SYNTHETIC DATA EXPLORATION OF MESSENGER/XRS SPATIAL RESOLUTION AND SENSITIVITY LIMITS. M. D'Amore[1], N. Verma[1], O. Barraud[1], K. Frizzell[2] , L. R. Nittler[2]. [1]Institute for Planetary Research, DLR, Rutherfordstrasse 2, 12489 Berlin, Germany (mario.damore@dlr.de), [2]ASU School of Earth and Space Exploration, Tempe, AZ 85287-6004, USA.

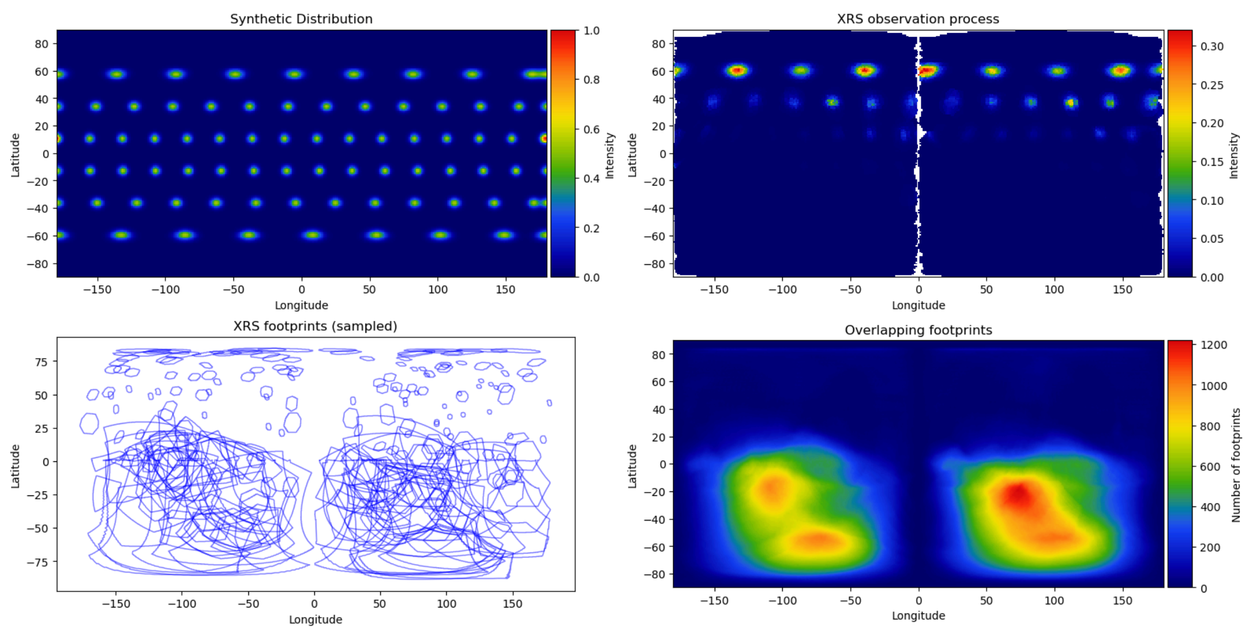
Introduction: The NASA MESSENGER mission, which orbited Mercury from 2011 to 2015, provided a wealth of data on the planet's surface composition, topography, and geology. One of the key instruments aboard MESSENGER was the X-ray Spectrometer (XRS)[1], which measured the elemental composition of Mercury's surface by detecting X-ray fluorescence emitted from the planet's surface when it was bombarded by solar X-rays. While the XRS provided valuable insights into Mercury's global composition, it suffered from limitations in spatial resolution, particularly at southern latitudes. This is due to the instrument's design and the geometry of MESSENGER's highly elliptical polar orbit. To address this limitation, we propose a novel approach to enhance the spatial resolution of XRS-derived compositional maps. By leveraging the redundancy in the XRS data and employing advanced image processing techniques, we aim to extract finer-scale details from the XRS mosaics. This method, which we refer to as *synthetic hyper-resolution*, has the potential to reveal new insights into Mercury's surface composition and geological history.

Methodology: The methodology for this study involves a comprehensive approach to simulate high-resolution elemental maps, process them through the XRS spatial resolution and mosaicking pipeline, and analyze the resulting maps. This approach is divided into two main steps: Synthetic Map Analysis and Inverse Modeling with Machine Learning. The machine learning approach is a future goal, and this work represents the first step towards achieving it.

