CLASSIFICATION OF PLANETARY ROCKS AND MINERALS BY COMBINING A CUSTOM MINERALOGICAL DATABASE WITH MACHINE LEARNING BASED MULTI-SPECTRAL UNMIXING. I. Drozdovskiy[1], F. Sauro[2], S.J. Payler[1, 3], S. Hill[4], P. Jahoda[4], K. Jaruskova[4], F. Venegas[4], A. Angellotti[4], M. Franke[4], P. Lennert[4], G. Ligeza[4], P. Vodnik[4], L. Turchi[1], L. Bessone[1] [1]Directorate of Human and Robotics Exploration, European Astronaut Centre (EAC) - European Space Agency (Linder Höhe, D-51147 Cologne, Germany; igor.drozdovskiy@esa.int), [2]Geological and Environmental Sciences, Italian Institute of Speleology - Bologna University, [3]Agenzia Spaziale Italiana, Rome, Italy, [4]ESA-EAC, CAVES & PANGAEA interns.

Introduction: The ESA-PANGAEA Mineralogical Toolkit is a combination of analytical methods together with reference datasets aiming to enhance the recognition of planetary minerals. It includes a custom structured database called the PANGAEA Mineralogical Database, which contains information on all known minerals found on the Moon, Mars and other planetary bodies [1]. This database then serves as the basis for a set of spectral classification methods using machine learning designed to perform in-situ spectroscopic identification of minerals [2]. Developed and tested together in the context of ESA's astronaut field science training using analogue environments, PANGAEA, the mineral library and the recognition software are conceived as real-time decision support tools for future planetary surface exploration missions.

PANGAEA Mineralogical Database: The Mineralogical database [1] can be viewed as two distinct products: a catalogue of petrographic information and an analytical library. The catalogue consists of petrographic information on all currently known minerals identified on the Moon, Mars, and in meteorites providing essential analytical information for rapid astromaterial identification and understanding of significance during planetary geological exploration. Each mineral entry includes: IMA recognized name, chemical formula, mineral group, surface abundance on planetary bodies, geological significance in context of planetary exploration (e.g., marker for important processes), number of collected VNIR and Raman spectra, their spectral discoverability and features. The database was compiled through systematic literature research, followed by the careful intercomparison of all mineral characteristic information. The second major part of the Mineralogical Database is a customized library of analytical data from all known planetary terrestrial analogue minerals. This covers reflective Visual-to-Near- & Shortwave-Infrared (VNIR), Raman vibrational (molecular) spectroscopy, Laser-Induced-Breakdown (LIBS), and X-Rays Fluorescence (XRF) atomic spectroscopy. This library also includes a set of reference spectra for evaluating the detectability of minerals with different analytical methods. The archive consists of high-quality spectra collected from available open access on-line catalogues, such as RRUFF (Raman), and USGS, RELAB and ECOSTRESS (VNIR) and our own collection of spectroscopic measurements of planetary analogue minerals taken by us and from different collections, and synthetic spectral libraries, such as LIBS NIST, see [2].

Machine Learning (ML) software for recognition of minerals from multispectral data: To utilize the Mineralogical Database for identifying minerals and their compositions from the output of analytical instrumentation, we also developed identification methods that combine types of material characteristics, mineral structure (obtained with VNIR and Raman spectra) and its chemical composition (from XRF and LIBS spectra). To achieve this, we evaluated various ML approaches used to identify mineral species from single analytical methods (Raman, VNIR or LIBS), and developed a flexible and modular algorithm that can classify minerals and their compositions (rocks, soils) either from one or pair-combined spectroscopic methods. Our new approach was then evaluated using our customized library of spectroscopic data from PANGAEA Mineralogical Database. Our cross-validation tests show that multi-method spectroscopy paired with ML paves the way towards rapid and accurate characterization of minerals [2], as well improving the quantification of mineral abundances in rocks and soils using ML-based spectral unmixing.

PANGAEA Mineralogical Tookit as an Analytical Toolset for Planetary Geological Exploration: The PANGAEA Mineralogical Toolkit is envisioned as a part of the PANGAEA Electronic Fieldbook Suite (EFB) [3], a deployable system supporting field science operations. The EFB can interface with handheld spectrometers intended for planetary exploration, simultaneously feeding their measurements into the embedded Mineralogical Toolkit. Combined within the EFB with various spectral analytical tools and benefiting from its instrument agnostic nature the PANGAEA Mineralogical Toolkit will enable fast and reliable in-situ recognition of rocks and minerals, thus becoming a crucial decision support tool for future human and robotic planetary surface exploration missions.

References: [1] Drozdovskiy, I. et al. 2020, *Data in Brief*, 31, 105985. [2] Jahoda, P. et al. 2020, *The Analyst*, 146(1), pp.184-195. [3] Turchi L. et al. *Planetary Space Science*, 197, p.105164.