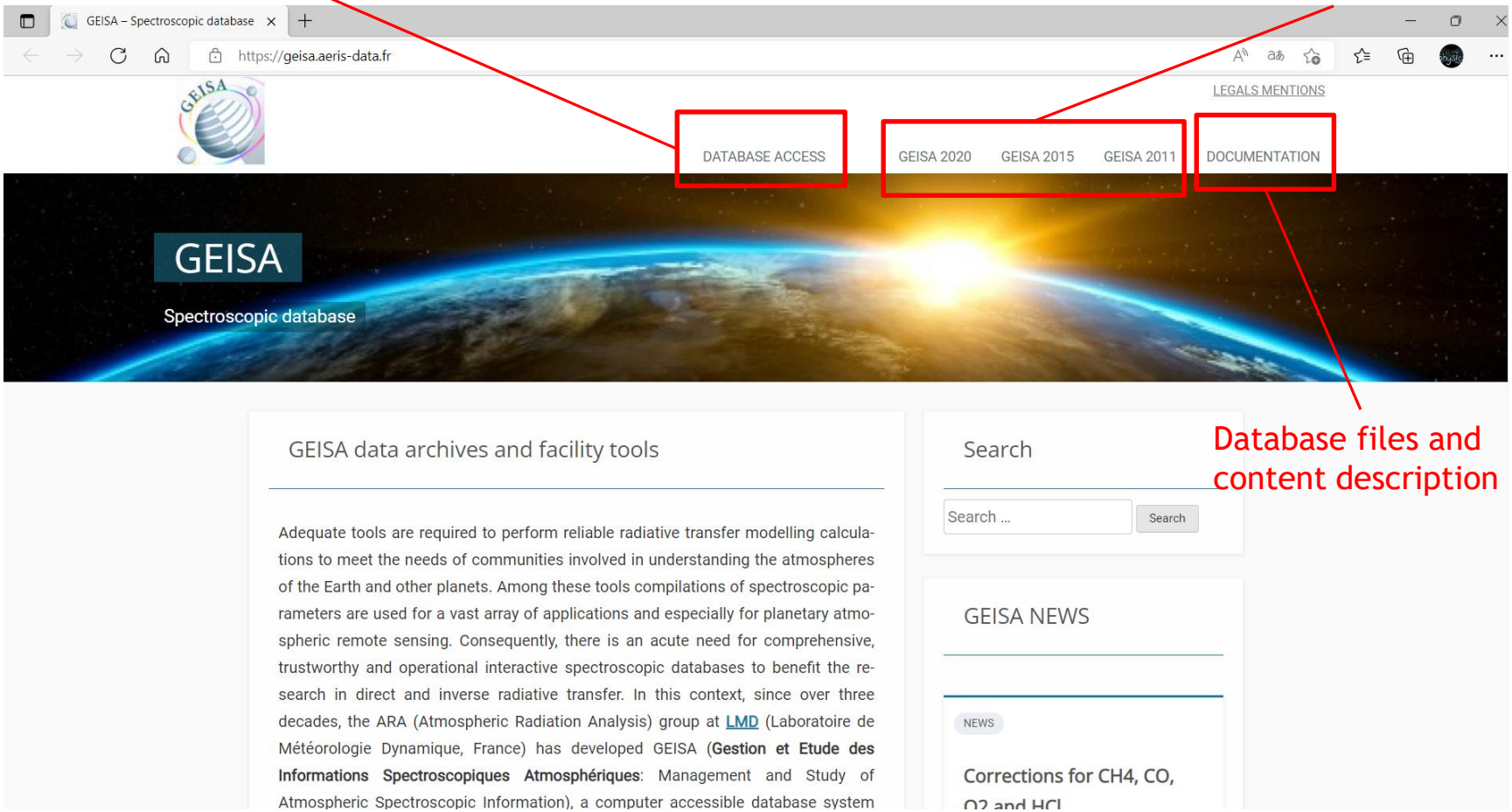


GEISA access

Main database access

https://geisa.aeris-data.fr/

