**PaNOSC USE CASE TEMPLATE**

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| **Title\*** | **Submitted by\*** |
| Short description of use case | Who submitted the use case |
| **Partner(s)\*** |
| PaNOSC partners involved |

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| **Scientist\*** | **Date\*** |
| Names of some scientists (and their affiliations) who have requested and will use the service | DD/MM/YYYY (creation date of use case) |

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| **Objective\*** |
| Longer description of the use case including a description of the scientific objectives of the use case |

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| **Description of needs \*** |
| Description of what the use case is requesting from PaNOSC |

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| **Main Contributors\*** | |
| Contributor 1 | Description of the contributors, their role in the use case and what they contribute |
| … |  |
| Contributor N |  |

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| **PaNOSC work packages** (to be filled in by PaNOSC) | |
| WP 1 | Name of PaNOSC WP use case is related to and which tasks |
| … |  |
| WP N |  |

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| **Use case action flow** | |
| 1: Step Name | Description of step 1 |
| … |  |
| N: Step Name |  |

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| **Impacts from the implementation\*** |
| Description of scientific and technical impacts for users |

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| **Generalisation of Use Case** | **Partners** |
| Description of the possible take up of the solution by other PaNOSC or ExPaNDS partners and the scientific community in general. A description of application of the use case to other users. | Other partners interested in this use case |

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| **Resources** |
| Description of software and/or source code repositories to be used. |

**USE CASE EXAMPLE – Jupyter notebooks for Cultural Heritage @ ESRF**

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| **Title\*** | **Submitted by\*** |
| Generic Jupyter notebooks for analysing cultural heritage data | A.Götz |

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| **Scientist\*** | **Date\*** |
| M.Cotte (ESRF), M.Burghammer (ESRF), V.Gonzalez (Rijks Museum), C.Rivard (SOLEIL) | 05/11/2020  (of use case) |

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| **Description\*** |
| The goal will be to perform 2µXRD maps on painting fragments from various historical paintings. |

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| **Objective(s)\*** |
| To improve the efficiency of the experiment (many different users, a possible regular beamtime, remote experiment), I think it would help a lot to have a dedicated Jupyter notebook for data processing. It would be a good way i) to save time, ii) to record which map has already been processed and how, iii) and have a coherent data processing between users and between sessions, and also for possible users who would like to reuse data after the embargo period. |

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| **Request\*** |
| Provide users with .hdf5 post azimuthal integration maps, so the Jupyter notebook should mainly take care of PyFAI integration of 2D maps.   It would be good as well to preliminary check the integration on the average of the map (on max or mean) (for example to check that there is no sudden modification of the set-up, such as energy, distances...)   To be discussed if the calibration of the set-up (obtaining the .poni file) should also be included or be available on a separate file (this will probably be of interest for many experiments at ID13). |

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| **Main Contributors\*** | |
| L.Huder | Scientific software developer will develop python scripts + notebooks + HDF5 |
| J.Kieffer | Scientific software developer author and expert in pyFAI and parallel computing |
| W.de Nolf | Expert in 2uXRD data analysis and HDF5 |

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| **PaNOSC work packages** | |
| WP 3 | Metadata definitions, HDF5 + Nexus formats |
| WP 4 | Data analysis services using Jupyter notebooks |

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| **Use case action flow** | |
| 1: Extract data | Write python scripts to extract data from raw data files |
| 2: Radial integration | Write python scripts to call pyFAI in highly optimised way |
| 3: Combine maps | Stitch integrated data together to make 2D/3D maps and output an HDF5 file |

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| **Impacts from the implementation\*** |
| The goal will be to perform 2µXRD maps on painting fragments from various historical paintings |

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| **Generalisation of Use Case** | **Partners** |
| The side goal from a methodological point of view is to assess the implementation of a "BAG" type proposal, but on a non-MX beamline: this means offering an efficient way to many users requiring the same set-up but for very few shifts to group their requests, such that we can welcome many users, and we do not lose too much time in the set-up (avoiding to have one proposal = one set-up per user). | SOLEIL  any sites doing mapping of cultural heritage samples |

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| **Resources** |
| pyFAI, Jupyter, slurm, silx, h5py, NeXus |