ÉCOLE DOCTORALE
SCIENCES DE LA TERRE ET DE L'ENVIRONNEMENT
ET PHYSIQUE DE L'UNIVERS, PARIS

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Subject title: Exploring nanoparticle dynamics in terrestrial and extraterrestrial environments using spICP-ToF-MS: Methodological advancements and challenges.

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Host lab/ Team: **IPGP – Teams CAGE, ACE – UMR 7154**

Financing: Doctoral contract with or without teaching assignment

Scientific context. Nanoparticles (NPs) play crucial roles in natural systems, including the lithosphere, hydrosphere, atmosphere, and extraterrestrial environments. Understanding their behavior, composition, and distribution is essential for various fields, including nano-geochemistry and cosmochemistry. However, existing analytical techniques face challenges in accurately characterizing NPs, hindering comprehensive insights into their roles in natural terrestrial and extraterrestrial processes.

The emergence of single-particle time-of-flight inductively coupled plasma mass spectrometry (spICP-ToF-MS) has revolutionized NPs characterization by allowing unparalleled investigations. However, analytical and methodological challenges persist, necessitating advanced data-driven approaches to maximize the information returned by the analyses.

Challenges.

1. Sensitivity enhancing: improve the sensitivity of spICP-ToF-MS for pinpoint detection of nanoparticles.
2. Noise nixing: tackle background noise to reveal clear nanoparticle signals.
3. NPs Source investigating: develop versatile methodologies to characterize nanoparticles from different sources and identify their mineralogical composition.
4. Data mining: Explore deeper into nanoparticle behavior with advanced data analysis techniques.

Proposed research objectives.

Advances in analytical techniques is key to make progress for elucidating complex processes in extraterrestrial and terrestrial systems. At present, one major difficulty is to be able to describe the chemistry and mineralogy (and in some cases the isotopic composition) of thousands of nanoparticles from a given sample.

A critical challenge in nanoparticle characterization by spICP-ToF-MS is the accurate detection and characterization of nanoparticles amidst instrumental noise. By conducting comprehensive analysis and optimization of spICP-ToF-MS data acquisition parameters and instrument settings, we propose to enhance the accuracy and sensitivity of nanoparticle detection and characterization. Through meticulous calibration and tuning, we will minimize background noise and maximize signal sharpness, improving our ability to reconstruct the composition and size distributions of nanoparticles in a given sample.

The methodologies thus developed will be used to analyze nanoparticles extracted from various samples. A few case studies will be selected to (i) understand the dynamics of nanoparticles in environmental systems and provide information on processes such as element transport, weathering and pollutant dispersion, thus contributing to environmental monitoring and remediation efforts, and (ii) obtain a statistically significant characterization of sub-micrometric phases in the matrix of primitive chondritic meteorites in order to constrain the origin and dynamics of dust in the accretion disk during the early evolution of the solar system.

Methodology and expected contributions.

1. Analytical chemistry investigation: Conduct comprehensive analysis and optimization of spICP-ToF-MS data acquisition parameters and instrument settings to enhance the accuracy and sensitivity of NP detection and characterization.
2. Advanced data-driven approaches: Develop novel methodologies integrating Bayesian inference, neural networks, and clustering algorithms for robust noise modeling, signal detection, and NP characterization in spICP-ToF-MS data.
3. Comprehensive NP characterization: Apply the developed methodologies to analyze NPs extracted from diverse sources, providing insights into their composition, size distribution, and spatial distribution.
4. Enhanced analytical framework: Advance statistical and machine learning frameworks tailored for facilitating deeper insights into NP behavior and interactions in the different systems.
5. Geo- and cosmo-chemical insights: Explore the composition, size distribution, and spatial distribution of NPs within terrestrial and meteoritic materials, contributing to our understanding of the formation and evolution of the solar system and the Earth.

Work environment. The proposed project will be carried out at the Institut de physique du globe de Paris, in close collaboration with Pr. Leonard Seydoux (team Seismology). IPGP hosts a world-leading geochemistry platform (PARI), equipped with an operational spICP-ToF-MS instrument. We possess an extensive dataset of spICP-ToF-MS measurements for both engineered and natural NPs as well as glass standard NPs. This dataset will serve as the foundation for algorithm development and testing. Additionally, through various collaborations in France (LiPADE, Université Gustave Eiffel) and abroad (University of Graz, Colorado School of Mines...), we can simulate spICP-ToF-MS time-series for training and validation of the developed methodology.

Scientific background of the candidates. To be successful, the candidate should have a background in analytical chemist with knowledge in data science and geochemistry. He/She should demonstrate its teamwork capabilities and have good communications skills in English (written and oral).

Application. Application should be sent as soon as possible by email to the 3 supervisors. It should include:

1. A CV
2. A motivation letter (1 page maximum)
3. We also request at least one recommendation letter from previous supervisors

Interviews for pre-selected candidates will be made shortly after application deadline.