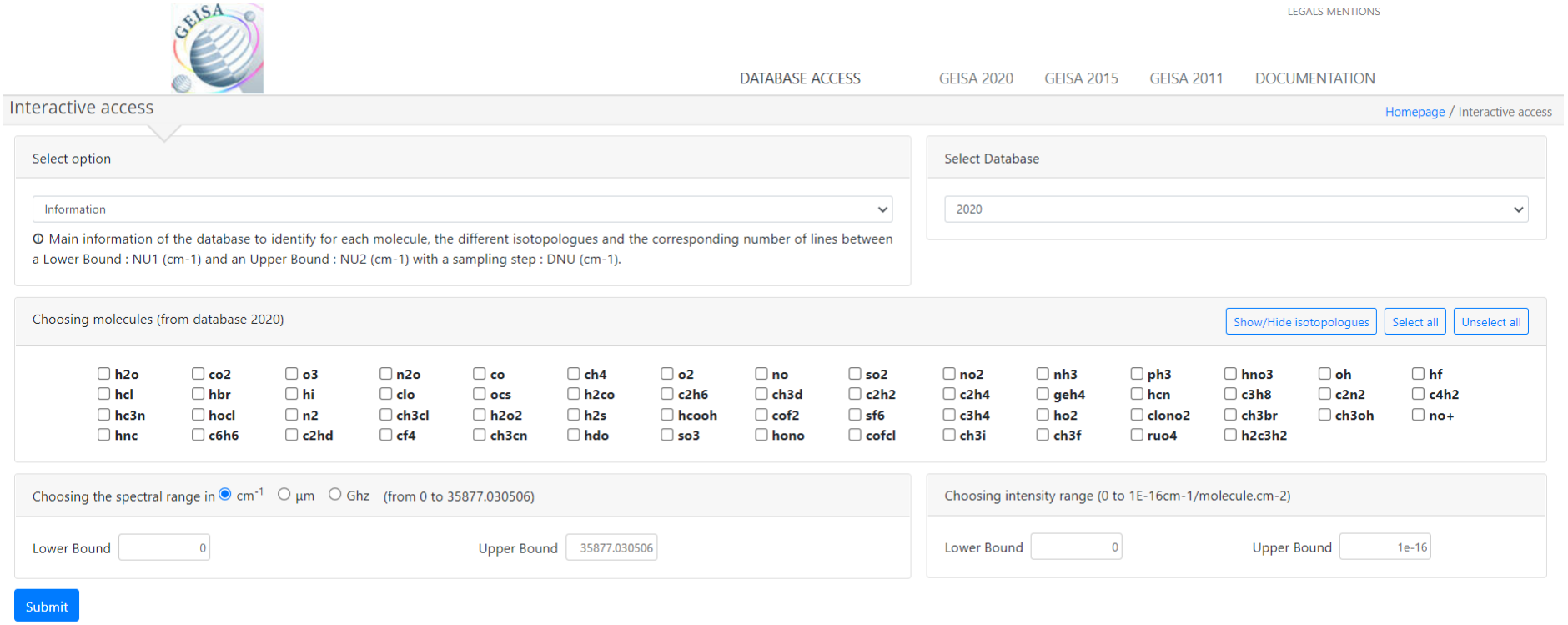
GEISA specific version description and access



