Grant Agreement No: 101057511

EURO-LABS

EUROpean Laboratories for Accelerator Based Science

HORIZON-INFRA-2021-SERV-01-07 Project EURO-LABS

MILESTONE REPORT

ML toolkit prototype (GeOFF) available on a shared platform

MILESTONE: MS37

Document identifier:	EURO-LABS-MS37
Due date of milestone:	End of Month: April 2023
Justification for delay:	[No]
Report release date:	19/04/2023
Work package:	WP5 Open, Diverse and Inclusive Science
Lead beneficiary:	GSI
Document status:	Final

Abstract:

Within EURO-LABS, the source code of the Machine Learning toolkit prototype has been made available on a shared platform as part of Task 5.3. The Generic Optimization Framework and Frontend (GeOFF) is available under the GNU Public License Version 3 (GPLv3) and hosted on CERN's Gitlab server. The current address is: "https://gitlab.cern.ch/geoff/geoff-app/". It can be reached from EURO-LABS webpage through the link https://web.infn.it/EURO-LABS/results/

The EUROpean Laboratories for Accelerator Based Science (EURO-LABS) project has received funding from the European Union's Horizon Europe Research Infrastructure (RI) services advancing frontier knowledge under Grant Agreement no. 101057511. EURO-LABS began in September 2022 and will run for 4 years.

Delivery Slip

	Name	Partner	Date
Authored by	**Sabrina Appel, Nico Madysa**	**GSI**	**04/04/23**
Authored by	**Sandrine Dobosz Dufrenoy**	**CEA**	**04/04/23**
Edited by	**Sebastian Rothe**	**CERN**	**04/04/23**
Reviewed by	**Maria Borge [WP coordinator]**	**CSIC**	**11/04/23**
Approved by	**Navin Alahari [Scientific coordinator]**	**GANIL**	**19/04/23**

TABLE OF CONTENTS

1. INTRODUCTION

EURO-LABS is a network of 33 research and academic institutions from 18 countries (25 beneficiaries and 8 associated partners) from European and non-EU countries, involving 47 Research Infrastructures in the Nuclear physics, Accelerators and Detectors for high energy physics pillars. Within this large network, EURO-LABS will ensure diversity and actively support researchers from different nationalities, gender, age, grade, and variety of professional expertise. The project brings together, for the first time, the three research communities of nuclear physics, accelerator and detector technologies for high energy physics, in a pioneering super-community of sub-atomic scientists. It provides effective access to a network of 47 Research Infrastructures (including 3 RIs with Virtual Access) to conduct curiosity-based research, addressing fundamental questions and technological challenges and advancing projects with broad societal impact, fostering knowledge sharing between scientific fields and enhancing Europe's potential for successfully facing future challenges.

EURO-LABS project is structured in six work packages (WP); of those one is dedicated to project management and another to ethical requirements. WP5 of EURO-LABS promotes several activities aiming at open, diverse and inclusive science.

One of the main goals of EURO-LABS is to enhance the competitiveness of our research infrastructure and its technical capabilities.

Within WP5, Task 5.3 aims to use Machine Learning (ML) methods to improve beam characteristics, transport efficiency and reproducibility of accelerator tuning, which will reduce the beam preparation time. The challenges of applying ML algorithms for accelerators are shared and tackled by several facilities. This task will focus on open tools and platforms, and will provide an platform where a development of ML and optimization toolkit will be available. We will develop a virtual accessible beam diagnostic data and an optimizer toolkit for accelerator experts and users.

The first objective is dedicated to beam control and optimization. To this aim we provide GeOFF (Generic Optimization Framework and Frontend), an ML and optimization toolkit for beam control that makes available a wide variety of open-source optimization routines and machine-learning algorithms. The main goal of Task 5.3 is to use GeOFF at different facilities for optimization and with it to be able to improve the accelerator performance at various facilities. This document describes GeOFF and reports on Milestone 5.3 (MS37), which involves the release of the source code as a prototype on the hosting platform.

2. THE ML OPTIMIZER TOOLKIT

The **Ge**neric **O**ptimization **F**ramework and **F**rontend (GeOFF) is an open-source toolkit being developed initially at CERN and has recently been introduced at GSI. Development continues in collaboration between the two institutes. The goal of GeOFF is to reduce the complexity of combining a variety of optimization and ML algorithms on one hand with any number of facility-specific optimization problems on the other. It is available under the GNU Public License Version 3 (GPLv3) on CERN's Gitlab instance at "https://gitlab.cern.ch/geoff/geoff-app/". This project page hosts the code, which is publicly accessible, as well as installation instructions, a bug reporting tool ("issue tracker") and a "wiki" in which frequently asked questions are answered.

