ML⁴NGP

Handbook of Operations

Document Information

Authors: Alexander Miguel Monzon (Action Chair); Zuzana Bednarikova (Action Co-chair); ML4NGP Core Group| (Document Version 1.0 | 10 May 2023)
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Abbreviations and acronyms

CG – Core Group

COST - European Cooperation in Science and Technology

EU – European Union

FAQ - Frequently Asked Questions

ITC – Inclusiveness Target Countries

ITC-CG – Conference Grants for Inclusiveness Target Countries participants

ML – Machine Learning

NGP – Non-Globular Proteins

ML4NGP – Machine Learning for Non-Globular Proteins

MC – Management Committee

WG – Working Groups

SCC – Science Communication Coordinator

STSM – Short Term Scientific Missions

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1. ML4NGP Action

1.1. Description

ML4NGP aims to establish a pan-European network to advance on non-globular protein (NGP) structure and function prediction by reassessing the interplay between experimental and computational data acquired through recent developments of machine learning (ML) approaches and methods for determining NGP structural ensembles. ML4NGP will enhance the primary experimental data generation, promote integrative structural biology approaches, benchmark the state-of-the-art ML methods and improve the functional characterization of NGPs. The generation of new computational techniques, best practices for NGP experimental and computational detection, and the creation of cutting-edge curated datasets will fundamentally contribute to a better understanding and characterization of the relationship between sequence-structure-dynamics-function of NGPs. ML4NGP integrative approaches also aim to raise awareness about NGPs in the scientific community, which has been biased toward globular proteins for many years. The collaborative network between European and non-European projects, societies and initiatives in the field will contribute to raising the awareness of non-globular proteins within and beyond the Action's participants and the scientific community.

1.2. Implementation

The project is carried out by a high-quality network of different participants from 37 COST member countries in Europe, including 20 Inclusiveness Target Countries (ITCs), plus one international partner country (Japan). It is led by the COST Action Chair Dr. Alexander Monzon of the University of Padova in Italy.
This interdisciplinary consortium from 37 countries will work together on 1) NGPs primary experimental data generation, curation and deposition, 2) Machine learning and NGP structural biology, 3) Assessment of state-of-the-art ML approaches in the NGP field, 4) Improving functional characterization of NGPs and 5) Communication, dissemination and exploitation of the Action results and activities. The expected duration of the Action is 48 months.

2. Purpose of the document

This document aims to complement and extend the procedures outlined in the [Annotated Rules for COST Actions](#) with ML4NGP-specific policies to ensure consistent and coherent procedures over time. It is not meant to replace the Annotated Rules, which always takes precedence in cases of

apparent contrast. All things written in this document are approved by the ML4NGP Management Committee.

3. Governance structure

ML4NGP is governed by the structure outlined in the Annotated Rules for COST Actions and related documents from the COST Association. The current structure is as follows:

- ➢ MC Chair: Alexander Monzon, University of Padova, Italy
- ➢ MC Vice-Chair: Zuzana Bednarikova, Institute of Experimental Physics SAS, Slovakia
- ➢ Grant Holder Scientific Representative: Silvio Tosatto, University of Padova, Italy
- ➢ Grant Holder Manager: Diana Battistella, University of Padova, Italy
- ➢ Grant Awarding Coordinator: Darius Šulskis, Vilnius University, Lithuania
- ➢ Science Communication Coordinator: Rita Vilaça, Instituto de Investigação e Inovação em Saúde, Portugal

3.1. Working Groups (WG)

Working Group Leaders

WG1 Lead: Pavel Kadeřávek, CEITEC, Czech Republic
WG2 Lead: Zsuzsanna Dosztanyi, Eötvös Loránd University, Hungary
WG3 Lead: Jovana Kovačević, Belgrade University, Serbia
WG4 Lead: R. Gonzalo Parra, Barcelona Supercomputing Center, spain
WG5 Lead: Rita Vilaça, Instituto de Investigação e Inovação em Saúde, Portugal

Working Group activities

WGs are the backbone of ML4NGP, coordinating and performing its scientific activity. As such, describing their goals and activities is of paramount importance. To this end, each WG shall produce a yearly document describing past and future activities, as well as relevant goals for the budget period, using the following procedure:

- Before the yearly meeting, the WG leads will prepare a short (1/2 page) draft document outlining goals and activities to be circulated to all ML4NGP members.
- The draft document will be discussed with the WG leads by all interested parties at the yearly meeting, first informally and then during the WG meeting.

- The WG leads will draw up an expanded document (> 1 page) detailing goals and activities after the meeting based on the discussions, including an additional round of consultation where warranted.
- The expanded document will be posted on the ML4NGP website to be also used to define the scope for STSMs and ITCCGs during the following year.
- Each WG is entitled to organize an additional event (e.g., workshop) per year as part of its official activities, with funding to be determined based on overall available resources.
- Events falling outside the goals of any WG are discouraged, with the exception of general interest ML4NGP training schools.

3.2. Core Group (CG)

The CG is composed by MC Chair & Vice-Chair, GHSR, Grant Awarding Coordinator, Science Communication Coordinator, all WG leads and co-leads.

Core Group activity

The Core Group will hold a regular teleconference to coordinate ML4NGP activities and monitor progress, usually on a monthly basis, with the following scope:

1) The MC Chair initiates a Doodle poll typically one week ahead of the proposed dates.
2) The date with the most preferences is selected.
3) The teleconference is chaired by the MC Chair (or Vice-Chair).
4) Topics include upcoming events and ongoing WG activities.
5) An agenda is prepared, and short minutes are collected during the teleconference to be published on the ML4NGP MC shared folder.