Database files and content description

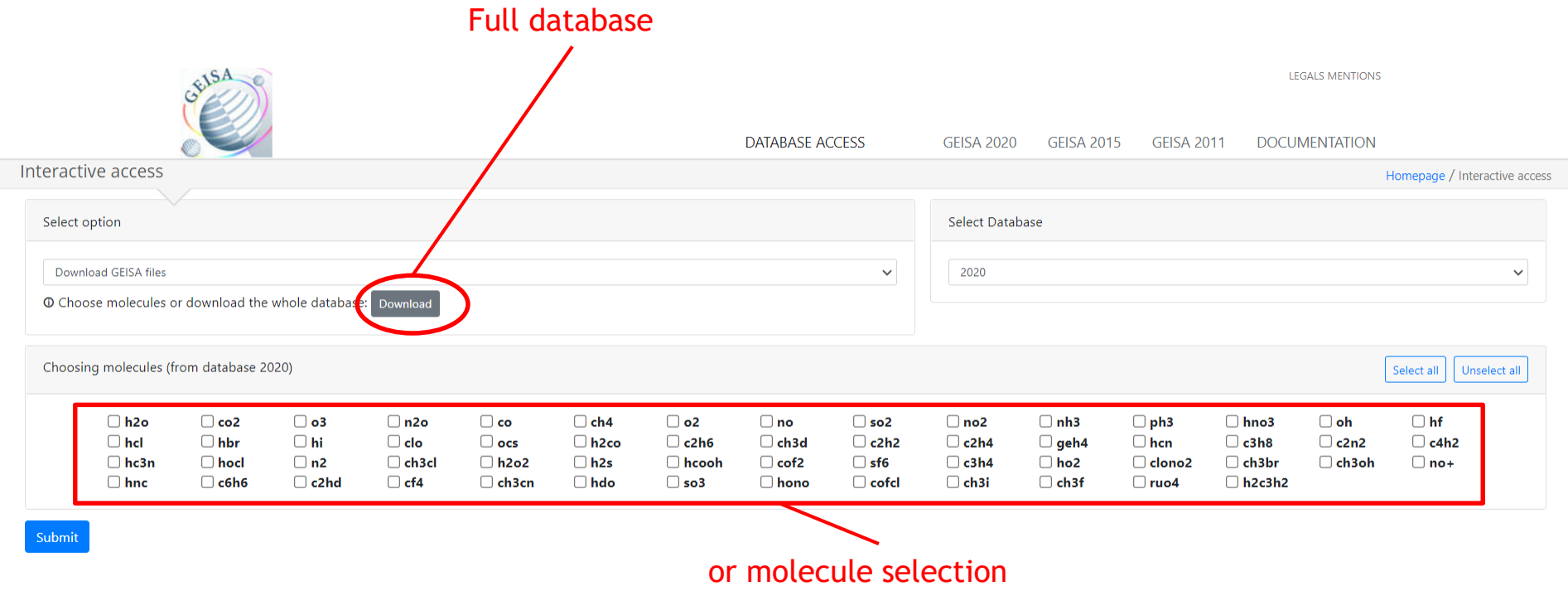
GEISA line parameters

- GEISA2020 line parameters: 6,746,987 lines (+33% vs GEISA-2015) on the spectral range 10^{-6} - 35,877 cm^{-1}.
- 23 updated and 6 new molecules (HONO, COFCl, CH_3F, CH_3I, RuO_4, $H_2C_3H_2$ (isomer of C_3H_4) – total of 58 molecules and 145 isotopologues.



GEISA line parameters

- Download the full database: Database Access -> Interactive access -> Download GEISA files
- The user can choose the version (2020, 2015, 2011) and download the full database or specific molecule files (ASCII format).



- The user can also extract a part of the database in the ‘Database extract’ tab.

Useful links

- GEISA database

  https://geisa.aeris-data.fr/

- Radis package

  https://github.com/radis/radis

- Simple spectrum calculation (RADIS-app)

  https://www.radis.app/

- Online environment for advanced spectrum processing and comparison with experimental data (RADIS-Lab)

  https://radis.github.io/radis-lab/

- Anaconda python distribution (for simple Radis installation)

  https://www.anaconda.com/products/distribution
  install RADIS using ‘cmd prompt’ executing ‘pip install radis -v’

Spectrum simulation

- For online spectrum simulation purpose, GEISA is interfaced with RADIS.