In its current state, GeOFF is a graphical application for generic numerical optimization and reinforcement learning. It is widely used at CERN, see Figure 2.1. With GeOFF, the user can easily define facility-specific optimization problems, switch between algorithms without modifying the program code and directly evaluate and compare both algorithms and optimization problems.

Conceptually, *GeOFF* has three components. The first component is a program library that provides a number of open-source optimization and ML libraries. The user can switch between algorithms without having to adjust any part of their own program due to a uniform program adapter interface. For example, COBYLA – the popular derivative-free optimization algorithms invented by Michael J. D. Powell – and BOBYQA – its successor – are implemented in separate packages. The two packages follow slightly different conventions in how they are invoked, e.g. parameter names and shapes. The adapter interface provided by GeOFF hides these differences and provides the same interface to both algorithms.

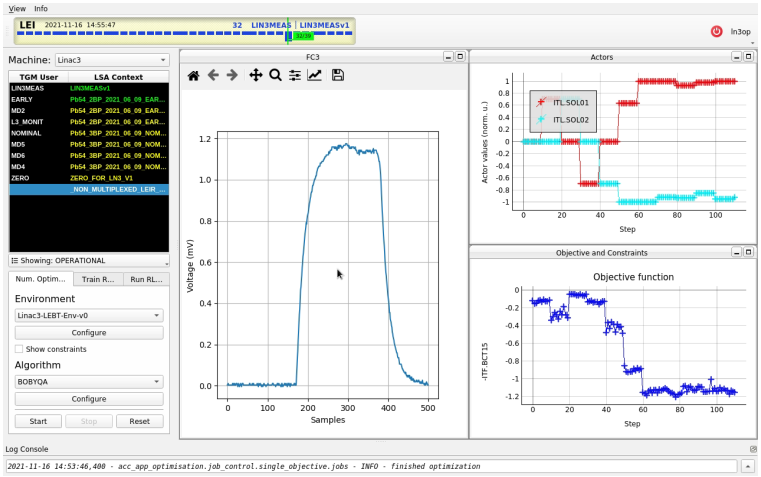

Figure 2.1: Generic Optimization Frontend and Framework (GeOFF) is the graphical application for generic numerical optimization and reinforcement learning. GeOFF has been used extensively for accelerator optimization at CERN. Here the Linac3 solenoid optimization is shown.

The second component of GeOFF specifies a standardised programming interface for optimization. This encapsulates the technical details of any user case so that a generic application can solve a given

problem without being aware of its concrete intricacies. This concept constitutes the major advantage for the user of GeOFF. Although GeOFF is in a prototype state, the experience at CERN shows that the integration of new accelerators and optimization problems is easy and possible in only a few hours. A website extensively documenting the programming interface is available at "https://cernml-coi.docs.cern.ch/index.html". It is partially supported by a suite of validation routines. A number of written tutorials and examples make it easy to introduce to technical and scientific staff having only moderate programming experience to the framework, see Figure 2.2.