3.3. Scientific Advisory Board

The SAB (see MoU) is composed by Silvio Tosatto, Andrey Kajava, Miguel Andrade, Sonia Longhi, Sandra Macedo-Ribeiro, Salvador Ventura, Peter Tompa and Christos A. Ouzounis.

4. Management Committee (MC) meetings

The Action MC will meet at least once a year by virtual means or in hybrid mode. Action MC Members and Observers will be invited to the Action MC meetings by default. The Action MC may invite to its meetings any other individual relevant for the progress of the Action in an advisory position.

In order to ensure that most of the Action budget goes to networking activities, the reimbursement of expenses for attending to Action MC face to face meetings is limited to one Action MC Member per COST Full or Cooperating Member:

- The Action MC Members from each COST Full or Cooperating Member will have to decide among themselves whom of them shall be the one benefiting from reimbursement, also considering if one of them is already being reimbursed for other co-located scientific activities or meetings;
- The other Action MC Member will be able to be present in the MC meeting or via virtual means.

5. Short Term Scientific Missions (STSMs)

The procedure for the submission and evaluation of STSM applications is explained in the [Annotated Rules for COST Actions](#). STSMs of ML4NGP COST Action are handled by a dedicated Committee and represented by Grant Awarding Coordinator. A detailed description of the exact procedure, including daily subsistence rates, can be found on the [ML4NGP webpage](#). At least two calls for applications will be published per budget year. Applications are collected after the application deadline and evaluated taking into account the following policies:

- Allocated budget. A maximum of 80% of the yearly STSM budget may be spent on a single call for application. Where necessary, applications will be ranked accordingly.
- Participation in ML4NGP. Both the sending and hosting lab shall be actively involved in ML4NGP Action, i.e., listed as MC or WG members on the website.
- Relevance to current WG activities. The application must clearly demonstrate the links to WG goals and activities for the budget period.

- Repetitive applications. Applications by the same individual to visit the same lab may be discarded unless properly justified.
- The Committee will discard applications failing any of the above policies even in the presence of remaining funds.

6. ITC Conference Grants (ITC-CGs)

The procedure for the submission and evaluation of ITC-CG applications is explained in the Annotated Rules for COST Actions. ITC-CGs of ML4NGP COST Action are handled by a dedicated Committee and represented by Grant Awarding Coordinator. At least two calls for application will be published on the ML4NGP webpage per budget year. Applications are collected after the application deadline and evaluated taking into account the following policies:

- Allocated budget. A maximum of 80% of the yearly ITC-CG budget may be spent on a single call for application. Where necessary, applications will be ranked accordingly.
- Participation in ML4NGP Action. The sending lab shall be actively involved in ML4NGP, i.e., listed as MC or WG members on the website.
- Relevance to current WG activities. The application must clearly demonstrate the links to WG goals and activities for the budget period.
- Relevant high-profile events. Strong preference will be given to high-profile scientific events in Europe. Relevance to ML4NGP Action has to be justified.
- Repetitive applications. Applications by the same individual will be discarded unless properly justified.
- The Committee will discard applications failing any of the above policies even in the presence of remaining funds.

7. Conflict of Interest

To ensure a fair and impartial selection process, we will avoid assigning reviewers to applications/abstracts from their own country or research group. Reviewers will be selected based on their expertise and qualifications, and will be required to disclose any potential conflicts of interest. In cases where a reviewer has a conflict of interest, they will be recused from the review

process. By implementing these measures, we aim to promote diversity, inclusivity, and excellence in our selection process.

During relevant ML4NGP committee meetings (e.g. Core Group, MC) any member shall abstain from expressing opinions related to other people belonging to their same institution or country in order to avoid potential conflicts of interest.

8. FAQs about Communication, Dissemination and Acknowledgement of the Action

What is the Action communication channel?

The website of the COST Action ML4NGP – www.ml4ngp.eu – is the central repository channel with all relevant information about research, events and timeline.

Any important subject related to the website should be sent by email to info@ml4ngp.eu with the topic "ML4NGP website" on the subject line.

Are you producing something that relates to the Action?

The acknowledgement of COST funding is a mandatory communication requirement.

The following acknowledgement shall always be added to any publication produced with COST funding:

"This [article] [publication] [project] is based upon work from COST Action ML4NGP, CA21160, supported by COST (European Cooperation in Science and Technology)."

Do you have a presentation to make or something to write about the ML4NGP COST Action?

A ML4NGP Communication Toolkit was designed for internal and external communication that includes the ML4NGP logo, funding logos, typefaces, PowerPoint and Word templates. The official

font is Poppins, a free Google-font. If you don't have it, please don't forget to first install it on your computer to ensure correct document formatting. The ML4NGP Communication Toolkit is available on the internal communication repository of the project (link). If you need any extra information or other logo/branding material with color variations please make a request by email to info@ml4ngp.eu with the topic "ML4NGP Toolkit" on the subject line.

Are you organizing an event sponsored by the Action?

The acknowledgement of COST funding is a mandatory communication requirement.
The following acknowledgement shall always be added to dissemination material about any event funded or sponsored with COST funding:

"This event is part of the activities of the COST Action ML4NGP, CA21160, supported by COST (European Cooperation in Science and Technology)."

The ML4NGP logo and COST and EU funding logos should be included on every visual dissemination material (webpages, event flyers and/or posters).

How to refer to the Action on social media?

To easily find messages with a specific theme or content related to the Action activities, always use the following on Twitter:
- hashtags: #ML4NGP, #COSTactions, #ScienceWithoutBorders
- handles: @ml4ngp, @COSTprogramme, @EU_Commission