https://github.com/radis/radis

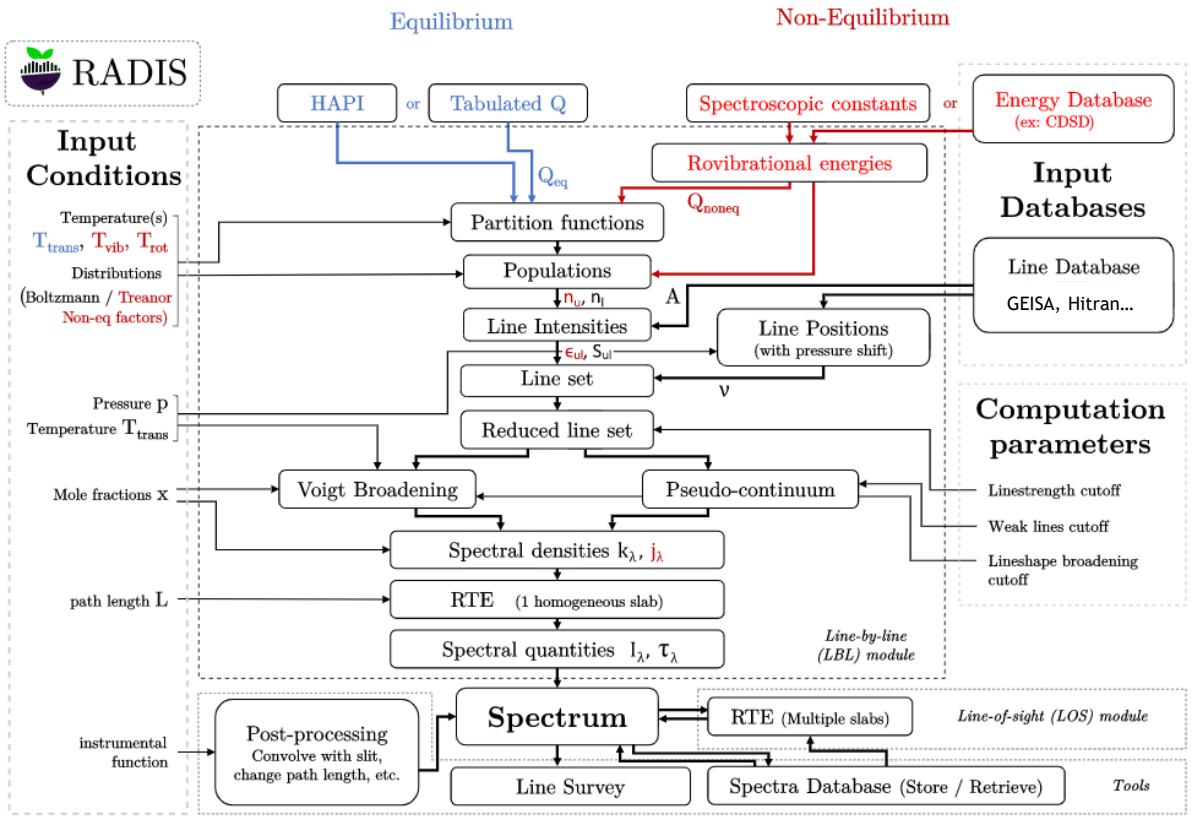
- RADIS is a fast line-by-line code for high resolution infrared molecular spectra (emission / absorption) based on GEISA/HITRAN/HITEMP/ ExoMol.

- It includes post-processing tools to compare experimental spectra and spectra calculated with RADIS or other spectral codes.