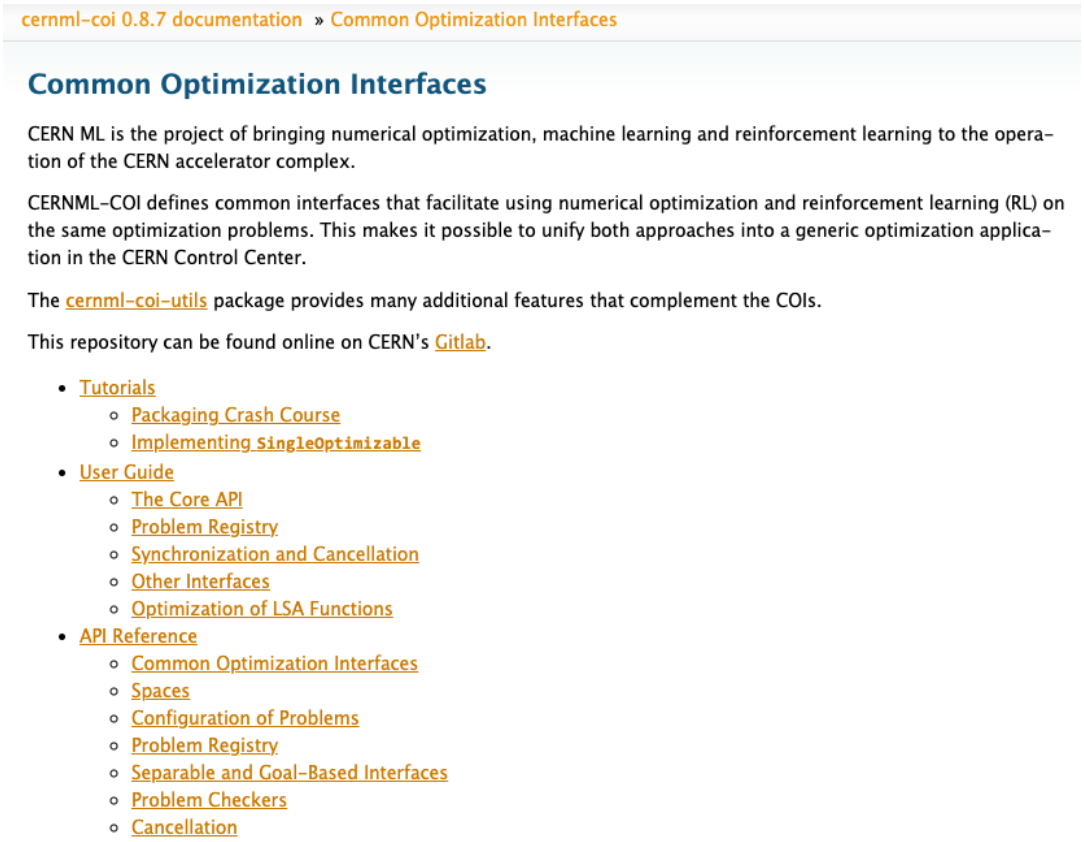

Figure 2.2: List of supporting documents for the programming interface including written tutorials and examples available on the website.

The third component is an application with a graphical user interface (GUI) that unifies the first two components and exchanges messages between them. With this, any supported optimization algorithm can be applied to any supported optimization problem. This facilitates experimentation and evaluation of algorithms and optimization problems. The framework is modular and encourages extension and customization to adjust it to each facility's specific needs. For example, the GUI allows optimization problems to generate their own graphs that are updated on-line during optimization to monitor progress. Optimization problems can further be made *configurable*, i.e. they can declare settings that the user can change in the GUI before optimization. In such cases, the GUI automatically generates a dialog window in which the user can make these changes.

A survey has shown that it has been used extensively by machine experts of most of the CERN accelerators during the commissioning phase. Feedback was generally positive and suggestions for further development have been made. All respondents expressed their desire to continue or even extend the use of GeOFF.

One of the next immediate goals for the EURO-LABS project is to further modularize the GUI application to remove dependencies on CERN-internal libraries; this makes it easier for other facilities to use the tool. Another important goal is to extract the core logic of the application into a separate program package that can be used in contexts that do not allow for graphical interfaces; e.g. a server that monitors certain variables of a machine and automatically starts an optimization job whenever they leave specified bounds. Cooperation with stakeholders at CERN is currently underway to perform this separation while keeping a convenient interface for users.

Finally, it is planned to improve support for Bayesian optimization algorithms and to add support for multi-objective optimization – two techniques that have shown promising results in isolation and that would benefit from more extensive evaluation and comparison to other techniques.
Testing new algorithms and machine learning routines with GeOFF will be done regularly at the Offline 2 facility, a recent mass separator beamline of ISOLDE@CERN.
It is important to indicate that preparations are underway for the use of GeOFF for the accelerators at GSI and they are progressing well. It is planned at the end of 2023 to use GeOFF for the first time for injection optimization of the SIS18 synchrotron and possibly for beam steering into the FRagment Separator (FRS). In the near future this toolkit will be used at CEA Saclay and be applied to a laser-driven system.

3. HIRING PROCESS

GSI has hired Nico Madysa on 01.03.2023 for the three-year position funded under EURO-LABS. Nico has a large experience in Machine Learning. He previously worked at CERN for three years on the development of GeOFF.

The strategy that has been adopted by CEA is to adapt the toolkit developed for conventional accelerators by GSI to the specificities of the laser-driven particle source. The post-doctoral researcher that will be hired will be in charge of implementation of GeOFF toolkit and of modification related to laser and gas target properties to finally generate new parameters for optimization.

The laser-driven electron source was moved from one site to another in 2020. The environment is completely new (new experimental configuration inducing new safety radioprotection calculations and validation) the final authorization from the Nuclear Safety Authority is mandatory for exploitation and has not been issued yet.

Due to these two reasons (adaptation of the Toolkit developed by GSI and Nuclear Safety Authorization), it has been decided to open the one-year postdoctoral position next April for a start scheduled next September. Having access to experimental data is essential to validate the modification of GeOFF toolkit.