RACER (RApid Calculation of Exoplanetary Radiative Opacities): a new PYTHON Package to Efficiently Calculate Opacities

David Haegele[1,2] and Paul Mollière[1]

[1] Max-Planck-Institut für Astronomie, Königstuhl 17, 69117 Heidelberg, Germany,

[2] Universität Heidelberg, Grabengasse 1, 69117 Heidelberg, Germany

With the expected revolution in high-resolution characterization of exoplanets with the ELT, accurate modeling of spectral features requires precise cross-sections of atoms and molecules. In this talk, I will present a new, easy-to-use Python package I am developing for calculating high-resolution opacities. A key feature is its numerical efficiency as the line lists are growing. For instance, the ExoMol methane line list currently contains about 50 billion lines, which significantly increases the computational time for opacity calculations. The rapid calculation of the individual line profiles is therefore crucial. To tackle this, our package combines a sampling method for molecular lines (M. Min, 2017) with the Humliček approximation of the Voigt profile to speed up the line profile calculations. This combination enables processing up to 2×10^6 lines per second per CPU core (depending on the pressure and resolution), making it possible to handle even the largest line lists efficiently. The package also allows the user to include sub-Lorentzian line wing treatments and multiple line broadening approaches, offering flexibility for various use cases. As input, the package supports the major spectroscopic databases ExoMol, HITRAN, HITEMP, VALD, and Kurucz. The resulting opacity data can be used directly with petitRADTRANS, a widely used atmospheric modeling and retrieval code, but can also be formatted in any other way that is specified by the user. At this workshop, I will ask for community input regarding additional features that may enhance usability in the community.