ELSEVIER
Journal of Quantitative Spectroscopy and Radiative Transfer
Volumes 222–223, January 2019, Pages 12-25

RADIS: A nonequilibrium line-by-line radiative code for CO_2 and HITRAN-like database species

Erwan Pannier, Christophe O. Laux



RADIS-app

- Simple online spectrum calculation RADIS-app (GEISA available in some days).
- Flexible gaz mixture configuration https://www.radis.app/

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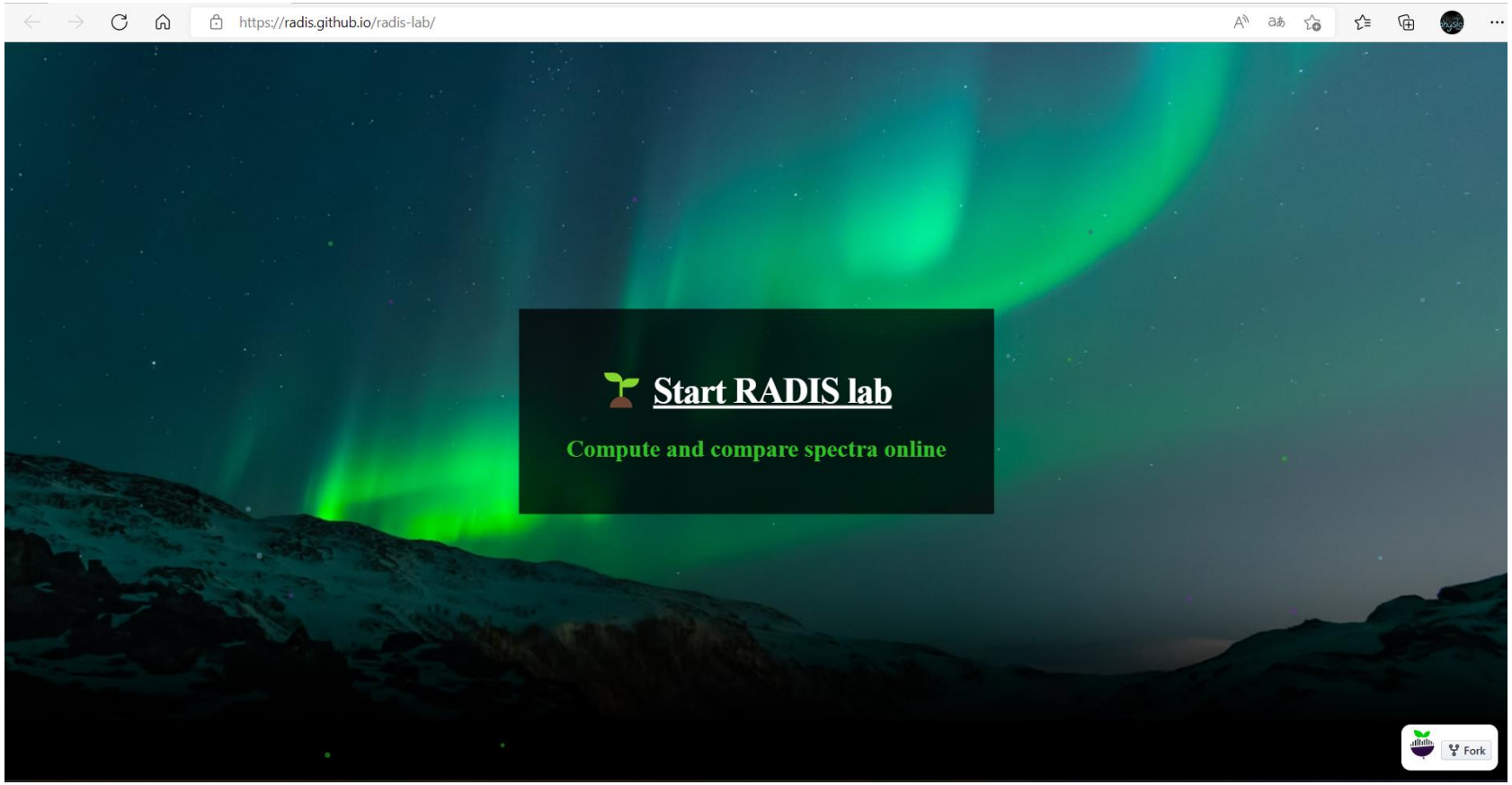
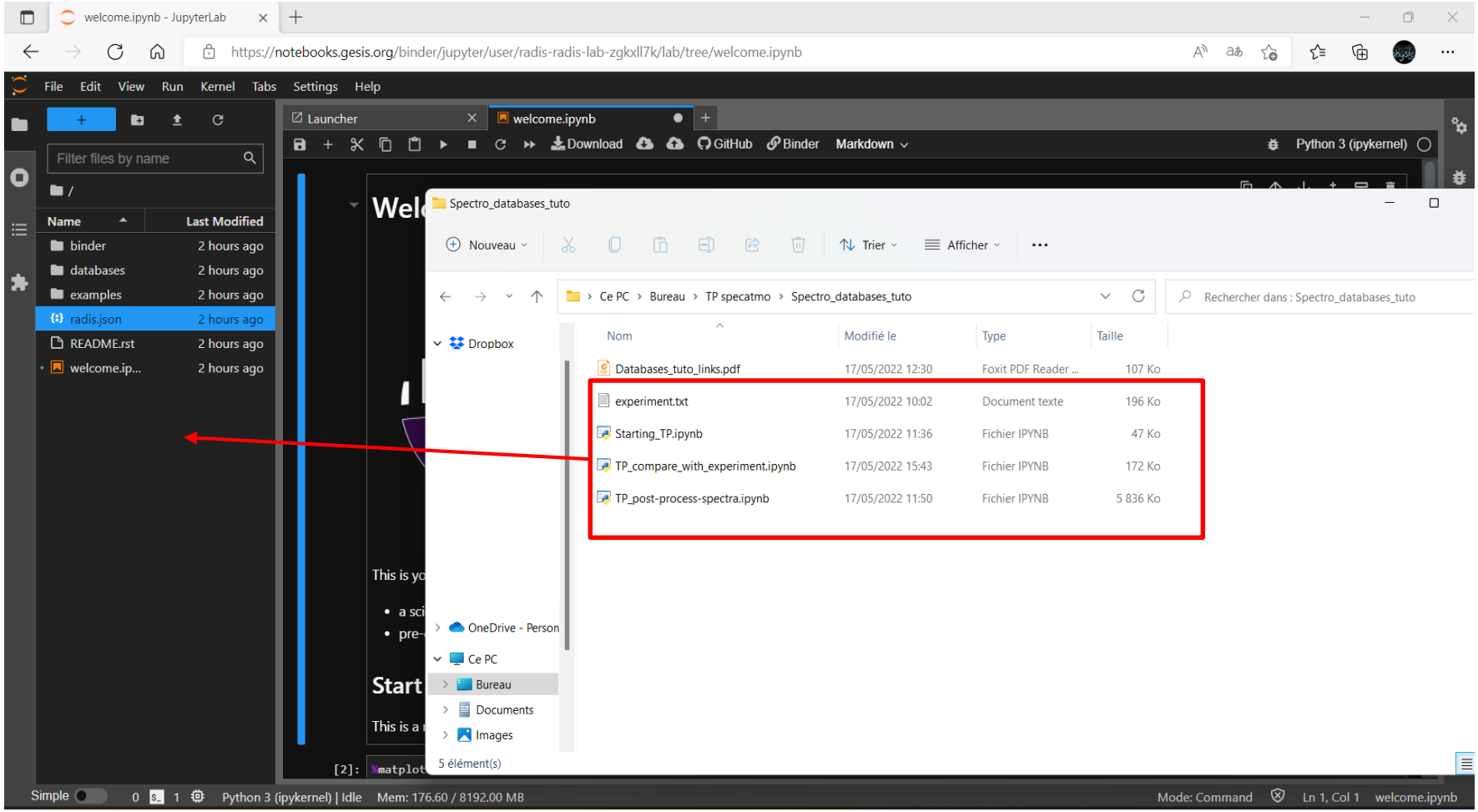


After the notebook is loaded, just drag and drop the following 4 files at the root:



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