In this first step, several high-resolution synthetic elemental maps are created to represent different surface distributions of elements such as Mg/Si, Al/Si and so on. Each element required a minimum threshold solar activity to generate enough signal, so each one was observed in a different set of XRS observations, tied to solar activity.

These maps are designed to mimic realistic geological scenarios on Mercury's surface and to address key questions about the XRS data. One key aspect of the synthetic map generation is to determine the source separation that the XRS can detect. By placing synthetic single sources in the maps and varying their separation in kilometers, we can evaluate the minimum distance at which the XRS can distinguish between two sources. This analysis takes into account the variable footprint size of the XRS instrument with latitude, particularly noting that the resolution decreases in the southern hemisphere due to the MESSENGER spacecraft's orbit.

Another important aspect is to analyze groups of synthetic single sources to understand how they contribute to enrichment patterns observed in the XRS



Mg map. By placing groups of sources in different configurations and locations on the synthetic maps, we can identify regions on Mercury's surface where these groups result in enrichment patterns similar to those detected by the XRS. This helps in understanding the spatial distribution and concentration of elements like magnesium

Next, the synthetic maps are processed through a simulated XRS spatial resolution filter, which accounts for the variable footprint size of the XRS instrument with latitude. This step reduces the resolution of the maps to match the XRS data.

In this work, each single XRS FOV is loaded as a Polygon, rasterised to the same pixel resolution as the synthetic maps. Finally we extract the average values under the FOV from each map and assemble in a 3 dimensional data cube (longitude, latitude, n. FOVs). The data cube is compressed to a map calculating the median or each pixel. These lower-resolution maps are then passed through a mosaicking process to create final maps that resemble the actual XRS mosaics produced by the MESSENGER mission.

The analysis phase involves evaluating the impact of spatial resolution on the detection of small-scale features by comparing the high-resolution input maps with the processed lower-resolution maps. The point spread function (PSF) of the XRS mosaics is estimated by analyzing how point sources in the synthetic maps are spread out in the final maps. Additionally, the minimum detectable size of high-concentration regions is determined by varying the size and separation of high-value spots in the synthetic maps and observing their detectability in the final maps.

Future work: In a future step, Inverse Modeling with Machine Learning, a large number of independent random distributions are automatically generated to create a diverse dataset for training and testing. The generation of synthetic maps and processes them through the established XRS pipeline, creating a comprehensive dataset of input-output pairs. This step lays the groundwork for future machine learning applications. A neural network will be designed to take the lower-resolution XRS maps as input and predict the original high-resolution elemental distributions. The neural network will be trained using the dataset of synthetic maps and their corresponding XRS-processed maps. The training process will include techniques to handle noise and variability in the data. Finally, the trained neural network will be used to infer the original high-resolution distribution from the lower-resolution XRS maps, providing uncertainty estimates for the inferred distributions. Machine learning tools will be employed to account for errors and uncertainties in the data, enhancing the robustness of the inferred results. By integrating these future steps and current work, this methodology provides a detailed and practical approach to quantify the uncertainties and limitations of the XRS data from the MESSENGER mission. The combination of synthetic map analysis and future machine learning-based inverse modeling offers valuable insights into the spatial resolution and detectability of elemental distributions on Mercury's surface.

Conclusions: This work presents a detailed methodology for quantifying the uncertainties and limitations of the XRS data from the NASA MESSENGER mission. By generating high-resolution synthetic elemental maps and processing them through a simulated XRS spatial resolution and mosaicking pipeline, we can better understand the impact of spatial resolution on the detection of small-scale features and the overall quality of the XRS mosaics. The synthetic map analysis evaluates key characteristics of the XRS observations, such as the minimum source separation detectable by the instrument and the spatial distribution of elemental enrichments. This approach provides valuable insights into the capabilities and limitations of the XRS instrument, helping to quantify detection limits and point spread functions. While the machine learning approach for inverse modeling is a future goal, this study establishes a robust pipeline for synthetic map generation and analysis. By addressing the uncertainties and limitations of the XRS data, this work contributes to a more accurate and detailed understanding of Mercury's surface and its geological processes, with potential applications to other planetary missions with similar instruments.

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References: [1] Nittler L. R. *et al.*, *Icarus*, Feb. 2020.